

Two-channel Kondo phases in coupled quantum dots

Andrew Keith Mitchell
Balliol College, Oxford

A thesis submitted for the degree of
Doctor of Philosophy
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Abstract

We investigate systems comprising chains and rings of quantum dots, coupled to two metallic leads. Such systems allow to study the competition between orbital and spin degrees of freedom in a nanodevice, and the effect this subtle interplay has on two-channel Kondo (2CK) physics. We demonstrate that a rich range of strongly correlated electron behaviour results, with non-Fermi liquid 2CK phases and non-trivial phase transitions accessible. We employ physical arguments and the numerical renormalization group (NRG) technique to analyse these systems in detail, examining in particular both thermodynamic and dynamical properties.

When leads are coupled to either end of a chain of dots, we show that the resulting behaviour on low temperature/energy scales can be understood in terms of simpler paradigmatic quantum ‘impurity’ models. An effective low-energy single-spin 2CK model is derived for all odd-length chains, while the behaviour of even-length chains is related fundamentally to that of the classic ‘two-impurity Kondo’ model.

In particular, for small interdot coupling, we show that an effective coupling mediated through incipient *single*-channel Kondo states drives all odd chains to the 2CK fixed point (FP) on the lowest temperature/energy scales. A theory is also developed to describe a phase transition in even chains. We derive an effective channel-anisotropic 2CK model, which indicates that the critical FP of such models must be the 2CK FP. This physical picture is confirmed using NRG for various chain systems.

We also examine the effect of local frustration on 2CK physics in mirror-symmetric ring systems. The importance of geometry and symmetry is demonstrated clearly in the markedly different physical behaviour that arises in systems where two leads are either connected to the same dot, or to neighbouring dots. In the latter case, we show for all odd-membered rings that two distinct 2CK phases, with different ground state parities, arise on tuning the interdot couplings. A frustration-induced phase transition thus occurs, the 2CK phases being separated by a novel critical point for which an effective low-energy model is derived. Precisely at the transition, parity mixing of the quasidegenerate local trimer states acts to destabilise the 2CK FPs, and the critical FP is shown to consist of a free pseudospin together with effective *single*-channel spin quenching. While connecting both leads to the same dot again results in two parity-distinct phases, a simple level-crossing transition now results due to the symmetry of the setup. The proposed geometry also allows access to a novel ferromagnetically-coupled two-channel local moment phase.

Driven by varying the interdot couplings and occurring at the point of inherent magnetic frustration, such transitions in ring structures provide a striking example of the subtle interplay between internal spin and orbital degrees of freedom in coupled quantum dot systems, and the resulting effect on Kondo physics.

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CHAPTER 1

Introduction

Strongly-correlated electron systems have fascinated theorists and experimentalists alike since it was realised that collective, emergent phenomena resulting from the complex interactions of a macroscopically-large number of particles can be fundamentally different from that arising in non-interacting systems [1]. Perhaps just as remarkably however, many systems behave as though there was little or no interaction between the electrons. Understanding the microscopic origin of the incredibly rich range of physical behaviour that is observed in such systems lies at the heart of modern condensed matter science.

Classic examples which illustrate the diversity of the field include materials such as the manganites and the cuprates. The behaviour of both is characterized by strong electron correlation, but in the former it results in colossal magnetoresistance [2], while in the latter it is responsible for high temperature superconductivity [3, 4] (although a complete understanding of the fundamental physics at work in each case remains somewhat elusive). Other important examples include correlated electron multilayer structures [5], heavy fermion and Kondo insulators [6, 7].

But one of the most enduring paradigms in quantum many-body theory is the so-called Kondo effect [8, 9]. Originally, the classic spin- $\frac{1}{2}$ Kondo effect was associated with bulk condensed matter systems — particularly those in which magnetic impurities are found in otherwise clean metals. Experimentally [10], it was found in the 1930s that metals such as gold follow the Curie law at high temperatures, but that anomalous contributions to various transport properties arise at low temperatures. It was only later realised that this effect was due to the presence of impurities such as iron.

At high temperatures, the Curie law susceptibility implies the existence of localized moments, but the very question of how these could survive in a metallic host was not immediately understood. Later, it was suggested by Anderson [11] that such local moments might arise due to local electron correlations on the impurity.

He proposed a model — known as the ‘Anderson impurity model’ (AIM) — which describes a single impurity with an on-site Coulomb interaction, U , and which is coupled to the non-interacting metallic host by a hopping matrix element V . We discuss the AIM (see Eq. 2.4 *ff*) in detail in Chapter 2, but here we consider the difficulties in solving this apparently ‘simple’ model, and the richness of the underlying physics.

The local electron-electron correlation U in the AIM renders the problem deeply non-trivial. The large number of interacting electrons obviously means that any *ab initio* method is totally inapplicable, and so approximate solutions have been sought. Anderson originally approached the problem at the mean-field level of unrestricted Hartree-Fock, where the impurity correlations are neglected. Such an analysis suggested the presence of a phase transition in the AIM between magnetic and non-magnetic ground states as a function of the interaction strength U . But subsequent work [12, 13] has shown that the ground state is *always* nonmagnetic: only at higher temperatures is the mean field approach even qualitatively correct.

The natural place to turn next is perhaps finite-order perturbation theory in powers of the interaction strength, but obviously this approach is only of use for small U [14–16], and yet the most interesting physics of the problem is only observed when the impurity electrons are *strongly* correlated. Indeed, perturbation theory in the hopping V is also problematical, since the analysis is about a ground state which is itself inherently correlated. Thus Wick’s theorem does not hold and hence the standard diagrammatic techniques cannot be employed here. In an attempt to capture the low-temperature/energy physics of strongly correlated systems, other more radical techniques have been developed. Perhaps most notably, a generalization of the AIM which describes an impurity with spin-degeneracy N is used in the ‘ $1/N$ ’ expansion, the non-crossing approximation, and the slave-boson mean field approach [8]. In all of these techniques, the $N \rightarrow \infty$ limit is taken, and while important physical insight into the problem can be obtained, the direct application to the spin- $\frac{1}{2}$ $N = 2$ case is rather dubious. Indeed, none of the aforementioned examples captures the physical behaviour of the AIM correctly on all energy scales.

To make progress with the problem, a simplified model was introduced, in which the presence of a spin- $\frac{1}{2}$ object on a single impurity is presupposed. The impurity spin is then exchange-coupled to a host of non-interacting metallic conduction band electrons. This is the so-called ‘Kondo model’ (see Eq. 2.10 *ff*), which we will analyse in more detail in the following chapter.

In fact, it was later realised that the Kondo model (with an additional trivial potential scattering term) can in fact be derived from the Anderson model in the regime where the impurity site is singly-occupied [17], and so all of the physics of the Kondo model is accessible also in the Anderson model (this is discussed further in Sec. 2.2). Importantly, Kondo was able to show [18] that the total resistivity of

such an impurity system is of the form

$$R(T) = a + bT^5 + c \ln \left(\frac{k_B T}{D} \right), \quad (1.1)$$

which was obtained for the Kondo model using perturbation theory to third-order in the impurity-host exchange interaction. The first term is simply a temperature-independent contribution arising from the scattering due to the impurity atoms, while the second is the phonon contribution, which naturally decays rapidly with decreasing temperature. The third term arises from the exchange coupling between the localised impurity spin and the conduction electrons (with D the width of the conduction band), and gives rise to a resistivity minimum at low temperatures. This was found to be in very good agreement with the available experimental data, and so in this sense, the anomalous behaviour of such systems was explained. But the question of what happens in the Kondo model as $T \rightarrow 0$ remained a mystery. Clearly the divergent logarithm in Eq. 1.1 indicates that the ground state properties cannot be described at the level of third-order perturbation theory. Indeed, as with the Anderson model, all perturbative attempts at answering this question have failed to capture the behaviour of the model on the lowest temperature scales. This problem has since come to be known as the ‘Kondo problem’.

An important breakthrough came with the development of so-called ‘renormalization group’ (RG) approaches, which provide an effective way of treating these impurity systems. Essentially, a transformation is generated by which the system is considered on different energy scales, and then the evolution of the behaviour upon successive application of the transformation is examined. Anderson developed such an approximate RG scheme for the Kondo model known as ‘poor man’s scaling’ [19], which we discuss in detail in Sec. 2.3 of Chapter 2. The approach is again inherently perturbative, and breaks down as $T \rightarrow 0$, but does indicate the existence of an exponentially-low energy scale (the Kondo temperature), which depends *non-analytically* on the spin-exchange between the impurity and the conduction band of the host.

Therefore, a key difficulty in tackling the Kondo problem is that one has to consider a very wide range of energies. The bandwidth itself is on the order of several eV, but since the conduction band consists of a continuum of states, excitations around the Fermi level (down to the exponentially-small Kondo temperature) are also important. Indeed, it is the *interactions* on an impurity coupled to this continuum that result in the infrared divergences in any perturbational treatment.

As such, an inherently non-perturbative approach is required to capture the low-temperature/energy physics of the Kondo model. The breakthrough came in the 1970s, when Wilson developed the numerical renormalization group (NRG) technique [12], and successfully applied it to the Kondo model. The key idea was to

discretize the conduction band *logarithmically*, so that the behaviour of the model on all energy scales of interest can be studied (effectively from the bandwidth to the Fermi level).

A great advantage of the NRG is that all system parameters are treated non-perturbatively — but the calculations must therefore be performed numerically. We describe the NRG approach in detail in Chapter 3, and explain that essentially-exact results for the thermodynamics and dynamics [20, 21] on all temperature and energy scales of interest can be calculated. For the Kondo model, it was rigorously shown [12] that as $T \rightarrow 0$, the impurity is locked into a many-body singlet state with the conduction electrons, and hence the impurity spin is completely screened. This is known as the ‘Kondo effect’. Viewed on the lowest energy scales, it appears as though the impurity is *non-interacting*: for example, the magnetic susceptibility is found to be constant as $T \rightarrow 0$ [22]. This effect is reminiscent of Landau’s Fermi liquid [23] description of certain metals, where the large Coulomb interaction between the electrons is effectively screened by the positive background charge. Such metals are thus well-described by non-interacting fermions, but with renormalized effective parameters. The low-energy excitations of these non-interacting ‘quasiparticles’ are then in a one-to-one correspondence with the original electronic excitations of the fully interacting system. In the present context therefore, the formation of the Kondo singlet thus implies that the Kondo and Anderson models describe systems which are fundamentally Fermi liquids [22].

Another important result established definitively from the NRG solution of the Kondo model is that the onset of the Kondo effect is characterized by a single low-energy scale — the Kondo temperature — as obtained earlier by Anderson’s approximate scaling approach [19]. Crucially, all of the low-temperature thermodynamics were shown to exhibit universal scaling in terms of the Kondo temperature, meaning that the fundamental physics of the Kondo effect is intrinsically universal.

Indeed, the NRG provides a framework for understanding the Kondo problem and this underlying universality in terms of renormalization group transformations. As will be seen in the course of this thesis, the NRG approach can provide key insights into the physical behaviour of other, more complex systems.

Wilson’s solution of the Kondo model using NRG did not result in a cessation of interest in the area. In fact, it stimulated a great deal of new research. The NRG approach itself was extended to tackle the Anderson model by Krishnamurthy *et al* [13], and the mapping of the Anderson model onto the Kondo model in the singly-occupied impurity regime was confirmed. Indeed, the full solution also allowed access to new results outside the ‘Kondo regime’. In fact, in the early 1980s, both the Kondo [24] and the Anderson [25] models were solved *analytically* using the Bethe *ansatz* technique, which confirmed the NRG results for the thermodynamics and ground state properties. However we note that dynamical properties calculable within the

NRG [26, 27] cannot be obtained exactly¹ from the Bethe *ansatz* solution. Indeed, the solution necessitates that the model be integrable, and since many interesting extensions of the basic quantum impurity paradigm are non-integrable, the NRG arguably represents a rather more powerful tool.

Indeed, the AIM and Kondo models are still being studied today. For example, conformal field theory techniques have been successfully applied to both [29], while the ‘local moment approach’ [30–33] for the single-particle dynamics of the AIM, has more recently been shown to capture both high- and low-energy spectral features known from NRG studies [26, 27].

Other models were also proposed, such as the gapped [34] and pseudogapped [35] Anderson impurity model, multi-impurity models [36, 37], and even systems where quantum impurities are coupled to bosonic baths [38, 39]. Such systems have been shown to exhibit novel physical behaviour and interesting phase transitions. Indeed, non-Fermi liquid behaviour — in which the system cannot be thought of in terms of non-interacting quasiparticles, even at the Fermi level — has also been predicted.

One classic variant on the standard quantum impurity paradigm is the ‘two-channel Kondo’ (2CK) model proposed by Nozières and Blandin [40], which describes a spin- $\frac{1}{2}$ symmetrically coupled to two independent metallic leads. We discuss the 2CK model (see Eq. 2.20 *ff*) in more detail in the next chapter, since the work of this thesis focuses on systems where 2CK physics is important. The single-spin 2CK model itself has now been extensively studied theoretically, with various solutions using NRG [41, 42], the Bethe *ansatz* [43–45] and conformal field theory [46–48] elucidating many aspects of the resulting physical behaviour (for a comprehensive review, see [49]). In particular, it is known to exhibit a number of unusual non-Fermi liquid properties [43–45, 49], including a residual $T = 0$ entropy of $\frac{1}{2}k_B \ln(2)$ and a magnetic susceptibility which diverges logarithmically at low temperature. However, the necessity for symmetrical exchange couplings and a strict impurity *spin* means that the underlying physics is rather delicate, and so its experimental observation in real systems was not initially anticipated.

In parallel with these considerable theoretical developments, important experimental advances have also been made. A huge resurgence of interest in the field of Kondo physics was generated by the observation of the Kondo effect in so-called ‘quantum dot’ structures [50]. Quantum dots are mesoscopic ‘droplets’ of an electron gas, which are coupled to metallic ‘leads’. The small size of the dot results in appreciable quantization of its electron energy levels, and as they are effectively isolated from their environment, the number of electrons occupying these levels is in

¹The so-called ‘spinon approximation’ [28] does allow *approximate* spectra to be calculated within the Bethe *ansatz*, however.

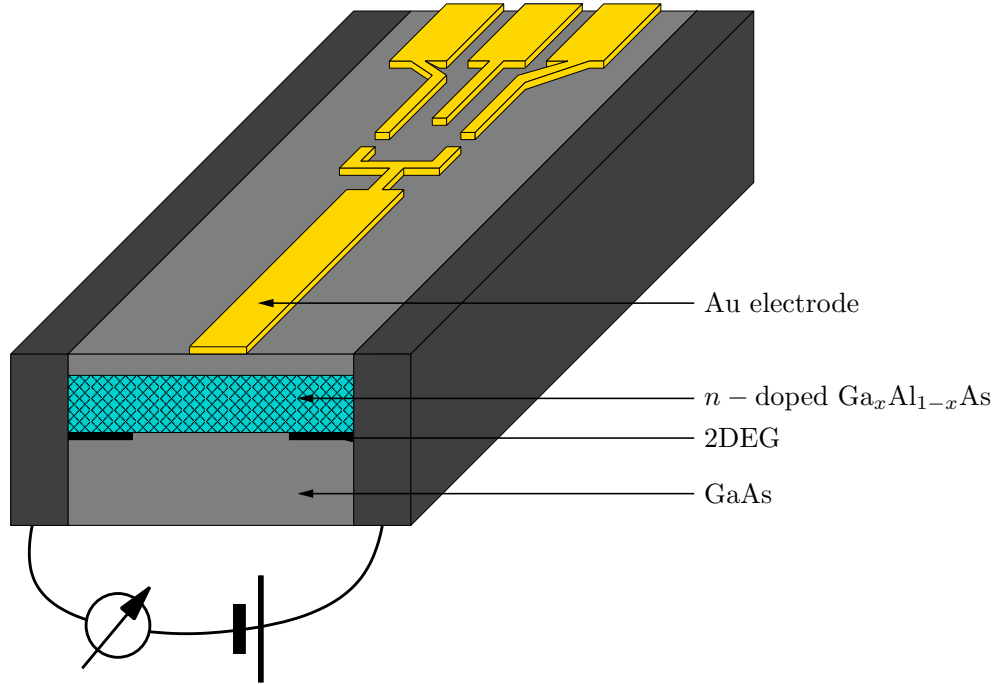


Figure 1.1: Schematic illustration of the single quantum dot device studied in Ref. [50]; diagram reproduced with permission from Ref. [51]. Gold electrodes are deposited on the surface of a heterostructure comprising semiconducting wafers of GaAs and $\text{Ga}_x\text{Al}_{1-x}\text{As}$. The shape of the 2-dimensional electron gas (2DEG) between the latter can be controlled by charging the electrodes, and in so doing, a small ‘dot’ can be defined.

general a well-defined quantity [9,50]. As such, quantum dots have been described as ‘artificial atoms’ [9]. However, exceptional experimental control is available over the size and capacitance of the dots, and (by tuning their proximity to nearby regions of high electron density) the tunnel-coupling to a metallic lead. The properties of quantum dots can thus be fine-tuned at will, and since they can be built into electronic circuits, the resulting physical behaviour can be probed with unprecedented clarity. We consider the theoretical models used to describe quantum dots in the next chapter, but first describe briefly how such structures are made. We go on to consider some variants on the basic setup, describing how novel strongly-correlated electron systems can be created with such devices.

The first quantum dot systems to exhibit the Kondo effect were created and studied by Goldhaber-Gordon *et al* and Cronenwett *et al* [50, 53]. A schematic illustration of the experimental setup used is presented in Fig. 1.1. The basic components of the device comprise a semiconductor heterostructure consisting of a wafer of n -doped $\text{Ga}_x\text{Al}_{1-x}\text{As}$, sandwiched between two undoped wafers of GaAs . As a result of the different band structure of the doped and undoped semiconductors, a 2-dimensional electron gas (2DEG) forms between the layers. The electrons are itinerant, but confined to the plane of the interface between the layers. Once this 2DEG

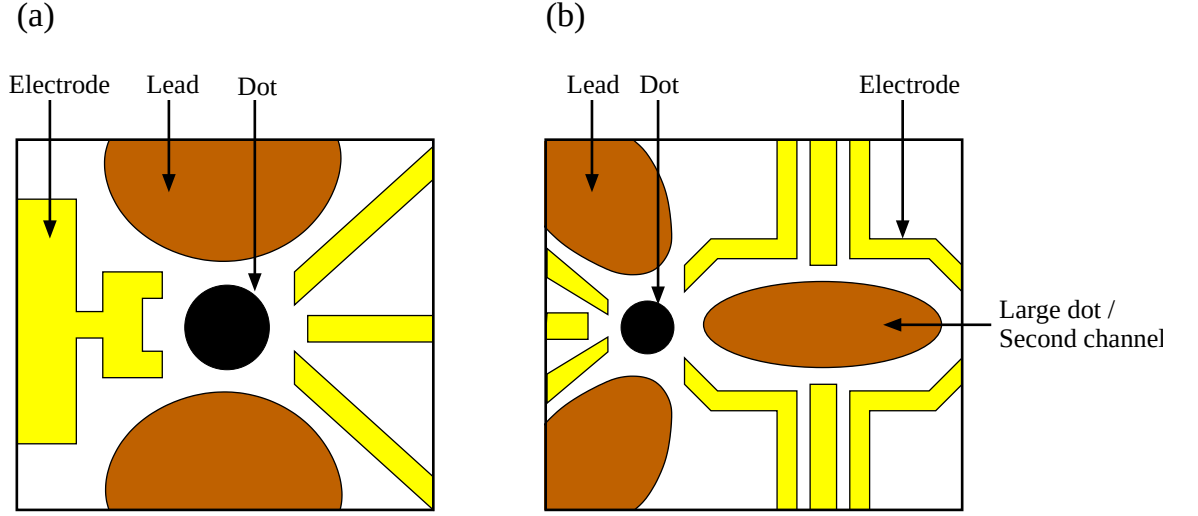


Figure 1.2: (a) Geometry of a single-channel, single dot device, as used in Ref. [50]. (b) Geometry of the two-channel device used in Ref. [52], where a second large dot acts as a second conduction band channel. In both cases, the size, capacitance and the dot-lead couplings can be controlled by charging the various electrodes.

has formed, the electron density can be manipulated by placing negatively-charged electrodes on the surface of the device, which deplete the 2DEG beneath. The electrodes themselves can be manufactured into any shape, and indeed the degree of charging also allows to fine-tune the system.

The basic idea is to position the electrodes as shown in Fig. 1.1 so that a small region of electron density is defined (the dot itself), separated from two large regions of the 2DEG (which constitute the ‘leads’). The desired shape of the 2DEG is illustrated in Fig. 1.2(a) for the setup shown in Fig. 1.1. The narrow barriers between the dot and the leads allow electrons to tunnel to and from the dot; the size of the barrier and the dot can be easily controlled by varying the potential of the various surface electrodes. Transport measurements from a ‘source’ lead to a ‘drain’ lead through the dot can then be made by connecting the leads to an external circuit and applying a bias.

To understand why the Kondo effect might arise in such a system, consider first the depleted 2DEG illustrated in Fig. 1.2(a). For very small dots, the quantised energy levels are widely spaced. Thus, for a given odd number of electrons on the dot, N , the charge excitations to the $(N \pm 1)$ -electron states are high in energy. Since the dot levels above the Fermi energy are essentially unoccupied, while the levels below are full, the system can then be thought of as being a *single* level, with an on-site Coulomb interaction U . The dot is also connected to the leads by tunneling matrix elements. For such ‘single-level’ dots at equilibrium, the setup is thus wholly

equivalent [9, 54–56] to the AIM (as shown rigorously in Sec. 2.1 of the next chapter).

Thus, single quantum dots represent a beautifully direct and tunable realisation of the standard spin- $\frac{1}{2}$ Kondo effect, with impressive experimental control now available in manipulating the microscopic interactions responsible for Kondo physics [8, 50, 53, 54, 57–59]. But perhaps the real importance of these developments is that one is not restricted to the simple geometries illustrated in Figs. 1.1 and 1.2(a). Since the electrodes can be engineered in any shape desired, a wide range of nanodevices can now be constructed.

Experimentalists are in fact now able to build some of the more complex models proposed by theorists. In particular, *coupled* quantum dot devices allow to study the interplay between internal spin and orbital degrees of freedom, and the effect this has on Kondo physics. A diverse range of strongly correlated electron behaviour is accessible in such systems, with subtle variants of the standard Kondo effect [60–65], quantum phase transitions [63, 64, 66–68] and non-Fermi liquid phases [69–72] having been studied theoretically. In particular, both double [61, 63, 66, 73–78] and triple [62, 65, 79–86] quantum dots have been shown to demonstrate low-temperature behaviour quite different from their single-dot counterparts [60].

Recent advances in nanofabrication techniques [50, 52–54, 59, 87–94], and atomic-scale manipulation using scanning tunneling microscopy [95, 96], now allow for the construction of such coupled quantum dot structures, in which the geometry and capacitance of the dots can be controlled, and their couplings fine-tuned [57, 90]. Experimental access to a rich range of Kondo and related physics is thus within reach.

One obvious area of interest was the 2CK model, since unusual non-Fermi liquid properties are expected, as discussed above. Previous attempts to observe 2CK behaviour had proved somewhat elusive, due to the necessity that a single spin couples *symmetrically* to two *independent* conduction band channels [49]. Indeed, for many decades, it was far from clear whether such behaviour could exist in any real system. Experimental realizations of 2CK physics have been variously sought in *eg.* heavy fermion systems containing Uranium [97–99], scattering from 2-level systems using ballistic metal point contacts [100, 101], systems with tunneling between nonmagnetic impurities in metals [102, 103], and even from impurities in graphene [104]. The interpretation that the observed behaviour is the result of 2CK physics is far from clear [105], however.

Quantum dots provide the ideal opportunity to manipulate the microscopic conditions which are required to observe this delicate effect. The fundamental difficulty however (as we discuss in Sec. 2.1 of the following chapter), is that the tunnel-coupling of dots to two leads allows charge transfer processes between the leads, which destroys the two-channel physics. There is thus no *direct* Andersonian analogue of the 2CK model. It has however been shown theoretically that an $O(3)$

Anderson model [106,107] maps onto the 2CK model when the Coulomb interaction U is large. A quadrupolar Anderson model [108], where the dot couples to both the spin and charge degrees of freedom in an attached lead, has also been studied theoretically, and shows 2CK physics, but realizing such models in quantum dot systems has not been so far accomplished.

The breakthrough came when it was suggested by Oreg and Goldhaber-Gordon [70] that a certain *coupled* dot system would map onto the 2CK model on fine tuning of the parameters. On the lowest possible energy scales however, finite charge transfer between the leads must ultimately destroy 2CK physics [47,68,78], but it was argued that at finite temperatures, two-channel physics would be observed.

The proposal [70] was to couple a small quantum dot to a lead, but also to another large quantum dot, as illustrated schematically in Fig. 1.2(b). The large dot would then act as a second lead, as the level spacing would be so small as to approximate a continuum of states; but it would be an *interacting* lead. The device could then be tuned so that the second dot was in the ‘Coulomb blockade’ regime, where successive addition or removal of electrons is disfavoured due to strong inter-electron repulsions (embodied in the parameter U for the large dot). Thus charge transfer to this second dot would be suppressed, the total number of electrons essentially being conserved. Finally, the couplings between the small dot and the two ‘leads’ would have to be tuned to be equal so that the 2CK physics could be accessed.

This incredibly ambitious and delicate experiment was successfully performed recently by Potok *et al* [52], who finally demonstrated unambiguous 2CK physics in such a coupled quantum dot device.

Studying coupled quantum dot systems in a two-channel environment has attracted considerable theoretical interest recently [65,67,68,71,85,109–111], in part because non-Fermi liquid states are accessible. The two-impurity two-channel Kondo model [36,37,109] (where two antiferromagnetically coupled dots are each coupled to their own lead) is a prime example, in which the tendency to form a local singlet state on the two dots competes with the formation of two separated single-channel Kondo states [36,37,78,109]. The quantum critical point separating these phases is again the 2CK fixed point [112,113]. Triple quantum dot models with three dots coupled to two leads in a mirror-symmetric fashion have also been studied [65,68,85,111,114]. Recently, Numata *et al* have studied a TQD comprising tunnel-coupled sites [65], showing that various interesting variants on the standard spin- $\frac{1}{2}$ Kondo effect are observed on tuning the gate voltage. Other work on a TQD ring of spins by Žitko and Bonča [85] has shown in particular that 2CK physics predominates, but that a range of fixed points familiar from simpler quantum impurity models are also accessible. Indeed both two-channel and two-impurity Kondo effects are realised, on tuning the interdot couplings, as a third dot is coupled to the two-impurity two-channel system [85].

In this thesis we examine the rich and subtle interplay between the internal spin and orbital degrees of freedom in coupled dot nanodevices, and the effect this has on two-channel Kondo physics. Specifically, we examine chains and rings of dots connected to two leads and show that while much of the underlying physical behaviour can be understood in terms of simpler paradigmatic quantum impurity models, novel phases and quantum phase transitions are also accessible. NRG techniques together with physically motivated arguments are used to obtain a detailed understanding of such problems, including the study of both thermodynamic and dynamic properties.

Having discussed the coupled dot models of interest in this work, and provided physical motivation for their study, we conclude this Introduction by giving an outline of the rest of this thesis.

In Chapter 2, we consider the theoretical models used to study single quantum dot systems. In particular, we examine single-level dots and demonstrate that tunnel-coupling such structures to two leads results inevitably in an inherently *single-channel* model. We show that the presence of a strong on-site Coulomb interaction (which disfavors double-occupancy of the dot level) favors local moment formation at low temperatures when the gate voltages are suitably tuned. An effective spin-only model — known as the single-channel Kondo (1CK) model — is then derived via the Schrieffer-Wolff transformation [8, 17]. We point out that it is the suppression of inter-lead charge transfer that allows access to *two-channel* physics [47, 68, 78], and introduce the two-channel Kondo (2CK) model, proposed by Nozières and Blandin [40]. The 2CK model describes a single dot *spin*- $\frac{1}{2}$ coupled to two metallic leads. We analyse both the single-channel and two-channel Kondo models with Anderson’s poor man’s scaling technique [19, 40], showing in particular that both models are characterized by a scaling invariant — the exponentially-small Kondo scale.

In Chapter 3, we move on to consider Wilson’s numerical renormalization group (NRG) technique [12, 13], which is an inherently non-perturbative approach to solving quantum ‘impurity’ problems. We describe in detail how the NRG can be extended to tackle a problem with two conduction band channels. We explain the main approximations made within the approach, including the logarithmic discretization procedure on which the technique is founded. An iterative solution to the two-channel Kondo model is then made possible [41]. But the real importance of the NRG is in the formulation of the iterative process in terms of a renormalization group (RG) transformation. The key concept of a ‘fixed point’ (FP) is introduced, and we explain how RG flow between such FPs can be interpreted in terms of evolution of physical properties on reducing the temperature. We show how both thermodynamics and dynamics of the 1CK and 2CK models can be calculated essentially exactly,

and survey some key results.

In Chapters 4–5, we study chains of quantum dots coupled to two leads, while in Chapters 6–8 we examine ring structures in a two-channel environment. We employ both physically motivated arguments and the NRG to obtain a detailed understanding of the underlying behaviour of these systems.

Specifically, Chapter 4 is concerned with chains of spins, with a non-interacting metallic lead connected to each end, in the regime where the interdot couplings are large. We show that the resulting behaviour on low temperature/energy scales can be simply understood in terms of simpler paradigmatic quantum ‘impurity’ models. An effective low-energy single-spin 2CK model can be derived for all odd-length chains, while the behaviour of even-length chains is related fundamentally to that of the classic ‘two-impurity Kondo’ (2IK) model. The situation is shown to be rather trivial for even chains, which simply decouple from the leads as the temperature is lowered. By contrast, for mirror-symmetric odd chains, the lowest chain doublet state is overscreened by conduction electrons, embodied in the infrared 2CK FP describing the non-Fermi liquid ground state. The resulting partially-quenched spin is characterized [43–45, 49] by an unusual residual entropy of $\frac{1}{2}k_B \ln(2)$, and a spectral density which reaches *half* the unitarity limit at the Fermi level [106, 108].

In Chapter 5 we consider the same chain systems, but in the limit of small interdot couplings. We again find that the 2CK FP characterizes the ground state properties for all odd chains. Using physical arguments and perturbative scaling, we derive an effective model to describe such systems at low temperatures, in terms of which the results of the NRG can be simply understood. An effective coupling mediated through incipient *single*-channel Kondo singlet states (forming at low temperatures between the terminal dots and their attached lead) is shown to drive all odd chains to the 2CK FP on the lowest temperature/energy scales. A theory is also developed to describe a transition in asymmetrically-coupled even chains [78]. An effective low-energy channel-anisotropic 2CK model is shown to characterize this transition, and so a physically transparent explanation of the 2CK nature of the critical point naturally follows. This physical picture is confirmed by direct NRG calculations for various chain systems.

The role of inherent magnetic *frustration* in ring systems is examined in Chapters 6–8. Specifically, in Chapter 6 we consider a ring of three quantum dots mutually coupled by antiferromagnetic exchange interactions, and tunnel-coupled to two metallic leads. As such, it is arguably the simplest system in which the consequences of local frustration arising from internal degrees of freedom of a nanodevice may be studied within a two-channel environment. 2CK physics is found to predominate at low-energies in the mirror-symmetric systems considered, with a residual spin- $\frac{1}{2}$ overscreened by coupling to both leads. It is however shown that two distinct 2CK phases, with different ground state parities, arise on tuning the interdot ex-

change couplings. In consequence a frustration-induced quantum phase transition occurs. The 2CK phases are separated by a quantum critical point for which an effective low-energy model is derived. Precisely at the transition, parity mixing of the quasi-degenerate local trimer states acts to destabilise the 2CK fixed points, and the critical fixed point is shown to consist of a free pseudospin together with effective *single*-channel spin quenching. Numerical renormalization group techniques and physical arguments are used to obtain a detailed understanding of the problem, including study of both thermodynamics and single-particle dynamics of the system.

In Chapter 7, we turn to larger rings with the same basic geometry and symmetry. We now focus specifically on Heisenberg rings of *spins*, showing in particular that the same underlying behaviour results for a trimer of spins exchange-coupled to leads as does when it is tunnel-coupled to leads — provided that the interdot interactions are again pure exchange. We go on to consider other odd rings, demonstrating that 2CK physics again predominates, but that two phases of distinct parity must ubiquitously arise on tuning the interdot couplings. A transition of the same type as that elucidated in Chapter 6 is found in each case, with the universality of the low-temperature/energy behaviour demonstrated explicitly using NRG.

In Chapter 8, we consider a different geometry for the TQD, and demonstrate that markedly different physical behaviour results. We consider a system in which two leads are coupled to the same dot, but we maintain the mirror symmetry of the setup. While two parity-distinct phases again result, we demonstrate that the symmetry of the model means that this parity is now carried by the *local* trimer states alone. This results in a simple level-crossing transition, the nature of which is shown to be rather different from that considered in Chapters 6 and 7. A low-energy effective model is developed to describe the transition, and it is found that both an antiferromagnetically-coupled phase (described by the 2CK FP on the lowest energy scales) and a *ferromagnetically*-coupled phase arises. In the latter, the slow approach to the stable local moment FP is characterized by leading irrelevant logarithmic corrections, as evidenced most clearly in the low-frequency behaviour of the spectrum. But at the Fermi level, the trimer is shown to be completely decoupled from the leads; meaning in particular that the phase is a ‘singular Fermi liquid’.

Near the transition, even in the LM phase, the antiferromagnetically-coupled trimer doublet may still undergo the 2CK effect, leading to an overscreened non-Fermi liquid state — even though it is not the ground state. On the lowest temperature scales, however, this many-body state must be destroyed and projected out, leaving a simple unscreened free spin on the decoupled trimer. Interestingly therefore, *warming* a system in the ferromagnetically-coupled LM phase gives rise to a revival of the antiferromagnetic 2CK effect.

The results and analysis presented in Chapters 4–8 thus provide a clear demonstration that the competition between orbital and spin degrees of freedom in cou-

pled quantum dot nanodevices may give rise to novel strongly-correlated electron behaviour and unusual quantum phase transitions.

The thesis ends with a short summary. Finally, we mention that the work of Chapter 6 has been submitted for publication (a preprint is available in Ref. [115]), while a single-channel variant of the work presented in Chapter 8 has appeared recently in Ref. [64].

CHAPTER 2

Models of quantum dots and scaling

In this chapter, we introduce briefly the models used to describe simple quantum dot (QD) systems, and the behaviour that is expected to occur at low temperatures, based on perturbative scaling arguments.

Interacting quantum dot nanodevices may in general be described by a pair of non-interacting metallic conduction bands H_L (the ‘source’ and ‘drain’ leads discussed in the previous chapter), the dot/nanodevice itself H_D , and a tunnel-coupling between these two subsystems, H_{hyb} . We consider the equilibrium case where the chemical potentials of the leads are the same, and for simplicity, take a single dot comprising a single level. This setup is illustrated schematically in Fig. 2.1(a), and its corresponding Hamiltonian is thus generically of the form $H = H_L + H_D + H_{\text{hyb}}$, with

$$H_L = \sum_{\mathbf{k}, \alpha=L,R} \epsilon_{\mathbf{k}} \hat{n}_{\alpha\mathbf{k}}, \quad (2.1a)$$

$$H_D = \epsilon(\hat{n}_{d\uparrow} + \hat{n}_{d\downarrow}) + U \hat{n}_{d\uparrow} \hat{n}_{d\downarrow}, \quad (2.1b)$$

$$H_{\text{hyb}} = \sum_{\substack{\alpha=L,R \\ \mathbf{k}, \sigma}} V_{\alpha} (d_{\sigma}^{\dagger} a_{\alpha\mathbf{k}\sigma} + a_{\alpha\mathbf{k}\sigma}^{\dagger} d_{\sigma}). \quad (2.1c)$$

Each lead described by Eq. 2.1a thus consists of a dense set of levels of energy $\epsilon_{\mathbf{k}}$ (with $\mathbf{k}$ labelling the momentum), and the bandwidth is taken to be $2D$ (see Fig. 2.1). The total number operator for a level in lead $\alpha = L, R$ describes its occupancy, and is given by $\hat{n}_{\alpha\mathbf{k}} = \hat{n}_{\alpha\mathbf{k}\uparrow} + \hat{n}_{\alpha\mathbf{k}\downarrow}$ with $\hat{n}_{\alpha\mathbf{k}\sigma} = a_{\alpha\mathbf{k}\sigma}^{\dagger} a_{\alpha\mathbf{k}\sigma}$ where $a_{\alpha\mathbf{k}\sigma}^{\dagger}$ creates a $\sigma = \uparrow, \downarrow$ spin electron in the $\alpha = L, R$ lead with momentum $\mathbf{k}$, and $a_{\alpha\mathbf{k}\sigma} = (a_{\alpha\mathbf{k}\sigma}^{\dagger})^{\dagger}$ destroys an identical electron¹. Thus H_L gives the total energy associated with the occupied levels of each lead.

¹The antisymmetry under permutation of two electrons is of course described by the fermion anticommutation relations [116], which for the conduction electrons are simply $\{a_{\alpha\mathbf{k}\sigma}^{\dagger}, a_{\alpha\mathbf{k}'\sigma'}\} = \delta_{\mathbf{k}\mathbf{k}'} \delta_{\sigma\sigma'}$ and $\{a_{\alpha\mathbf{k}\sigma}^{\dagger}, a_{\alpha\mathbf{k}'\sigma'}^{\dagger}\} = \{a_{\alpha\mathbf{k}\sigma}, a_{\alpha\mathbf{k}'\sigma'}\} = 0$, where $\{\hat{A}, \hat{B}\} = \hat{A}\hat{B} + \hat{B}\hat{A}$ as usual.

H_D describes the total energy of the dot itself (see Fig. 2.1, Eq. 2.1b), which has a single level at an energy ϵ , and U is the Coulomb interaction, corresponding to the energy penalty for placing a pair of electrons (with different spin) on the dot. As for the lead electrons, the number operator is $\hat{n}_{d\sigma} = d_\sigma^\dagger d_\sigma$ where $d_\sigma^\dagger$ is the creation operator for a $\sigma = \uparrow, \downarrow$ spin electron on the dot. We note here that real dots have many levels, but gate voltages may be tuned such that the gap between the levels is sufficiently large that levels far below the Fermi level are essentially filled, while those far above are empty, and thus play no role².

Finally, H_{hyb} describes the single-electron tunneling processes between the dot and the leads, which we assume is independent of the spin or lead momentum, $V_{\alpha\mathbf{k}\sigma} \equiv V_\alpha$.

2.1 Prevalence of single-channel models

The above picture can be simplified conceptually in the case of single-level dots (considered here). Performing a canonical transformation³ of the lead operators, viz:

$$\begin{aligned} a_{L\mathbf{k}\sigma} &= a_{A\mathbf{k}\sigma} \cos \theta + a_{B\mathbf{k}\sigma} \sin \theta \\ a_{R\mathbf{k}\sigma} &= a_{A\mathbf{k}\sigma} \sin \theta - a_{B\mathbf{k}\sigma} \cos \theta, \end{aligned} \quad (2.2)$$

which is of course valid for any value of θ . Using Eq. 2.2 in the Hamiltonian Eq. 2.1, we obtain $H_L = \sum_{\mathbf{k}, \alpha=A,B} \epsilon_{\mathbf{k}} \hat{n}_{\alpha\mathbf{k}}$, which again describes two non-interacting leads, $\alpha = A, B$. The dot contribution H_D remains unaltered, while the tunnel-coupling between the dot and the leads now becomes

$$\begin{aligned} H_{\text{hyb}} = \sum_{\mathbf{k}, \sigma} [& (d_\sigma^\dagger a_{A\mathbf{k}\sigma} + a_{A\mathbf{k}\sigma}^\dagger d_\sigma)(V_L \cos \theta + V_R \sin \theta) \\ & + (d_\sigma^\dagger a_{B\mathbf{k}\sigma} + a_{B\mathbf{k}\sigma}^\dagger d_\sigma)(V_L \sin \theta - V_R \cos \theta)], \end{aligned} \quad (2.3)$$

and now a judicious choice of $\tan \theta = V_R/V_L$ ensures that the second term vanishes. Thus, the dot only couples to a *single* lead, the other playing no role. Eq. 2.1 is wholly equivalent therefore to a single lead model, known as the single-impurity Anderson model (SIAM), illustrated pictorially in Fig. 2.1(b), and described by

²Conversely, the level energies can also be tuned so that two or more levels do become important to the low-energy physics [117], but this is beyond the scope of the current work.

³It can be readily shown that such a transformation preserves the anticommutation relations of the fermion operators.

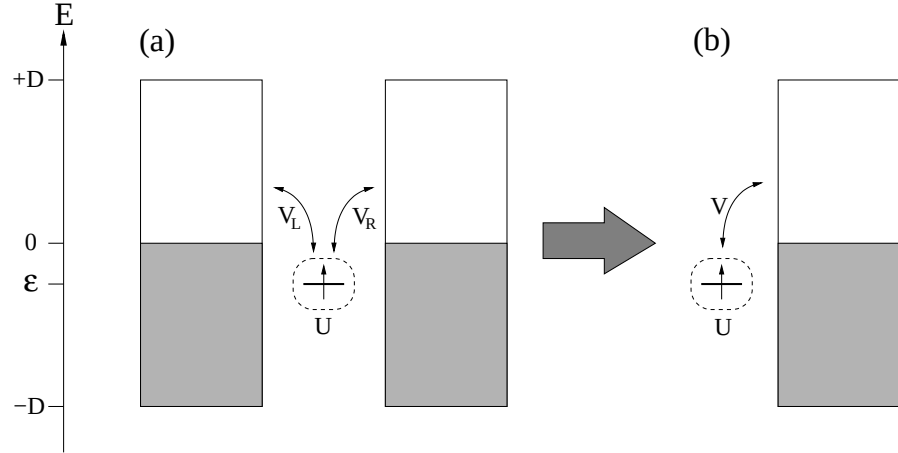


Figure 2.1: Schematic illustration of (a) a quantum dot tunnel-coupled to two leads and (b) the equivalent single-lead setup.

$H_{\text{And}} = H'_L + H_D + H'_{\text{hyb}}$, where

$$H'_L = \sum_{\mathbf{k}} \epsilon_{\mathbf{k}} \hat{n}_{\mathbf{k}}, \quad (2.4a)$$

$$H_D = \epsilon(\hat{n}_{d\uparrow} + \hat{n}_{d\downarrow}) + U \hat{n}_{d\uparrow} \hat{n}_{d\downarrow}, \quad (2.4b)$$

$$H'_{\text{hyb}} = \sum_{\mathbf{k}, \sigma} V (d_{\sigma}^{\dagger} a_{\mathbf{k}\sigma} + a_{\mathbf{k}\sigma}^{\dagger} d_{\sigma}), \quad (2.4c)$$

with $V^2 = V_L^2 + V_R^2$. In general, the above argument demonstrates that a single-level dot tunnel-coupled to two leads⁴ is actually formally a single-channel system. The obvious question is: how might multi-channel physics be observed? We consider this question in Sec. 2.4, but first derive an effective spin model for the QD, known as the ‘Kondo’ model.

2.2 Schrieffer-Wolff transformations and the Kondo model

The SIAM, Eq. 2.4, was first used to describe systems of dilute magnetic impurities in metals, and has since been applied widely to quantum dot systems. In the ‘atomic’ limit, when the dot is detached from the lead ($V = 0$), the SIAM is immediately and trivially soluble. In particular, for $\epsilon < \mu$ and $\epsilon + U > \mu$ (with μ the chemical potential of the system), the dot is singly-occupied, and as will be seen, this situation gives rise to interesting and subtle physical behaviour when the leads are reattached. The so-called Kondo model assumes that the impurity/dot is a pure spin from the outset,

⁴The argument can also be extended to more complicated tunnel-coupled nanodevices and those with several levels, provided [117, 118] that there is a constant ratio of couplings to left and right leads for all dot levels.

and models the coupling to the leads as Heisenberg exchange. The Kondo model itself can be obtained perturbatively from the Anderson model using a Schrieffer-Wolff (SW) transformation [8, 17], and we sketch the derivation below.

We consider the case where the ground state of the SIAM for $V = 0$ is one in which the dot is singly-occupied, the other dot configurations being excited states. The key idea of the SW transformation is to project H_{And} into the $\mathcal{N} = 1$ -electron (singly-occupied) manifold, perturbatively eliminating virtual excitations to the $\mathcal{N} = 0$ and 2 electron sectors to second-order⁵ in H_{hyb} (and neglecting retardation effects [8] as usual). Thus we define a unity operator for the reduced local (dot) Hilbert space of singly-occupied states,

$$\hat{1}_{s.o.} = |\uparrow\rangle\langle\uparrow| + |\downarrow\rangle\langle\downarrow|, \quad (2.5)$$

and an operator $\hat{P} = \hat{1}_{\text{tot}} - \hat{1}_{s.o.}$, which projects into the excited manifold. After lengthy manipulation, it can be shown that the resultant effective dot Hamiltonian $H_{\text{eff}}^{SW} = \hat{1}_{s.o.} H'_{\text{hyb}} (\epsilon - H_D)^{-1} \hat{P} H'_{\text{hyb}} \hat{1}_{s.o.}$ then follows as

$$\begin{aligned} H_{\text{eff}}^{SW} = & \mathfrak{J} \sum_{\mathbf{k}, \mathbf{k}'} \left[\hat{S}^z (a_{\mathbf{k}\uparrow}^\dagger a_{\mathbf{k}'\uparrow} - a_{\mathbf{k}\downarrow}^\dagger a_{\mathbf{k}'\downarrow}) + \hat{S}^+ a_{\mathbf{k}\downarrow}^\dagger a_{\mathbf{k}'\uparrow} + \hat{S}^- a_{\mathbf{k}\uparrow}^\dagger a_{\mathbf{k}'\downarrow} \right] \\ & + \mathfrak{K} \sum_{\mathbf{k}, \mathbf{k}', \sigma} \left(a_{\mathbf{k}\sigma}^\dagger a_{\mathbf{k}'\sigma} \right), \end{aligned} \quad (2.6)$$

where $\hat{S}^z = \frac{1}{2}(|\uparrow\rangle\langle\uparrow| - |\downarrow\rangle\langle\downarrow|)$, $\hat{S}^+ = |\uparrow\rangle\langle\downarrow|$ and $\hat{S}^- = |\downarrow\rangle\langle\uparrow|$ define a spin- $\frac{1}{2}$ operator $\hat{\mathbf{S}}$ for the dot (with $\hat{S}^\pm = \hat{S}^x \pm i\hat{S}^y$), and

$$\mathfrak{J} = V^2 \left(\frac{1}{\epsilon + U} - \frac{1}{\epsilon} \right), \quad (2.7a)$$

$$\mathfrak{K} = V^2 \left(\frac{1}{\epsilon + U} + \frac{1}{\epsilon} \right). \quad (2.7b)$$

The first term of Eq. 2.6 thus couples the dot spin to the lead, while the second term corresponds to potential scattering [8]. This can be recast in a deceptively simple form,

$$H_{\text{eff}}^{SW} = J_K \hat{\mathbf{S}} \cdot \hat{\mathbf{s}}_0 + K \hat{n}_0, \quad (2.8)$$

⁵As H'_{hyb} contains single dot creation or destruction operators, corresponding to the ‘hopping’ of electrons between the dot and lead, to first-order H'_{hyb} always projects into the excited manifold of dot states.

where $\hat{\mathbf{s}}_0$ is the spin density of the lead at the dot, given by

$$\hat{\mathbf{s}}_0 = \sum_{\sigma, \sigma'} f_{0\sigma}^\dagger \boldsymbol{\sigma}_{\sigma\sigma'} f_{0\sigma'} \quad (2.9a)$$

$$f_{0\sigma}^\dagger = \frac{1}{\sqrt{N}} \sum_{\mathbf{k}} a_{\mathbf{k}\sigma}^\dagger, \quad (2.9b)$$

with $\boldsymbol{\sigma}$ the Pauli matrices and $f_{0\sigma}^\dagger$ the creation operator for an orbital which couples directly to the dot (known as the ‘0’-orbital of the Wilson chain: see Chapter 3), and N is the number of orbitals in the lead. The couplings are then readily shown to be $J_K = 2N\mathfrak{J}$ and $K = 2N\mathfrak{K}$. The standard Kondo model itself is the particle-hole symmetric limit of Eq. 2.8, where there is no potential scattering, which occurs when the second term of H_{eff}^{SW} vanishes. From Eq. 2.7b, this arises for $\epsilon = -\frac{1}{2}U$, whence we obtain

$$H_K = H'_L + J_K \hat{\mathbf{S}} \cdot \hat{\mathbf{s}}_0 \quad (2.10)$$

with $\rho J_K = 8\Gamma/(\pi U)$ given in terms of the hybridization strength, $\Gamma = \pi V^2 \rho_T$, with total lead density of states $\rho_T = N\rho \equiv N/(2D)$ such that NV^2 , and hence Γ , is finite in the continuum limit $N \rightarrow \infty$. It should also be noted that $\rho J_K > 0$ and so the coupling is always *antiferromagnetic*.

The Kondo model is thus the low-temperature/energy effective model of the full Anderson model. While the latter has different physics at $T \gg \Gamma$, the low-temperature behaviour (and importantly, the ground state itself) of both models is equivalent, and this can be shown explicitly using renormalization group methods [13].

The Kondo and Anderson models are both of course genuine many-body problems and, as will be seen shortly, their low-temperature behaviour and ground states (which should be equivalent, as discussed above) cannot be obtained by perturbative techniques. Attempts to calculate the resistivity, entropy, magnetic susceptibility or magnetization [8, 119] perturbatively generate logarithmically divergent terms as $T \rightarrow 0$, and even resummation of certain terms to infinite order fails to capture the physics on the lowest temperature scales.

Anderson developed an approach based on perturbative scaling arguments [19] to study Eq. 2.10, which provides key insights into the resulting many-body behaviour of the Kondo model at low temperatures, although again it ultimately fails as $T \rightarrow 0$. In the next section we discuss briefly these results, and in so doing provide an introduction to the ideas of scaling, universality and Wilson’s non-perturbative numerical renormalization group [12], which we discuss more extensively in Chapter 3.

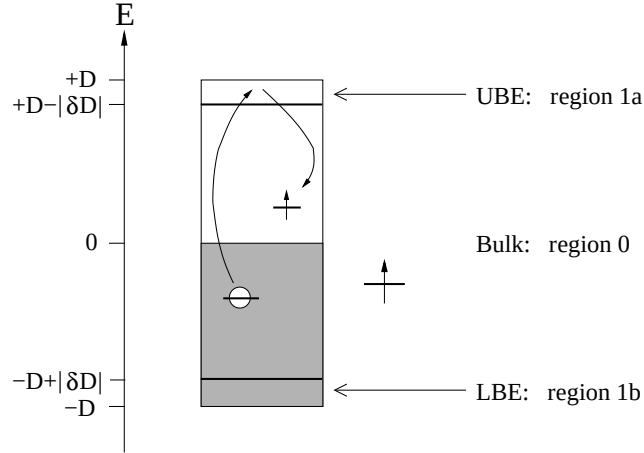


Figure 2.2: Division of the lead conduction band into regions: the band is of total width $2D$, while the upper band edge (labelled UBE) and lower band edge (LBE) are each of width $|\delta D|$. Also illustrated with curly arrows is a virtual excitation of an electron from a filled level to the UBE, then back down to an unfilled level. In poor man's scaling, such excitations to the band edges are perturbatively eliminated, and the bandwidth reduced.

2.3 Poor man's scaling

In the previous section, we used second-order perturbation theory to eliminate virtual excitations from the singly-occupied dot manifold to the higher lying empty or doubly-occupied states (the SW transformation [8, 17]). An effective Hamiltonian valid on a lower energy scale was derived, in which the effect of these virtual excitations was encompassed in the exchange coupling between the dot spin and the leads (see Eqs. 2.6–2.10).

As discussed in the previous section, standard perturbative techniques for tackling the Kondo model itself fail at low temperatures due to the appearance of $\ln(T/D)$ terms (with $2D$ the conduction bandwidth as usual), which diverge as $T \rightarrow 0$. Equivalently, the limit $D \rightarrow \infty$ cannot be taken, implying that the higher energy excitations are important to the low-energy physics, and cannot simply be ignored. The crucial advance was made by Anderson who developed a technique known as ‘poor man's scaling’ [19]⁶, which adopts a similar approach to that of the SW transformation. Anderson progressively reduced the width of the lead conduction band, but calculated the renormalized coupling of the dot spin to the rest of the lead by perturbatively eliminating virtual excitations to the band edges.

The first step is to divide up the lead conduction band, as shown in Fig. 2.2, with an upper band edge (UBE: region 1a) and a lower band edge (LBE: region 1b) both of width $|\delta D|$, with the bulk of the band (region 0) thus running from

⁶In fact, Anderson's poor man's scaling derived simply a result which he had previously obtained by mapping the Kondo model onto a classical one-dimensional gas [120, 121]

$(-D + |\delta D|) \rightarrow (+D - |\delta D|)$. For notational simplicity, we will label the Kondo Hamiltonian Eq. 2.6 according to the bandwidth and coupling $\mathfrak{J}$, as these quantities will be renormalized by the scaling procedure (and we will consider the particle-hole symmetric limit where $\mathfrak{K} = 0$). For a band with $A \leq \epsilon_{\mathbf{k}} \leq B$ (and so of width $B - A$) and exchange coupling $\mathfrak{J}$, we define

$$H_K(\mathfrak{J}; A, B) = \mathfrak{J} \sum_{\mathbf{k}, \mathbf{k}'} \theta(\epsilon_{\mathbf{k}} - A) \theta(B - \epsilon_{\mathbf{k}}) \theta(\epsilon_{\mathbf{k}'} - A) \theta(B - \epsilon_{\mathbf{k}'}) \times \left[\hat{S}^z (a_{\mathbf{k}\uparrow}^\dagger a_{\mathbf{k}'\uparrow} - a_{\mathbf{k}\downarrow}^\dagger a_{\mathbf{k}'\downarrow}) + \hat{S}^+ a_{\mathbf{k}\downarrow}^\dagger a_{\mathbf{k}'\uparrow} + \hat{S}^- a_{\mathbf{k}\uparrow}^\dagger a_{\mathbf{k}'\downarrow} \right], \quad (2.11)$$

where the Heaviside step function $\theta(x) = 1$ for $x \geq 0$ but vanishes otherwise. Thus $H_K(\mathfrak{J}; -D, +D)$ describes the first term of Eq. 2.6 over the entire band. We now consider excitations to the band edges as a perturbation, and so divide the full Hamiltonian up as $H_K(\mathfrak{J}; -D, +D) = H_0 + H_1$, with

$$H_0 = H_K(\mathfrak{J}; -D + |\delta D|, +D - |\delta D|), \quad (2.12)$$

and the perturbation $H_1 = H_K(\mathfrak{J}; -D, +D) - H_0$ so defined. The latter can be broken into two parts, $H_1 = H_{1a} + H_{1b}$, with H_{1a} corresponding to spin-scattering processes between the bulk (region 0) and the UBE⁷ (region 1a), while H_{1b} scatters conduction band electrons between the bulk and the LBE (region 1b). We now use the Brillouin-Wigner perturbation expansion [122] of $H_K(\mathfrak{J}; -D, +D)$, and project onto the states of H_0 with a unity operator $\hat{1}_0$, which acts only on the reduced Hilbert space of the bulk, region 0 (see Fig. 2.2), viz:

$$H_{\text{eff}} = \hat{1}_0 (H_0 + H_1 + H_1(E - H_0)^{-1} H_1 + \dots) \hat{1}_0. \quad (2.13)$$

The first term is simply $\hat{1}_0 H_0 \hat{1}_0 = H_0$, while the second term vanishes entirely, $\hat{1}_0 H_1 \hat{1}_0 = 0$, since H_1 scatters bulk electrons (region 0) into the band edges (regions 1a and 1b), which we neglect. As with the SW transformation considered in the previous section, the non-trivial contribution comes from *virtual* excitations from the bulk (region 0) to the band edges (regions 1a or 1b) and then back into the bulk. These processes are embodied in the second-order term of Eq. 2.13, given by $\hat{1}_0 H_1 (E - H_0)^{-1} H_1 \hat{1}_0$, and are represented most simply diagrammatically. One such example is shown in Fig. 2.3: the horizontal line represents the state of the dot, while the other lines represent states of the lead. Specifically, the dashed line corresponds to the virtual excitation in the band edge (which we label with momentum $\mathbf{q}$).

Summing over all such second-order diagrams, we obtain the second-order contribution to H_{eff} . Assuming that the UBE is initially empty and the LBE is initially

⁷We assume that the UBE is initially empty and the LBE is initially full, and thereby neglect the contributions to H_1 for scattering processes *within* the band edges themselves.

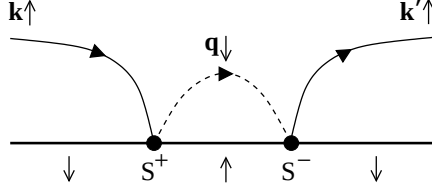


Figure 2.3: Example of a second-order poor man's scaling diagram for the single-channel Kondo model. The horizontal line represents the state of the dot, whose spin is flipped twice by interactions (represented by circles) with conduction band states (curly arrows). The dashed line corresponds to a virtual excitation in the band edge.

full, and neglecting the energies of $\epsilon_{\mathbf{k}}$ and $\epsilon_{\mathbf{k}'}$ compared with the bandwidth $2D$, it can be shown [8, 19] that $\hat{1}_0 H_1 (E - H_0)^{-1} H_1 \hat{1}_0 = H_K(\delta\mathfrak{J}; -D + |\delta D|, +D - |\delta D|)$, with

$$\delta\mathfrak{J} = 2\mathfrak{J}^2 \rho_T \frac{|\delta D|}{D}, \quad (2.14)$$

Thus up to second-order in $\mathfrak{J}$ we obtain,

$$H_{\text{eff}} = H_K(\mathfrak{J} + \delta\mathfrak{J}; -D + |\delta D|, +D - |\delta D|). \quad (2.15)$$

which is a Hamiltonian of exactly the same form as the original Kondo Hamiltonian, but valid on a reduced bandwidth $\tilde{D} = 2(D - |\delta D|)$, and with renormalized coupling $\tilde{\mathfrak{J}} = (\mathfrak{J} + \delta\mathfrak{J})$. This process can be continued, with the bandwidth reduced progressively, and the flow of the renormalized coupling analysed. Taking the limit $|\delta D| \rightarrow -dD$ (δD being negative) and $\delta\mathfrak{J} \rightarrow d\mathfrak{J}$, it immediately follows from Eq. 2.14 that

$$\frac{d\mathfrak{J}}{d \ln(D)} = -2\rho_T \mathfrak{J}^2 + \mathcal{O}(\rho_T^2 \mathfrak{J}^3). \quad (2.16)$$

Integrating Eq. 2.16 from an initial band cutoff D and bare Kondo coupling $\mathfrak{J}$, to a reduced band cutoff $\tilde{D}$ and renormalized coupling $\tilde{\mathfrak{J}}$, we obtain the scaling trajectory,

$$D \exp(-1/2\rho_T \mathfrak{J}) = \tilde{D} \exp(-1/2\rho_T \tilde{\mathfrak{J}}) \sim T_K^{1CK}, \quad (2.17)$$

where T_K^{1CK} is a *scaling invariant*, known as the Kondo temperature. As the bare Kondo Hamiltonian $H_K(\mathfrak{J}; -D, +D)$ and the effective model $H_K(\tilde{\mathfrak{J}}; -\tilde{D}, +\tilde{D})$ are of the same form, systems with different D and $\mathfrak{J}$ must have the same low-energy behaviour if they lie on the same scaling trajectory — *ie.* they have the same T_K^{1CK} .

Indeed, decreasing the bandwidth is effectively the same as reducing the *temperature*; excitations to progressively lower and lower energy states are eliminated by the scaling, with the effect of these processes on the low-energy physics incorporated into a renormalized Kondo coupling. Thus, the immediate implication of the existence of a scaling invariant is that at low temperatures all properties of a system,

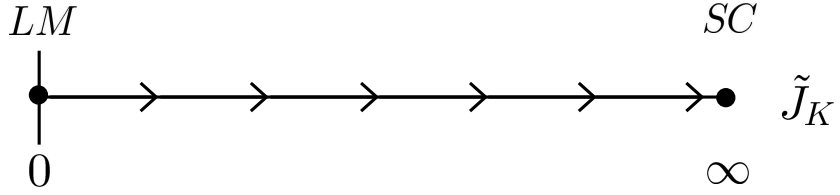


Figure 2.4: Scaling trajectory for the single-channel Kondo model, as derived from poor man’s scaling. The circles indicate the ‘fixed points’ of the model, where successive reduction of bandwidth causes no further renormalization of the effective coupling $\tilde{J}_K$. The ‘local moment’ (LM) fixed point corresponds to $\tilde{J}_K = 0$ while the ‘strong coupling’ (SC) fixed point corresponds to $\tilde{J}_K = \infty$.

such as thermodynamic functions like the uniform spin susceptibility or entropy, depend only on this single parameter T_K^{1CK} , and are universal functions of it. This is also seen clearly from renormalization group arguments, which we discuss fully in Chapter 3.

The above calculation can be extended to third-order in $\mathfrak{J}$ to obtain a better estimate of T_K^{1CK} , but the principle is exactly the same. The scaling equation then becomes [8, 19]

$$\frac{d\mathfrak{J}}{d \ln(D)} = -2\rho_T \mathfrak{J}^2 + 2\rho_T^2 \mathfrak{J}^3 + \mathcal{O}(\rho_T^3 \mathfrak{J}^4), \quad (2.18)$$

and the single-channel scaling invariant up to third-order is then simply

$$T_K^{1CK}/D = \sqrt{\rho J_K} \exp(-1/\rho J_K), \quad (2.19)$$

where we have used the definitions $J_K = 2N\mathfrak{J}$ and $\rho_T = N\rho$ to express T_K^{1CK} in terms of the bare coupling of the Kondo model Eq. 2.10.

Finally, we note that the form of Eq. 2.18 indicates that as the bandwidth/temperature is reduced, the effective coupling *increases*, as illustrated in Fig. 2.4. Also shown by circles in Fig. 2.4 are the so-called ‘fixed points’ (FPs) of the Kondo model. These are points where further scaling (reduction of bandwidth) causes no further change in the renormalized coupling $\tilde{J}_K$. There are only two such points for the single-channel Kondo model, which correspond to $\tilde{J}_K = 0$ and ∞ . For $\tilde{J}_K = 0$, the dot decouples from the lead; this is referred [13] to as the ‘local moment’ (LM) FP as the dot spin remains free under further renormalization/reduction of the energy scale. However, the scaling from Eq. 2.18 indicates that for any small positive $\tilde{J}_K$, reduction of the bandwidth/temperature leads to an increase in the effective coupling. The LM FP is thus said to be ‘unstable’, and as such cannot describe the properties of the system on the lowest temperature scales.

For any antiferromagnetic bare coupling, instead $\tilde{J}_K$ begins to increase as the bandwidth/temperature is reduced (see Fig. 2.4). Indeed, one might expect that as the strength of the coupling becomes very large, the dot spin would form a singlet

state with the lead electrons. The $\tilde{J}_K = \infty$ limit is referred to as the ‘strong coupling’ (SC) FP, and from the above argument, the dot spin would be screened/quenched by the lead electrons.

These conclusions are based on the behaviour of the effective coupling under renormalization from Eq. 2.18. However, poor man’s scaling, as outlined above, is an inherently *perturbative* approach, necessarily treating $\tilde{J}_K$ as a small parameter. As $\tilde{J}_K$ increases, the analysis breaks down, so that in particular for $T < T_K^{1CK}$, nothing can be said about the system. We might surmise that the SC FP is in fact reached as $T \rightarrow 0$ by extrapolating the flow of $\tilde{J}_K$, but the ground state properties cannot be definitively or rigorously obtained in this way.

While Anderson’s approach represents a hugely important step in understanding the low-temperature behaviour of the Kondo model through the presence of an exponentially-small low-energy scale, fundamentally, a non-perturbative approach is required. We consider such an approach in the next chapter, but first explore the possibilities and implications for a *two-channel* Kondo model.

2.4 Behaviour of a two-channel Kondo model

In Sec. 2.1 we discussed how systems comprising a single-level dot tunnel-coupled to two leads are described ubiquitously by single-channel models (at equilibrium). The possibility of realizing systems in which a quantum dot is coupled to several *distinct* channels would therefore seem impossible. However, a strict *spin* model, with the dot coupled to two leads by pure exchange interactions, would in principle display two-channel physics. In the Introduction, we discussed possible routes to access this behaviour experimentally; here we simply introduce such a model directly, and analyse the low-temperature behaviour expected from a poor man’s scaling perspective. We write the two-channel Kondo (2CK) model as $H = H_L + H_{2CK}$, with $H_L = \sum_{\mathbf{k},\alpha} \epsilon_{\mathbf{k}} \hat{n}_{\alpha\mathbf{k}}$ describing two non-interacting leads $\alpha = L/R$ as before, and

$$H_{2CK} = J_{KL} \hat{\mathbf{S}} \cdot \hat{\mathbf{s}}_{L0} + J_{KR} \hat{\mathbf{S}} \cdot \hat{\mathbf{s}}_{R0}, \quad (2.20)$$

where $\hat{\mathbf{s}}_{\alpha 0}$ is the spin density of the $\alpha = L/R$ lead at the dot (*cf.* Eq. 2.9), and $J_{K\alpha}$ is the antiferromagnetic exchange coupling of the dot spin $\hat{\mathbf{S}}$ to that lead. Unlike a tunnel-coupled model, no rotation of the lead basis states or transformation of this 2CK Hamiltonian can eliminate the exchange coupling to each lead. In fact, it is the suppression of charge transfer processes between the leads which makes the channels strictly distinct, and therefore fundamentally different from the single-channel model Eq. 2.1 considered above.

The possibility of realizing novel physics in such a model was first pointed out theoretically by Abrikosov and Migdal [123], and later analysed in more detail by

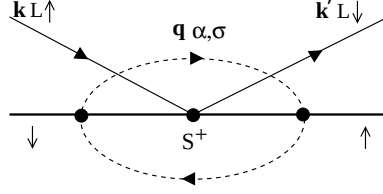


Figure 2.5: Example of a third-order poor man's scaling diagram for the two-channel Kondo model. The dot spin is flipped by the interaction with the left lead, but the virtual excitations (dashed line) to the band edges occur in *both* leads.

Nozières and Blandin [40], with the numerical study of Cragg and Lloyd [41] confirming these conjectures.

In this section we discuss the expected behaviour of the 2CK model Eq. 2.20 using poor man's scaling, following Nozières and Blandin [40]. We show that the low-temperature physics in the channel-isotropic (mirror symmetric) $J_{KL} = J_{KR}$ case must be fundamentally different from that of the single-channel Kondo model considered in Sec. 2.3.

A poor man's scaling approach to the 2CK model Eq. 2.20 proceeds in exactly the same way as described in Sec. 2.3. Each lead is subdivided into the bulk and the band edges, and then virtual excitations to the band edges are eliminated perturbatively. To second order, it is easy to see that an analogous scaling equation to Eq. 2.16 must arise for each lead, because an excited state generated in the band edges of a given lead must be subsequently destroyed. Thus we obtain a pair of separate scaling equations for the flow of the effective coupling between the dot and each lead $\alpha = L/R$ on progressive reduction of the bandwidth:

$$\frac{d\rho J_{K\alpha}}{d \ln(D)} = -(\rho J_{K\alpha})^2 + \mathcal{O}((\rho J_{K\alpha})^3), \quad (2.21)$$

where we have used $\rho J_{K\alpha} = 2\rho_T \mathfrak{J}_\alpha$. To third-order, however, there is a key difference from the single-channel case. To illustrate this, we show an example of a third-order poor man's scaling diagram in Fig. 2.5: the horizontal line again corresponds to the state of the dot, while the solid arrow labelled with momentum $\mathbf{k}$ represents a state in the left lead which is scattered by the dot into a state $\mathbf{k}'$ (also in the left lead). The dashed lines however are the virtual excitations in the band edges, but these can occur in *both* leads. Thus, the contribution from third-order diagrams is *double* that of the single-channel model.

Collecting all such terms is a laborious process, but the result is again simple:

$$\frac{d\rho J_{K\alpha}}{d \ln(D)} = -(\rho J_{K\alpha})^2 + 2(\rho J_{K\alpha})^3 + \mathcal{O}((\rho J_{K\alpha})^4). \quad (2.22)$$

A scaling invariant for each lead $\alpha = L/R$ is then readily shown to be

$$T_K^\alpha/D = \rho J_{K\alpha} \exp(-1/\rho J_{K\alpha}), \quad (2.23)$$

so that decreasing the bandwidth of lead α again leads to an increase in the effective coupling $\tilde{J}_{K\alpha}$. This implies that if for example $J_{KL} > J_{KR}$, the coupling to the left lead would increase faster than the coupling to the right lead as the bandwidth/temperature is reduced. Thus it might be expected from this calculation that at the lowest temperatures, the dot couples strongly to the left lead (to which it was initially more strongly-coupled) and decouples from the right lead, essentially recovering single-channel behaviour⁸.

However, it was argued by Nozières and Blandin [40] that the situation is markedly different when there is left/right mirror symmetry in the model: $J_{KL} = J_{KR} \equiv J_K$. The symmetric 2CK model is simply

$$H_{2CK} = J_K \hat{\mathbf{S}} \cdot (\hat{\mathbf{s}}_{L0} + \hat{\mathbf{s}}_{R0}), \quad (2.24)$$

where there is now a single scaling invariant for the whole system, which is the two-channel Kondo scale,

$$T_K^{2CK}/D = \rho J_K \exp(-1/\rho J_K). \quad (2.25)$$

The couplings to each lead now increase at the same rate as the bandwidth/temperature is reduced. In contrast to the asymmetric case, the dot spin is now ‘overscreened’ by the conduction electrons, as a singlet state cannot be formed by strong coupling to *both* leads simultaneously. The combined lead spin ($\hat{\mathbf{s}}_{L0} + \hat{\mathbf{s}}_{R0}$) must be either a singlet or a triplet (as $\hat{\mathbf{s}}_{\alpha 0}$ is a spin- $\frac{1}{2}$ operator), and as J_K is antiferromagnetic, the dot forms a *doublet* state with the leads. It can then be shown [49] that the residual coupling of this doublet to the rest of the lead states is antiferromagnetic, which itself must be renormalized as the bandwidth/temperature is decreased. As such, the strong coupling FP must be unstable. The above heuristic argument suggests that there must be another FP in the 2CK model which describes the lowest temperature behaviour.

As FPs correspond to points on the scaling trajectory where further reduction of the bandwidth/temperature causes no further renormalization of the effective coupling, we should be able to obtain them directly from the scaling equations derived above, provided $\rho \tilde{J}_K < 1$, where the perturbative analysis holds. Setting

⁸The effect of channel anisotropy has been studied using conformal field theory [46], the Bethe ansatz [124] and the numerical renormalization group [45], and this picture has been confirmed.

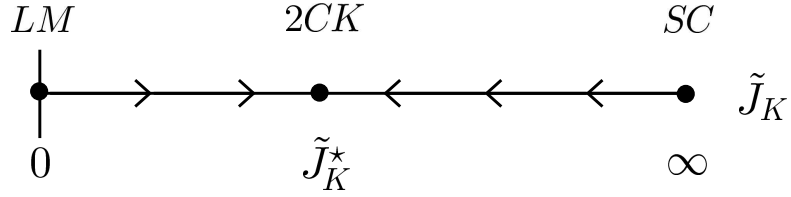


Figure 2.6: Scaling trajectories and FPs of the two-channel Kondo model. The SC FP ($\tilde{J}_K = \infty$) is destabilised when another lead is coupled symmetrically to the dot. An intermediate ‘2CK’ FP at finite coupling $\tilde{J}_K^*$ now arises.

Eq. 2.22 to zero, to third-order we find an intermediate FP at finite coupling,

$$\rho J_K^* = \frac{1}{2}, \quad (2.26)$$

which is referred to as the 2CK FP. The flow of the renormalized coupling $\tilde{J}_K$ on successive reduction of the bandwidth/temperature is shown schematically in Fig. 2.6. Recently, this physical picture has been confirmed [125] by renormalization group techniques, and the effective intermediate-coupling at the 2CK FP established as $\rho J_K^* \approx 0.35$. We shall return to this in Chapter 3.

From poor man’s scaling, it would seem that for any non-zero or non-infinite bare coupling J_K , the effective coupling $\tilde{J}_K$ tends toward this 2CK FP value $\tilde{J}_K^*$. However, as before, this perturbative approach breaks down for $T \ll T_K^{2CK}$, so the exact nature of the ground state cannot be definitively established. Indeed, the properties of a system described by the 2CK FP cannot be determined from this analysis: all we can say is that T_K^{2CK} is a low-energy scale for the 2CK model, and plays the part of a scaling invariant, so that all low-energy/temperature properties of the system must be universal functions of it.

We note that this FP cannot exist in a single-channel model, and therefore the two-channel Kondo model must display fundamentally different physical behaviour at low temperatures [41, 49].

The perturbative approaches introduced in this chapter cannot describe the full behaviour of these models, and do not permit the analysis of critical behaviour and phase transitions. However, the notions of scaling and fixed points described here do provide an important introduction to the ideas underpinning the numerical renormalization group [12] (NRG) technique. As the NRG is a fundamentally non-perturbative approach and is essentially exact, we employ it in the current work to study in detail two-channel models of coupled quantum dots. In the next chapter, we demonstrate how the technique can be applied to such systems, and how it provides a different way of thinking about such many-body problems.

CHAPTER 3

The Numerical Renormalization Group

In this chapter, we discuss the numerical renormalization group (NRG) approach devised by Wilson [12, 13, 27], which is a very powerful tool for studying quantum ‘impurity’ problems, such as the two-channel Kondo (2CK) model, or other systems of quantum dots coupled to metallic leads. It gives essentially exact results for thermodynamic and dynamic properties of such systems on all energy scales of interest — in particular capturing accurately the *low-temperature* behaviour where perturbative approaches inevitably fail. The NRG also provides a non-perturbative conceptual framework for understanding the complex many-body behaviour of such systems in terms of renormalization, scaling and universality.

As we discussed in the previous chapter, serious problems arise when attempting to treat such problems theoretically. The metallic leads consist of a continuum of states where a wide range of energies is important — from the bandwidth, which is of the order of several eV, to arbitrarily small excitation energies near the Fermi level. The dot or nanodevice itself is an *interacting* system, and so the coupling to metallic leads can generate infrared divergences when treated by perturbation theory. In the single-channel and two-channel Kondo models, the low-temperature/energy behaviour is governed by an exponentially-small scale, T_K , which depends non-analytically on the spin-exchange J_K .

The NRG approach treats all parameters of the model non-perturbatively, but as a result, the calculation must be performed numerically. However, as we discuss in this chapter, once the underlying fixed points [12, 13, 27] and associated energy scales have been identified, much work can be done analytically. Indeed, systems with the same stable fixed points can be shown to be fundamentally alike on the lowest temperature/energy scales, thus demonstrating a universality between problems which are often apparently dissimilar.

We use the NRG extensively in the current work (see Chapters 4–8) to examine and study a range of 2CK systems. Thus it is important to provide an account of the

formulation of the method, and introduce the conceptual framework which we will rely heavily on throughout the rest of the thesis. Inevitably, much of the discussion here follows closely the seminal work of Wilson [12] who first solved the Kondo model using NRG, and Krishnamurthy, Wilkins and Wilson [13] who applied the technique to the Anderson model. More fulsome mathematical and technical details can be found in those original papers, and in the excellent recent review by Bulla *et al* [27]. In this chapter we introduce the NRG approach, and show specifically how it can be applied to the 2CK model.

At the end of the chapter, we also discuss more recent developments, focusing mainly on accurate calculation of the proper electron self energy [126] and other dynamic properties through the ‘full density matrix’ extension of the technique [20,21]. Finally we examine the relationship between the scattering t-matrix and the single-particle spectrum for the Anderson model and by analogy calculate the spectrum of the standard single-channel Kondo model, following the approach of Ref. [127].

3.1 Transformations of the Hamiltonian

We will demonstrate the formulation of the NRG with the concrete and most relevant example of the 2CK model, Eq. 2.24, which we present again here for reference:

$$H = \sum_{\alpha, \mathbf{k}, \sigma} \epsilon_{\mathbf{k}} a_{\alpha \mathbf{k} \sigma}^{\dagger} a_{\alpha \mathbf{k} \sigma} + J_K \hat{\mathbf{S}} \cdot (\hat{\mathbf{s}}_{L0} + \hat{\mathbf{s}}_{R0}), \quad (3.1)$$

where, in the same notation as in Chapter 2, the first term describes two non-interacting metallic leads $\alpha = L/R$, while the second term is the exchange coupling between the dot spin and that lead. As in Sec. 2.2, we have used the definitions

$$\hat{\mathbf{s}}_{\alpha 0} = \sum_{\sigma, \sigma'} f_{\alpha 0 \sigma}^{\dagger} \boldsymbol{\sigma}_{\sigma \sigma'} f_{\alpha 0 \sigma'} \quad (3.2a)$$

$$f_{\alpha 0 \sigma} = \frac{1}{\sqrt{N}} \sum_{\mathbf{k}} a_{\alpha \mathbf{k} \sigma}, \quad (3.2b)$$

and combining Eqs. 3.1 and 3.2, we obtain the equivalent representation

$$H = \sum_{\alpha, \mathbf{k}, \sigma} \epsilon_{\mathbf{k}} a_{\alpha \mathbf{k} \sigma}^{\dagger} a_{\alpha \mathbf{k} \sigma} + \frac{J_K}{2N} \sum_{\alpha, \mathbf{k}, \mathbf{k}'} \left[\hat{S}^z (a_{\alpha \mathbf{k} \uparrow}^{\dagger} a_{\alpha \mathbf{k}' \uparrow} - a_{\alpha \mathbf{k} \downarrow}^{\dagger} a_{\alpha \mathbf{k}' \downarrow}) + \hat{S}^+ a_{\alpha \mathbf{k} \downarrow}^{\dagger} a_{\alpha \mathbf{k}' \uparrow} + \hat{S}^- a_{\alpha \mathbf{k} \uparrow}^{\dagger} a_{\alpha \mathbf{k}' \downarrow} \right]. \quad (3.3)$$

This Hamiltonian can be transformed [13] into the one-dimensional form required for the NRG, and with the lead conduction band operators expressed in terms of a continuous energy variable k (extending in the range of the band $-D \leq k \leq +D$)

rather than the discrete momentum vector $\mathbf{k}$. This is accomplished straightforwardly by expanding the conduction band states in terms of spherical harmonics centred around the dot, and assuming isotropy in $\mathbf{k}$ -space (full details of the rather lengthy manipulations involved are given in Appendix A of Ref. [13]). The resulting Hamiltonian retains only the minimum structure necessary to capture the physics, and only the dimensionless parameter ρJ_K enters the theory (with $\rho = 1/(2D)$ the density of states per orbital at the Fermi level), so that all temperature-dependent properties will be functions of T/D , and all frequency-dependent properties will be functions of ω/D . The transformed Hamiltonian is then of the form

$$\begin{aligned} \frac{H}{D} = & \sum_{\alpha, \sigma} \int_{-1}^{+1} dk \, k a_{\alpha k \sigma}^\dagger a_{\alpha k \sigma} \\ & + \frac{1}{2} \rho J_K \sum_{\alpha} \int_{-1}^{+1} dk \int_{-1}^{+1} dk' \left[\hat{S}^z (a_{\alpha k \uparrow}^\dagger a_{\alpha k' \uparrow} - a_{\alpha k \downarrow}^\dagger a_{\alpha k' \downarrow}) + \hat{S}^+ a_{\alpha k \downarrow}^\dagger a_{\alpha k' \uparrow} + \hat{S}^- a_{\alpha k \uparrow}^\dagger a_{\alpha k' \downarrow} \right], \end{aligned} \quad (3.4)$$

where the set of continuum operators $\{a_{\alpha k \sigma}\}$ for lead $\alpha = L/R$ satisfy the usual fermionic anticommutation relations $\{a_{\alpha k \sigma}^\dagger, a_{\alpha' k' \sigma'}\} = \delta_{\alpha \alpha'} \delta_{\sigma \sigma'} \delta(k - k')$.

3.2 Logarithmic discretization

To make progress with Eq. 3.4, it is necessary to make an approximation to the delocalized continuum of states in the leads. The conduction bands can be discretized, but as discussed in the previous chapter, excitations on exponentially low-energy scales of order T_K^{2CK} are important in the 2CK model. Wilson's solution [12] for the single-channel Kondo (1CK) model was to split the conduction band up *logarithmically*, so that the low-energy behaviour can be arbitrarily well-sampled. It is then possible to construct an approximate but complete set of discrete orbitals, localized around the dot. As we will show, the choice of a logarithmic discretization of the continuum in each lead means that there is a separation of energy scales between the orbitals, which allows for an iterative solution of the model.

The conduction band for a given lead $\alpha = L/R$ is divided into intervals distributed symmetrically around the Fermi level $k = 0$, and whose width decreases logarithmically. The n^{th} interval is defined such that $\Lambda^{-(n+1)} < \pm k \leq \Lambda^{-n}$ with the discretization thus controlled by the parameter $\Lambda \gtrsim 1$. Within each interval of each lead, we generate a complete set of orthonormal functions:

$$\psi_{np}^\pm(k) = \begin{cases} \frac{1}{\sqrt{d_n}} e^{\pm i \omega_n p k} & \text{if } \Lambda^{-(n+1)} < \pm k \leq \Lambda^{-n}, \\ 0 & \text{otherwise,} \end{cases} \quad (3.5)$$

where $p \in \mathbb{Z}$ is the harmonic index, and $d_n = \Lambda^{-n}(1 - \Lambda^{-1})$ is the width of the n^{th} interval, with $\omega_n = 2\pi/d_n$ its corresponding fundamental frequency. Thus, Eq. 3.5 defines a Fourier series in each interval, and we can then expand the conduction band operators for each lead in this basis:

$$a_{\alpha k \sigma} = \sum_{n,p} [a_{\alpha n p \sigma} \psi_{np}^+(k) + b_{\alpha n p \sigma} \psi_{np}^-(k)], \quad (3.6)$$

with the new operators $a_{\alpha n p \sigma}$ and $b_{\alpha n p \sigma}$ so defined. These operators form a complete set of *discrete* operators within each interval n for a given lead $\alpha = L/R$, and are readily shown to satisfy the usual fermionic anticommutation relations, *e.g.* $\{a_{\alpha n p \sigma}^\dagger, a_{\alpha' n' p' \sigma'}\} = \delta_{\alpha\alpha'} \delta_{nn'} \delta_{pp'} \delta_{\sigma\sigma'}$. Inverting Eq. 3.6 for a given harmonic index p , we obtain

$$a_{\alpha n p \sigma} = \int_{-1}^1 dk [\psi_{np}^+(k)]^* a_{\alpha k \sigma} \quad b_{\alpha n p \sigma} = \int_{-1}^1 dk [\psi_{np}^-(k)]^* a_{\alpha k \sigma} \quad (3.7)$$

Integrating over the energies of the interval, it can be shown by combining Eq. 3.5, 3.6 and 3.7 that all terms cancel except those involving the fundamental Fourier harmonic, $p = 0$:

$$\int_{-1}^1 dk a_{\alpha k \sigma} = \sum_{n=0}^{\infty} \sqrt{d_n} (a_{\alpha n 0 \sigma} + b_{\alpha n 0 \sigma}). \quad (3.8)$$

Using this result in the Hamiltonian Eq. 3.4, we immediately see that the dot only couples to the $p = 0$ conduction band states. This is illustrated in Fig. 3.1(a), where we show the logarithmic discretization of each conduction band, with the dot spin coupling to a single state in each interval.

It is natural to make one final transformation of basis,

$$\begin{aligned} f_{\alpha 0 \sigma} &= \frac{1}{\sqrt{2}} \sum_{n=0}^{\infty} \sqrt{d_n} (a_{\alpha n 0 \sigma} + b_{\alpha n 0 \sigma}) \equiv \frac{1}{\sqrt{2}} \int_{-1}^1 dk a_{\alpha k \sigma} \\ &\equiv \frac{1}{\sqrt{N}} \sum_{\mathbf{k}} a_{\alpha \mathbf{k} \sigma}, \end{aligned} \quad (3.9)$$

where the $\frac{1}{\sqrt{2}}$ factor in the definition ensures proper normalization of the operators so that $\{f_{\alpha 0 \sigma}^\dagger, f_{\alpha' 0 \sigma'}\} = \delta_{\alpha\alpha'} \delta_{\sigma\sigma'}$, and the equivalence of the second line can be shown explicitly from the above transformations. Thus, the $f_{\alpha 0 \sigma}$ operator is simply that defined in Eq. 3.2. However, transforming the conduction electron term, we see that

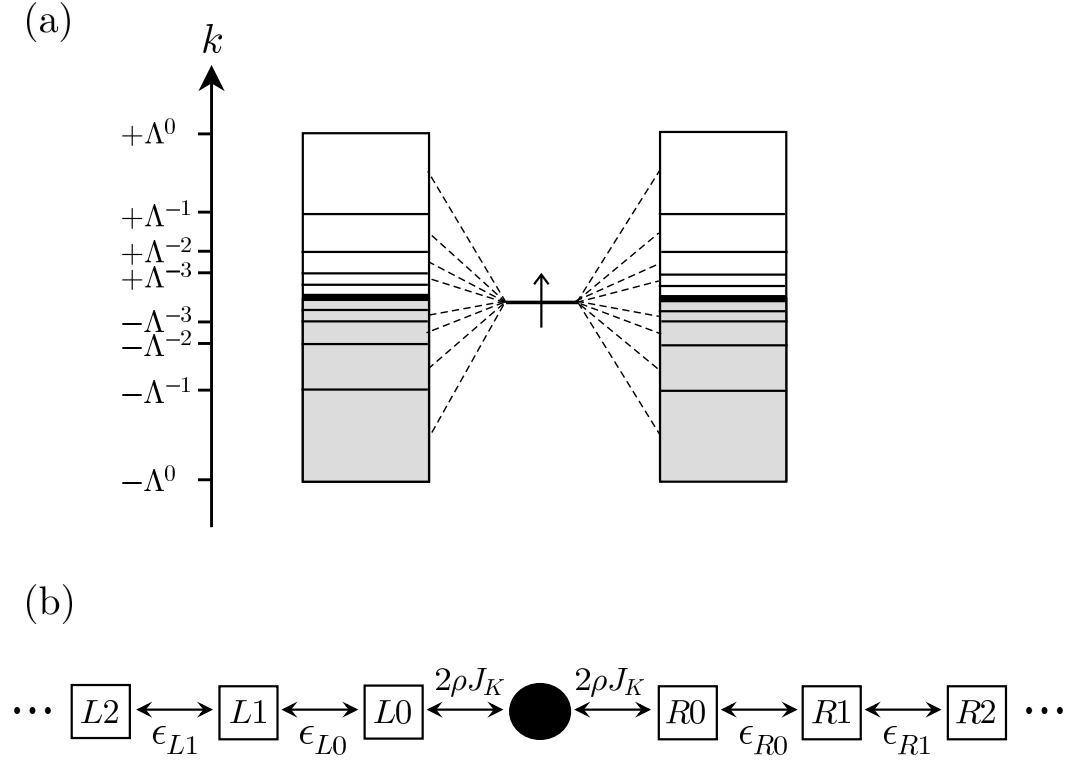


Figure 3.1: Transformations of the 2CK Hamiltonian Eq. 3.3 into a the final linear chain form used in NRG. (a) shows the logarithmic discretization of each conduction band, with the dot spin coupling only to a single state (the $p = 0$ Fourier harmonic) in each interval. (b) shows the tridiagonalized linear chain form, Eq. 3.11, with couplings between neighbouring sites of lead $\alpha = L/R$ given by $\epsilon_{\alpha n} \propto \Lambda^{-n/2} \xi_n$, which decrease exponentially down the chain.

the orbitals $a_{\alpha n p \sigma}$ and $b_{\alpha n p \sigma}$ (Eq. 3.7) for $p > 0$ *do* still enter the problem:

$$\begin{aligned} \int_{-1}^{+1} dk \, k a_{\alpha k \sigma}^{\dagger} a_{\alpha k \sigma} &= \frac{1}{2}(1 + \Lambda^{-1}) \sum_{n,p} \Lambda^{-n} \left(a_{\alpha n p \sigma}^{\dagger} a_{\alpha n p \sigma} + b_{\alpha n p \sigma}^{\dagger} b_{\alpha n p \sigma} \right) \\ &+ \sum_{n,p \neq p'} \frac{\exp[i\omega_n \Lambda^{-n}(p' - p)]}{i\omega_n(p' - p)} \left(a_{\alpha n p \sigma}^{\dagger} a_{\alpha n p' \sigma} - b_{\alpha n p \sigma}^{\dagger} b_{\alpha n p' \sigma} \right). \end{aligned} \quad (3.10)$$

It is worth noting at this point that all the transformations so far have been *exact*. The first and fundamental approximation of the NRG employed now is to ignore all orbitals with $p > 0$. This is justified from Eq. 3.10 for $\Lambda \rightarrow 1$, since in this limit $\omega_n = 2\pi/d_n \rightarrow \infty$. For $\Lambda = 1$, the continuum limit is thus recovered, but as will be seen, using much larger values of Λ still yields essentially-exact numerical results [12, 13]. In fact, a common choice is $\Lambda = 3$, and this is the value we work with throughout this thesis.

We mention briefly here that inaccuracies in the calculation of physical proper-

ties due to the above approximation can be reduced by averaging results over several different discretization schemes for a fixed Λ [128–130]. This so-called ‘interleaved NRG’ approach (also commonly referred to as the ‘z-trick’) takes modified discretization points at Λ^{-n+z} , where z covers the interval $[0, 1)$. Certain artifacts which arise in the NRG due to the discretization (such as low-energy oscillations [27]) are removed by this z -averaging [128–130], although integrating over z does not actually recover the $\Lambda = 1$ limit [27]. Indeed, in calculations which depend very sensitively on the parameters of the model (such as in the region of critical points or phase transitions), we have found that performing the z -averaging can be numerically unstable, and can ‘wash out’ important features of the low-temperature or low-energy properties. In much of the present work therefore, we have avoided the use of this modification.

A rather more reliable approach is to attempt to extrapolate to the $\Lambda = 1$ continuum limit through the use of a correction factor to the bare coupling J_K [13, 131], which can be taken into account from the outset. Replacing $J_K \rightarrow A_\Lambda J_K$ where $A_\Lambda = \frac{1}{2}(\Lambda + 1)(\Lambda - 1)^{-1} \ln(\Lambda)$ can be shown [13, 131] to give the exact continuum result for non-interacting systems, and appears to work well even for interacting systems.

Neglecting the higher Fourier harmonics, and using the definition of $f_{\alpha 0 \sigma}$ from Eq. 3.9, the remaining operators $f_{\alpha n \sigma}$ (for $n > 0$) can be obtained by an exact unitary transformation of $a_{\alpha n 0 \sigma}$ and $b_{\alpha n 0 \sigma}$. Using a standard tridiagonalization procedure, the conduction band part of the Hamiltonian can then be chosen [12] to be of the form of a tight-binding linear chain, with couplings between $f_{\alpha n \sigma}$ and $f_{\alpha(n+1)\sigma}$ only. This is referred to as the ‘Wilson chain’, with $f_{\alpha n \sigma}$ an operator for the n^{th} -orbital of that chain. The orbitals of the Wilson chain can be thought of as a sequence of shells centred on the dot [8, 12]. The ‘0’-orbital has the maximum of its wavefunction closest to the dot, and is coupled directly to the dot and to the neighbouring shell further out. The details of the rather lengthy mathematical manipulations necessary to derive this result for the 1CK model are expounded in Wilson’s original paper, Ref. [12]. The final result for the 2CK model is analogously:

$$\frac{H}{D} = 2\rho J_K \hat{\mathbf{S}} \cdot (\hat{\mathbf{s}}_{L0} + \hat{\mathbf{s}}_{R0}) + \sum_{\alpha=L,R} \sum_{n=0}^{\infty} \frac{1}{2} (1 + \Lambda^{-1}) \Lambda^{-n/2} \xi_n \left(f_{\alpha n \sigma}^\dagger f_{\alpha(n+1)\sigma} + f_{\alpha(n+1)\sigma}^\dagger f_{\alpha n \sigma} \right), \quad (3.11)$$

where $\hat{\mathbf{s}}_{\alpha 0}$ is a spin- $\frac{1}{2}$ operator for the ‘0’-orbital of the $\alpha = L/R$ Wilson chain (see Eq. 3.2), and the dot spin $\hat{\mathbf{S}}$ is exchange coupled to this orbital by $2\rho J_K \equiv J_K/D$. From Eq. 3.11, the couplings between sites n and $(n+1)$ in each chain are given by $\epsilon_{\alpha n} = \frac{1}{2}(1 + \Lambda^{-1})\Lambda^{-n/2}\xi_n$, with

$$\xi_n = (1 - \Lambda^{-n-1})(1 - \Lambda^{-2n-1})^{-1/2}(1 - \Lambda^{-2n-3})^{-1/2} = \mathcal{O}(1), \quad (3.12)$$

as obtained by Wilson [12] for a wide flat conduction band (with constant density of states), and with momentum-independent exchange couplings $J_{\mathbf{k}\mathbf{k}'} \equiv J_K/N$ as used in Eq. 3.3. This form of the Hamiltonian is illustrated in Fig. 3.1(b), with the dot indicated as the solid circle, and the sites of the left and right Wilson chains represented as squares. As $\xi_n = \mathcal{O}(1)$ (Eq. 3.12), and indeed $\xi_n \rightarrow 1$ for large n , the couplings between successive sites of the chains decrease exponentially with n , *ie.* $\epsilon_{\alpha n} \rightarrow \frac{1}{2}(1 + \Lambda^{-1})\Lambda^{-n/2}$. This might suggest that a good approximation to the full system could be made by truncating the chains at some suitably small value of n . However, orbitals with fairly large values of n are in fact required, as these are constructed from conduction band states close to the Fermi level. The poor man's scaling arguments presented in Chapter 2 indicate that excitations on the order of the exponentially-small energy scale T_K^{2CK} are important in the 2CK model, and these excitations can only be described accurately by including orbitals with *large* n . This makes the calculation intractable, because going from n to $(n + 1)$ sees the addition of an extra site on both left and right chains¹. This entails an increase of the size of the Hilbert space of the problem by a factor of 16, which means in practice that direct diagonalization is computationally impossible.

However, the fact that the couplings decrease exponentially down the chains has another important implication. For a chain of a given length N , the lowest energies of the discretized model are $\mathcal{O}(\epsilon_{\alpha N})$, meaning that there is an *exponential separation of energy scales* going from one orbital of the Wilson chain to the next. We discuss in the next section how this can be exploited in the NRG to solve the problem iteratively.

3.3 Iterative diagonalization

The transformations described in Secs. 3.1 and 3.2 map the original 2CK model Eq. 3.3 onto a linear chain Hamiltonian Eq. 3.11. As discussed above, the structure of the transformed Hamiltonian hints at the possibility of obtaining a converged solution for a finite chain length. But in fact the problem remains intractable as it stands because far too many sites of the Wilson chain must be retained to allow direct diagonalization. Wilson's solution [12] for the 1CK model was to begin with a simple cluster of the dot and the '0'-orbital of the chain (which can be diagonalized exactly), then couple on extra sites successively, rediagonalizing the Hamiltonian at each stage. Clearly the Hilbert space of the problem grows exponentially with each added site, and so this process might initially appear as intractable as simply attempting to diagonalize the entire chain in one go. However, the advantage of this approach, as Wilson showed, is that only the lowest few states need be retained

¹Left and right orbitals of the Wilson chains must be added simultaneously to maintain the mirror symmetry of the model.

at each iteration, and yet properties of the system on all energy scales can still be calculated accurately. The Hilbert space thus remains of constant size from iteration to iteration, and so arbitrarily many iterations can be performed. The iterative diagonalization procedure itself also implies the renormalization group (RG) structure of the problem, which provides key insights into the behaviour of the model on all energy scales, but in particular the universal character of the low-temperature properties. In this section we describe this iterative diagonalization approach, as applied to the 2CK model, and discuss its implications.

The first step is to consider a series of Hamiltonians of *finite* length, H_N (with $N = 0, 1, 2, 3, \dots$), which recover the chain Hamiltonian of the full system, Eq. 3.11 in the limit $N \rightarrow \infty$. We define a dimensionless Hamiltonian corresponding to a system comprising the dot coupled to the first N sites in each chain, viz:

$$H_N = \Lambda^{(N-1)/2} \left[\tilde{J}_K \hat{\mathbf{S}} \cdot (\hat{\mathbf{s}}_{L0} + \hat{\mathbf{s}}_{R0}) + \sum_{\sigma, \alpha=L,R} \sum_{n=0}^{N-1} \Lambda^{-n/2} \xi_n \left(f_{\alpha n \sigma}^\dagger f_{\alpha(n+1)\sigma} + f_{\alpha(n+1)\sigma}^\dagger f_{\alpha n \sigma} \right) \right], \quad (3.13)$$

with the dimensionless coupling given by

$$\tilde{J}_K = \frac{4\rho J_K}{1 + \Lambda^{-1}}, \quad (3.14)$$

so that Eq. 3.11 is obtained in the limit

$$H = \lim_{N \rightarrow \infty} \left\{ \frac{1}{2} D (1 + \Lambda^{-1}) \Lambda^{-(N-1)/2} H_N \right\}. \quad (3.15)$$

The factor of $\Lambda^{(N-1)/2}$ has been used in Eq. 3.13 to cancel the N dependence of the coupling between the last two sites in each Wilson chain, $\epsilon_{\alpha(N-1)}$, thus ensuring that the lowest energy scale of the H_N is a number $\mathcal{O}(1)$. This makes the diagonalization numerically stable, but the scaling is also useful when analysing the fixed points and RG flows (see Sec. 3.4 below).

A recursion relation follows from Eq. 3.13, which prescribes the generation of H_{N+1} from H_N , with energies measured relative to the ground state energy, E_G^{N+1} :

$$H_{N+1} = \sqrt{\Lambda} H_N + \sum_{\sigma, \alpha=L,R} \xi_N \left(f_{\alpha N \sigma}^\dagger f_{\alpha(N+1)\sigma} + f_{\alpha(N+1)\sigma}^\dagger f_{\alpha N \sigma} \right) - E_G^{N+1}. \quad (3.16)$$

Any H_N can thus be calculated iteratively from an initial Hamiltonian H_0 , which

(from Eq. 3.13) is simply

$$H_0 = \left(\frac{\tilde{J}_K}{\sqrt{\Lambda}} \right) \hat{\mathbf{S}} \cdot (\hat{\mathbf{s}}_{L0} + \hat{\mathbf{s}}_{R0}), \quad (3.17)$$

and can be calculated exactly ‘by hand’.

Below, we describe the truncation scheme necessary to permit successive application of the recursion relation, and then discuss the iterative process itself in terms of an RG transformation. First however, we demonstrate how Eq. 3.16 may be used in practice to obtain the energies and states of H_{N+1} for the 2CK model.

3.3.1 Use of the recursion relation

The original Hamiltonian Eq. 3.3 has various symmetries which can be exploited in the NRG process. For the 2CK model, three $SU(2)$ quantum numbers can be defined for the isospin² of the left/right chains, and total spin (for the dot and both chains). Classifying the states of the system according to these quantum numbers permits the Hamiltonian to be block-diagonalized at each iteration, which saves a huge amount of computational effort.

However the most general and useful description is one where only the left/right charge, $Q_{\alpha=L/R}$, and total z -component of the spin, S_{tot}^z , is specified. This allows the machinery described below to be used for more general models where, for instance, the particle-hole symmetry of the problem is broken, or when a magnetic field is applied. The use of additive quantum numbers is also much simpler in practice, and so we will describe the NRG process in terms of these, labelling the states of H_N as $|Q_L, Q_R, S_{tot}^z, r\rangle_N$, where r is an index which distinguishes different states with the same set (Q_L, Q_R, S_{tot}^z) . We define operators for these quantum numbers viz:

$$\hat{Q}_{\alpha,N} = \sum_{n=0}^N \hat{q}_{\alpha,n} \quad : \quad \hat{q}_{\alpha,n} = \hat{n}_{\alpha n \uparrow} + \hat{n}_{\alpha n \downarrow} - 1, \quad (3.18a)$$

$$\hat{S}_{tot,N}^z = \hat{S}^z + \sum_{\alpha=L,R} \sum_{n=0}^N \hat{s}_{\alpha,n}^z \quad : \quad \hat{s}_{\alpha,n}^z = \frac{1}{2}(\hat{n}_{\alpha n \uparrow} - \hat{n}_{\alpha n \downarrow}), \quad (3.18b)$$

where $\hat{S}^z$ is an operator for the dot as before, and $\hat{n}_{\alpha n \sigma} = f_{\alpha n \sigma}^\dagger f_{\alpha n \sigma}$ is a number operator for the n^{th} orbital of the $\alpha = L, R$ Wilson chain. We then obtain as desired,

$$\begin{aligned} \hat{Q}_{L,N} |Q_L, Q_R, S_{tot}^z, r\rangle_N &= Q_L |Q_L, Q_R, S_{tot}^z, r\rangle_N, \\ \hat{Q}_{R,N} |Q_L, Q_R, S_{tot}^z, r\rangle_N &= Q_R |Q_L, Q_R, S_{tot}^z, r\rangle_N, \\ \hat{S}_{tot,N}^z |Q_L, Q_R, S_{tot}^z, r\rangle_N &= S_{tot}^z |Q_L, Q_R, S_{tot}^z, r\rangle_N. \end{aligned} \quad (3.19)$$

²Isospin is a non-abelian quantum number related to spin by the Shiba transformation (probably first defined in [132]), and whose z -component is the charge.

As $\hat{Q}_{\alpha,N}$ and $\hat{S}_{tot,N}^z$ commute with each other and H_N , the states of H_N are eigenstates of $\hat{Q}_{\alpha,N}$ and $\hat{S}_N^z$, as shown above.

Since the iterative procedure involves successively building up the Wilson chains site by site, it will also be necessary to define the possible states of the $(N+1)^{th}$ orbital of the $\alpha = L/R$ chain, $|Q, S^z\rangle_{N+1}^\alpha$, as follows:

$$|-1, 0\rangle_{N+1}^\alpha \equiv |-\rangle_{N+1}^\alpha = |-\rangle_{N+1}^\alpha \quad (3.20a)$$

$$|0, -\frac{1}{2}\rangle_{N+1}^\alpha \equiv |\downarrow\rangle_{N+1}^\alpha = f_{\alpha(N+1)\downarrow}^\dagger |-\rangle_{N+1}^\alpha \quad (3.20b)$$

$$|0, +\frac{1}{2}\rangle_{N+1}^\alpha \equiv |\uparrow\rangle_{N+1}^\alpha = f_{\alpha(N+1)\uparrow}^\dagger |-\rangle_{N+1}^\alpha \quad (3.20c)$$

$$|+1, 0\rangle_{N+1}^\alpha \equiv |\uparrow\downarrow\rangle_{N+1}^\alpha = f_{\alpha(N+1)\uparrow}^\dagger f_{\alpha(N+1)\downarrow}^\dagger |-\rangle_{N+1}^\alpha \quad (3.20d)$$

As the $(N+1)^{th}$ orbitals must be added simultaneously to both left and right leads (to maintain mirror symmetry), it will be convenient to describe the resulting states via

$$|p\rangle_{N+1} \equiv |Q, S^z\rangle_{N+1}^L \otimes |Q', S^{z'}\rangle_{N+1}^R, \quad (3.21)$$

where $|p\rangle_{N+1}$ spans a 16-dimensional space, and has left charge $Q_{p,L} = Q$, right charge $Q_{p,R} = Q'$ and the total z -component of the spin $S_{p,tot}^z = S^z + S^{z'}$.

The basis states of the entire system with chains of length $(N+1)$ are then simply

$$|Q'_L, Q'_R, S_{tot}^{z'}, r; p\rangle_{N+1} = |Q_L, Q_R, S_{tot}^z, r\rangle_N \otimes |p\rangle_{N+1}, \quad (3.22)$$

where $Q'_\alpha = Q_\alpha + Q_{p,\alpha}$ and $S_{tot}^{z'} = S_{tot}^z + S_{p,tot}^z$. Diagonalizing H_{N+1} gives the states and energies of the system in terms of the basis states Eq. 3.22, and construction of H_{N+1} itself can be achieved through the use of the recursion relation, Eq. 3.16. In general, elements of the Hamiltonian matrix are readily shown to be of the form

$$\begin{aligned} & \langle Q'_L, Q'_R, S_{tot}^{z'}, r'; p' | H_{N+1} | Q_L, Q_R, S_{tot}^z, r; p \rangle_{N+1} = \\ & \sqrt{\Lambda} E_{Q_L, Q_R, S_{tot}^z, r}^N \times \delta(Q'_L, Q_L) \delta(Q'_R, Q_R) \delta(S_{tot}^{z'}, S_{tot}^z) \delta(r, r') \delta(p, p') \\ & + \sum_{\alpha, \sigma} \xi_N \left[\langle Q'_L, Q'_R, S_{tot}^{z'}, r'; p' | f_{\alpha N \sigma}^\dagger f_{\alpha(N+1)\sigma} | Q_L, Q_R, S_{tot}^z, r; p \rangle_{N+1} \right. \\ & \quad \left. + \langle Q_L, Q_R, S_{tot}^z, r; p | f_{\alpha N \sigma}^\dagger f_{\alpha(N+1)\sigma} | Q'_L, Q'_R, S_{tot}^{z'}, r'; p' \rangle_{N+1} \right]. \end{aligned} \quad (3.23)$$

The first term is simply the diagonal part, corresponding to the rescaled energies of states for the previous iteration. The final two terms involve the coupling between the N^{th} and $(N+1)^{th}$ sites of each chain (and we have taken the Hermitian conjugate

for the last term). The latter terms are simplified if we insert a complete set of states

$$\hat{1} = \sum_{Q_L'', Q_R'', S_{tot}'', r'', p''} |Q_L'', Q_R'', S_{tot}'', r'', p''\rangle \langle Q_L'', Q_R'', S_{tot}'', r'', p''| \quad (3.24)$$

so that the matrix elements we must calculate can be split up into two terms:

$$\begin{aligned} & \langle Q_L', Q_R', S_{tot}', r'; p' | f_{\alpha N \sigma}^\dagger f_{\alpha(N+1)\sigma} | Q_L, Q_R, S_{tot}^z, r; p \rangle_{N+1} \\ &= \sum_{Q_L'', Q_R'', S_{tot}'', r'', p''} \langle Q_L', Q_R', S_{tot}', r'; p' | f_{\alpha N \sigma}^\dagger | Q_L'', Q_R'', S_{tot}'', r'', p'' \rangle_{N+1} \\ & \quad \times \langle Q_L'', Q_R'', S_{tot}'', r'', p'' | f_{\alpha(N+1)\sigma} | Q_L, Q_R, S_{tot}^z, r; p \rangle_{N+1}. \end{aligned} \quad (3.25)$$

The first term of the expansion only involves the operator $f_{\alpha N \sigma}^\dagger$, which acts on states of chain length N , while the second term only involves an operator for the added orbitals, $f_{\alpha(N+1)\sigma}$. It thus follows that

$$\begin{aligned} & \langle Q_L', Q_R', S_{tot}', r'; p' | f_{\alpha N \sigma}^\dagger | Q_L'', Q_R'', S_{tot}'', r'', p'' \rangle_{N+1} \\ &= \langle \tilde{Q}_L', \tilde{Q}_R', \tilde{S}_{tot}', r'; p' | f_{\alpha N \sigma}^\dagger | \tilde{Q}_L'', \tilde{Q}_R'', \tilde{S}_{tot}'', r'' \rangle_N \times \delta(p', p'') \end{aligned} \quad (3.26)$$

where $\tilde{Q}_\alpha = (Q_\alpha - Q_{p,\alpha})$, and $\tilde{S}_{tot}^z = (S_{tot}^z - S_{p,tot}^z)$. Similarly, for the second term:

$$\begin{aligned} & \langle Q_L'', Q_R'', S_{tot}'', r'', p'' | f_{\alpha(N+1)\sigma} | Q_L, Q_R, S_{tot}^z, r; p \rangle_{N+1} \\ &= \langle p'' | f_{\alpha(N+1)\sigma} | p \rangle_{N+1} \times \delta(\tilde{Q}_L'', \tilde{Q}_L) \delta(\tilde{Q}_R'', \tilde{Q}_R) \delta(\tilde{S}_{tot}'', \tilde{S}_{tot}^z) \delta(r'', r) \end{aligned} \quad (3.27)$$

where the elements $\langle p'' | f_{\alpha(N+1)\sigma} | p \rangle_{N+1}$ are independent of N and are easily calculated explicitly from the definition of the states, Eqs. 3.20 and 3.21.

The key result of the above manipulations is that the Hamiltonian H_{N+1} can be constructed purely from a knowledge of the matrix elements of the operator $f_{\alpha N \sigma}^\dagger$ and the energies of H_N . Successive Hamiltonians can thus be generated and diagonalized in this recursive process.

3.3.2 Truncation of states

Due to the exponential growth of the Hilbert space with N , diagonalizing all the states of H_N becomes unfeasible for $N \gtrsim 3$, even exploiting the symmetries of the Hamiltonian to diagonalize matrices in the (Q_L, Q_R, S_{tot}^z) subspaces independently. As mentioned in Sec. 3.2 however, there is a separation of energy scales going from

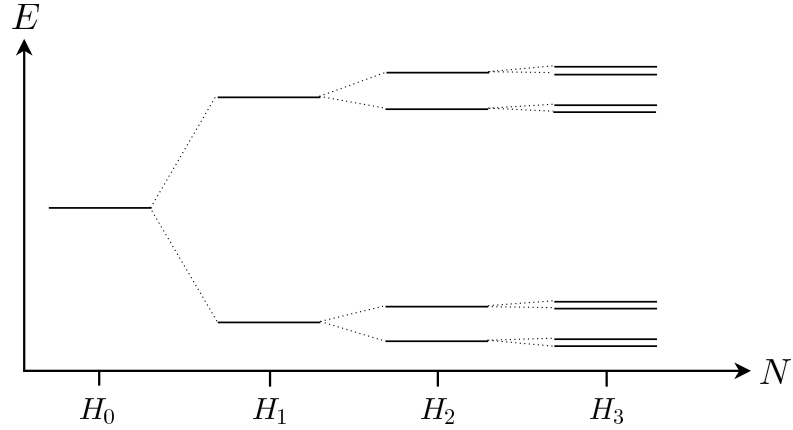


Figure 3.2: Illustration of the exponential reduction in the splitting of energy levels from iteration to iteration. Higher-lying states of H_N do not cross over to become low-lying states of H_{N+1} , thus allowing accurate determination of the lowest levels for large N , even though the higher levels were discarded at an earlier iteration.

one iteration to the next, because the coupling between successive sites of the Wilson chains decreases exponentially with N . The effect of this on the energies of H_N is illustrated in Fig. 3.2, where we show that the splitting of levels going from one iteration to the next decreases exponentially. This implies that high-energy states of H_N do not cross over and become low-lying states of H_M , for $M > N$. This is exploited in the NRG by truncating the number of states retained at each iteration. Keeping the lowest N_s states means that the Hilbert space remains of constant size from iteration to iteration: the calculation time thus scales linearly with N , and a converged solution of the problem³ can then hopefully be obtained for large N .

A summary of the overall NRG procedure is illustrated in Fig. 3.3, where we show schematically how the Wilson chains are built up iteratively. For a given iteration, the process can be broken up into four simple steps: (a) take only the lowest N_s states of the previous iteration; (b) rescale the energies by $\sqrt{\Lambda}$; (c) couple an extra orbital onto each chain using the recursion relation Eq. 3.16 and block diagonalize the new system; (d) give the energies of the new states relative to the ground state energy of that iteration. These steps can then be repeated, with the energies for each H_N spanning approximately the same range. This allows a direct comparison of the lowest lying levels from iteration to iteration, and we show in the next section that for some *finite* N we can then identify the convergence to the $N \rightarrow \infty$ limit.

We also note that in the simplified picture presented in Fig. 3.3, we have used $N_s = 3$ for clarity, and the Hilbert space doubles at each iteration. In the 2CK model, we retain typically $N_s \approx 4000$ and the Hilbert space increases by a factor of

³That the splitting of levels decrease exponentially with N does not in fact *guarantee* that truncated states would not become important at later iterations, but Wilson showed [12] that if one keeps enough states per iteration, then the physics is indeed captured to high accuracy.

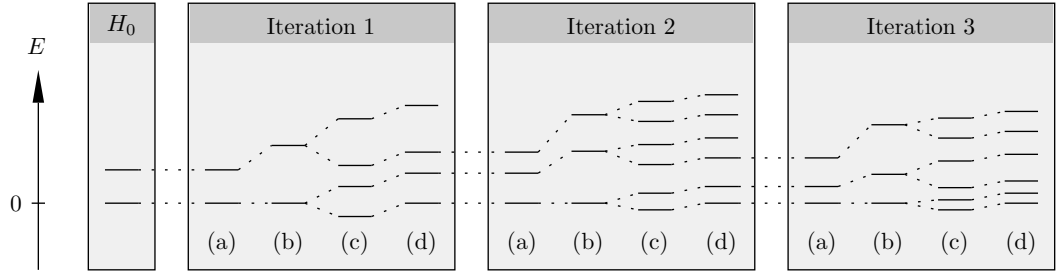


Figure 3.3: Schematic illustration of the NRG process, reproduced with permission from [51]. For a given iteration, (a) the lowest N_s states are retained from the previous iteration; (b) the energies are rescaled by $\sqrt{\Lambda}$; (c) an extra site of each chain is coupled on; (d) the energies are expressed relative to the ground state energy. The simplified illustration here is for $N_s = 3$, with a Hilbert space which doubles at each iteration.

16 at each iteration. The highest energy state retained at a given iteration N clearly depends on N_s , but is often chosen to be on the order of $10 \times \epsilon_{\alpha,N}$, where $\epsilon_{\alpha,N}$ is the coupling between the last two sites of the chain, and thus corresponds roughly to the lowest energy scale of H_N .

The obvious question which arises now is whether the above iterative procedure is of use in describing anything other than the ground state and very low-lying excitations of the system. It would appear that with every extra iteration, we obtain progressively more accurate information about proportionally fewer states. In fact, as we explain in Sec. 3.5, useful information can be extracted from *each* iteration, building up a description of the properties of the system on all energy scales.

First however, we discuss the concept of renormalization in the NRG, and show how the behaviour of the system can be thought of in terms of renormalization group ‘flows’ between ‘fixed points’. We make a connection between renormalization in the NRG and the poor man’s scaling technique discussed in the previous chapter, and then show in Sec. 3.5 that the temperature-dependent thermodynamic properties of the system can be understood in terms of these flows and fixed points.

3.4 Renormalization group flows and fixed points

The mathematical prescription discussed in the above sections was first applied to the single-channel Kondo model by Wilson [12], and later to the Anderson model by Krishnamurthy *et al* [13] and to the 2CK model by Cragg, Lloyd and Nozières [41] (as well as to numerous other problems since then). The technique as described so far does represent a triumph, as the ground state properties of these systems can be definitively established within a wholly non-perturbative approach. However, the real beauty of the NRG is that it allows such problems to be understood in terms of renormalization group (RG) transformations. This not only provides a useful

way of viewing the iterative process involved in applying the NRG in practice, but fundamentally it also provides an insightful conceptual framework for thinking about the energy- and temperature-dependent behaviour of the systems themselves. In this section we discuss the implications of the NRG formulation of the 2CK model in terms of RG ‘flows’ between ‘fixed points’, and the universality which arises as a consequence of this underlying structure.

The recursion relation, Eq. 3.16, can be understood as an RG transformation of the form

$$H_{N+1} = \hat{\mathcal{R}}(H_N). \quad (3.28)$$

With each new iteration (or equivalently, with each application of the operator $\hat{\mathcal{R}}$), the lowest states span an exponentially decreasing range of energies (see Sec. 3.2), but a fixed total number of states N_s is retained. Thus the RG transformation maps the problem onto a model with a reduced characteristic energy scale.

The RG transformation, Eq. 3.28, implies the existence of certain special points, which are referred to as fixed points (FPs), where the repeated action of $\mathcal{R}$ causes no further renormalization:

$$H^* = \hat{\mathcal{R}}(H^*), \quad (3.29)$$

where H^* is an FP Hamiltonian⁴ independent of N , since $H_N^* = H_{N+1}^* \equiv H^*$. Thus FPs represent possible exact $N \rightarrow \infty$ solutions of the model. The concept of the FP was introduced in Sec. 2.3 in the context of the poor man’s scaling technique of Anderson [19], where we defined an FP to be a point where successive bandwidth reduction did not result in further renormalization of the effective Kondo coupling.

The poor man’s scaling approach is an example of the simplest formulation of an RG transformation: a Hamiltonian specified by a set of parameters, $\vec{K}$, is mapped onto a Hamiltonian of the same form, but with renormalized parameters $\vec{K}'$ [27]. Thus in this scheme we would obtain $H(\vec{K}') = \hat{\mathcal{R}}H(\vec{K})$ (see especially Eq. 2.15). For the Kondo model, this approach is necessarily approximate since certain assumptions must be made so that the form of the Hamiltonian remains the same on progressive reduction of the bandwidth. There is in fact no known representation of H_N for the Kondo model (or the 2CK model) where such a transformation can be defined *exactly*. The poor man’s scaling approach is also fundamentally perturbative, and so breaks down when the effective parameters are renormalized to large values. By contrast, in the NRG, we do not impose any restrictions on the form of the Hamiltonian, but calculate instead the lowest energy levels numerically. The flexibility associated with allowing H_N to take any arbitrary form is an important part of the success of the NRG, although we shall see below that at FPs, the behaviour of the system can again be understood in terms of effective Hamiltoni-

⁴Normally in the NRG, FPs are defined by the transformation $H^* = \hat{\mathcal{R}}^2(H^*)$, as odd and even chains usually exhibit different behaviour. This is discussed further in Sec. 3.4.1.

ans with renormalized parameters (even though this is not strictly possible in the crossover region between FPs).

Before discussing the approach used to describe and understand RG flow in the NRG, we consider the general implications of the existence of the FPs themselves. Clearly, for systems with original ‘bare’ parameters which coincide with the FP parameters (*ie.* $H = H^*$), the iterative process of the NRG (or the reduction of the bandwidth in poor man’s scaling) simply yields the same Hamiltonian with the same parameters on all energy scales. While this is in itself an important result, it is rather more informative to consider what happens in the vicinity of the FPs.

As we show below, the presence of an FP strongly affects the behaviour of systems near them. In particular, we can classify FPs according to whether they ‘attract’ or ‘repel’ RG flow in their vicinity. Thus the FP structure of a model is extremely important, because it determines *how* systems renormalize under the RG transformation Eq. 3.28, and hence is fundamentally responsible for the resulting physical behaviour.

An FP is said to be ‘stable’ if it attracts nearby RG flow, while it is ‘unstable’ if it repels RG flow. Thus, to establish the stability of a given FP, we examine the flows close to them. This is done by linearizing the NRG flows around the FP, and then expanding them in terms of the eigenvectors of a linearized transformation. By analysing the N -dependence of the corresponding eigenvalues, one can determine whether the flows tend toward or away from the FP. We sketch the mathematical formulation of this process below.

First, we consider a Hamiltonian H_N which is close to an FP Hamiltonian H^* in the sense that the (effective) parameters of the two are similar. We define

$$\Delta H_N = H_N - H_N^* \quad (3.30)$$

where H_N^* is the FP Hamiltonian in the same Hilbert space as H_N , and both are assumed to have the same basic structure, so that ΔH_N is a Hamiltonian characterized by having small parameters. Similarly $\Delta H_{N+1} = H_{N+1} - H_{N+1}^*$, which may be related to ΔH_N via the RG transformation, viz

$$\begin{aligned} \Delta H_{N+1} &= \hat{\mathcal{R}}(H_N) - H_{N+1}^* \\ &= \hat{\mathcal{R}}(\Delta H_N + H_N^*) - H_{N+1}^* \\ &= \hat{\mathcal{R}}(\Delta H_N). \end{aligned} \quad (3.31)$$

We now approximate the final result by keeping only terms linear in ΔH_N ,

$$\Delta H_{N+1} \approx \hat{\mathcal{L}}(\Delta H_N) \quad (3.32)$$

where $\hat{\mathcal{L}}$ is a matrix which describes this transformation to first order, with eigen-

vectors defined by

$$\hat{\mathcal{L}}O_l = \lambda_l O_l, \quad (3.33)$$

which form a complete set in terms of which ΔH_N may be expanded. Thus we obtain

$$\Delta H_N = \sum_l a_l(N) O_l, \quad (3.34a)$$

$$\Delta H_{N+1} = \sum_l a_l(N+1) O_l, \quad (3.34b)$$

where the coefficients of the expansion are in general N -dependent, as indicated above. Combining Eqs. 3.32, 3.33 and 3.34(a) we now obtain

$$\begin{aligned} \Delta H_{N+1} &= \hat{\mathcal{L}} \sum_l a_l(N) O_l, \\ &= \sum_l \lambda_l a_l(N) O_l, \end{aligned} \quad (3.35)$$

which by comparison with Eq. 3.34(b) yields

$$a_l(N+1) = \lambda_l a_l(N). \quad (3.36)$$

The above relation implies that $a_l(N) = \lambda_l^N C_l$, where C_l is now N -independent. The key result now follows from Eq. 3.34(a) as

$$\Delta H_N = \sum_l \lambda_l^N C_l O_l. \quad (3.37)$$

The significance of this result becomes clear when we consider the behaviour of ΔH_N as N increases. There are three distinct possibilities which arise, depending on the eigenvalue λ_l . We consider first for simplicity the case where there is only a single eigenvector O_1 of the linearized transformation $\hat{\mathcal{L}}$, with corresponding eigenvalue λ_1 . If $\lambda_1 > 1$ then from Eq. 3.37, the (effective) parameters of ΔH_N clearly increase with each iteration, indicating that H_N itself is moving *away* from the FP Hamiltonian H_N^* . The FP is then said to be unstable, and the eigenvector O_1 is referred to as being ‘relevant’.

By contrast, if $\lambda_1 < 1$, then λ_1^N decreases with N so that H_N tends toward H_N^* . RG flow is thus attracted to the FP, which is said to be stable. The corresponding eigenvector O_1 is termed ‘irrelevant’.

The final case is when $\lambda = 1$, so that as N increases, there is no RG flow in the direction of the eigenvector O_1 , which is said to be ‘marginal’. In this case, further analysis is required, as the expansion of $\hat{\mathcal{R}}$ to higher orders of ΔH may in principle result in an eigenvector which could be either relevant or irrelevant. Often

the approach adopted here is in fact simply to examine the actual behaviour of the RG flows obtained numerically from NRG near the FP to establish its stability.

The above arguments can be extended straightforwardly to the general case where there are several eigenvectors of the linearized transformation $\hat{\mathcal{L}}$. A single relevant eigenvector will always result in RG flow away from the FP, which renders it unstable; we have a stable FP only when there are *no* relevant eigenvectors (all being irrelevant or precisely marginal).

The determination of the eigenvectors and eigenvalues of $\hat{\mathcal{L}}$ is somewhat lengthy, and so we do not expand upon it further here. For full details on the approach, the reader is directed to the original work on the Kondo model by Wilson [12] and the extension to the Anderson model by Krishnamurthy *et al* [13].

Before discussing the approach used to determine the FPs and analyse the RG flow from the results of the NRG, we consider briefly the simplified RG procedure where the form of the Hamiltonian does not change under transformation. As mentioned above, one specific example of this type of transformation is the poor man's scaling approach, and simple diagrams for the evolution of the effective coupling on bandwidth reduction were presented in Figs. 2.4 and 2.6 of the previous chapter for the 1CK and 2CK models. To illustrate some basic RG concepts, we consider now a generalized two-parameter Hamiltonian $H(x, y)$ which transforms under the action of an operator $\hat{\mathcal{R}}$ according to $H(\tilde{x}, \tilde{y}) = \hat{\mathcal{R}}[H(x, y)]$, and which maps onto a Hamiltonian valid on a lower energy scale (as in the NRG). We show schematically RG flow diagrams of two fictitious models in Fig. 3.4 which exemplify rather different behaviour and demonstrate the power of the underlying RG concept.

In Fig. 3.4, the circles represent the FPs of the model, while the arrows indicate the RG flow. For these systems, the flow is simply the trajectory of the effective parameters upon successive application of the renormalization group transformation $\hat{\mathcal{R}}$. In the left diagram, we show a model with a single stable FP: irrespective of 'bare' starting parameters, all systems eventually approach H_S^* . On the lowest possible energy scales (which corresponds to the $N \rightarrow \infty$ limit of Eq. 3.28), all systems are described precisely by H_S^* , and thus behave in fundamentally the same way, despite their obvious differences at high energies, where the physical behaviour is dominated by the different starting parameters. This gives rise to the notion of 'universality': two apparently very different systems may flow to the same stable FP on very different energy scales (or equivalently, iteration numbers), but when viewed on lower energy scales, their behaviour is essentially equivalent.

On the right of Fig. 3.4 we show a more complicated example where the model possesses two stable FPs. The key difference here is that the 'bare' starting system parameters now dictate which of these FPs describes the behaviour of the system on the lowest energy scales. Each stable FP (H_{S1}^* and H_{S2}^*) has its own 'basin of attraction': any system which starts off inside the basin of attraction for H_{S1}^*

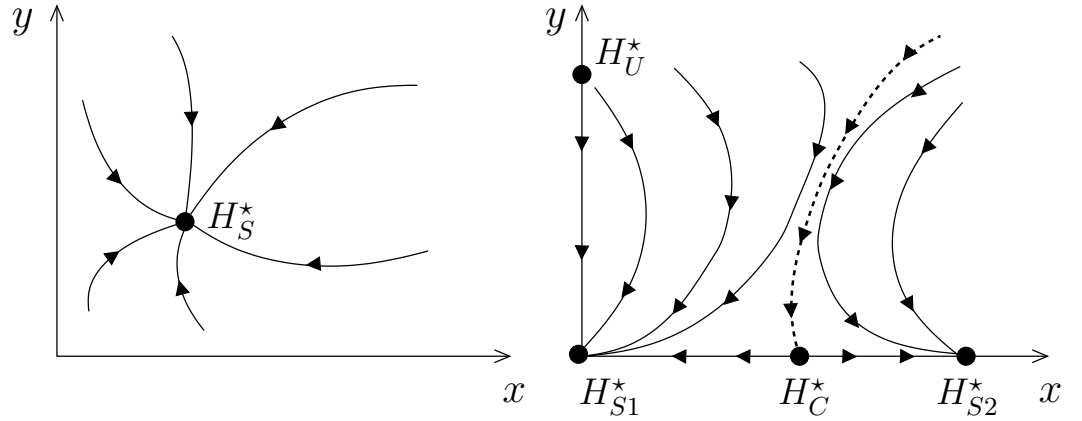


Figure 3.4: Schematic RG flow diagram of a two-parameter Hamiltonian $H(x, y)$. *Left:* shown for a model with a single ‘stable’ FP, H_S^* . All flows tend toward this FP, irrespective of the ‘bare’ starting parameters x and y . *Right:* the presence of two stable FPs means that the ‘bare’ system parameters dictate whether RG flow tends ultimately toward H_{S1}^* or H_{S2}^* . The model thus possesses a ‘quantum phase transition’, with the dashed line describing the phase boundary. Any system precisely at the transition flows to the critical FP, H_C^* . By contrast, RG flow is always repelled by the unstable FP H_U^* .

will always flow toward H_{S1}^* under renormalization. All such systems then share the common low-energy behaviour characteristic of that FP. However, systems with bare parameters which put them in the basin of attraction of H_{S2}^* will inevitably be described by that FP on the lowest possible energy scales. Thus the model has a so-called ‘quantum phase transition’ which occurs on tuning the bare system parameters, and the dashed line in the right panel of Fig. 3.4 shows the corresponding phase boundary. A system precisely on this line (and hence at the point of the transition itself) flows toward the critical FP, H_C^* . Any deviation from this line must of course result ultimately in flow away from the critical FP, and toward one or other of the stable FPs.

Finally, we see that even though the unstable FP H_U^* can never describe the behaviour of a system as $N \rightarrow \infty$, its presence does strongly affect the behaviour of the RG flow in its vicinity. Indeed, RG flow may persist in the vicinity of an unstable FP or a critical FP over many iterations, and hence systems may be well-described by such FPs over a range of energies. We shall see shortly in Sec. 3.5 that this has important implications for the temperature-dependent properties of the system.

Thus, the FP structure of a model determines the RG flows, and hence is responsible for the phase diagram and ultimate low-energy behaviour. The obvious question is: how does one determine the FPs of a given model?

3.4.1 Determination of FPs

There does not in fact exist a general method for determining analytically all the FPs of an arbitrary system within the NRG formulation. Indeed, in some cases (such as the so-called intermediate-coupling FP of the 2CK model, considered in Sec. 3.4.3), FPs can only be identified and classified via numerics obtained from the NRG. However, as was shown in Ref. [13], many FPs can be identified by setting the parameters of the bare model to special values of either zero or infinity. In the case of the 1CK and 2CK models, the FPs can then be understood in terms of a free conduction band, plus a simple isolated dot part. As the free conduction band Hamiltonian (denoted H_N^0), is itself invariant under an RG transformation, such effective Hamiltonians must be FPs. We show this below and study H_N^0 explicitly, as many of the NRG results presented in Secs. 3.4.2 and 3.4.3 can be interpreted in terms of the properties of it.

The free conduction band Hamiltonian we consider is the full Hamiltonian H_N , but with the dot removed. Thus for a two-channel problem, $H_N^0 = H_{LN}^0 + H_{RN}^0$, but as $H_{\alpha N}^0$ for $\alpha = L$ and R are wholly equivalent, we will focus on a single lead:

$$H_{\alpha N}^0 = \Lambda^{(N-1)/2} \sum_{\sigma, n=0}^{N-1} \Lambda^{-n/2} \xi_n \left(f_{\alpha n \sigma}^\dagger f_{\alpha(n+1)\sigma} + f_{\alpha(n+1)\sigma}^\dagger f_{\alpha n \sigma} \right). \quad (3.38)$$

For a given N , the above Hamiltonian can in principle be diagonalized exactly into $(N+1)$ single-particle levels [133]. However, as Eq. 3.38 is particle-hole symmetric, the levels must be symmetrically distributed about the Fermi level. The cases where N is even or odd are thus obviously fundamentally different: for even $(N+1)$, there must be $\frac{1}{2}(N+1)$ levels above the Fermi level⁵ $\eta_j(N) > 0$, and a corresponding set of $\frac{1}{2}(N+1)$ levels below it with energies $-\eta_j(N)$. For odd $(N+1)$ however, symmetry requires that we have a level at $\hat{\eta}_0(N) = 0$, with $\frac{1}{2}N$ of the remaining levels at $\hat{\eta}_j(N) > 0$ and $\frac{1}{2}N$ at $-\hat{\eta}_j(N)$.

The ground state of the system is obtained simply by filling all negative-energy levels (those below the Fermi energy), while excited states are generated by removing these electrons, or promoting them to higher unfilled levels. We cast the diagonalized form of Eq. 3.38 in terms of particle operators $g_{\alpha j \sigma}^\dagger$ which create electrons in levels of positive energy, while the hole operators $h_{\alpha j \sigma}^\dagger$ destroy electrons in the negative-

⁵We will measure the energies relative to the Fermi level, which is equivalent to setting $E_f = 0$.

energy levels. Considering the cases for even and odd N separately, we obtain

$$H_{\alpha N}^0 = \hat{\eta}_0 g_{\alpha 0 \sigma}^\dagger g_{\alpha 0 \sigma} + \sum_{j=1}^{\frac{1}{2}N} \hat{\eta}_j \left(g_{\alpha j \sigma}^\dagger g_{\alpha j \sigma} + h_{\alpha j \sigma}^\dagger h_{\alpha j \sigma} \right) \quad : N \text{ even}, \quad (3.39a)$$

$$H_{\alpha N}^0 = \sum_{j=1}^{\frac{1}{2}(N+1)} \eta_j \left(g_{\alpha j \sigma}^\dagger g_{\alpha j \sigma} + h_{\alpha j \sigma}^\dagger h_{\alpha j \sigma} \right) \quad : N \text{ odd}. \quad (3.39b)$$

The single-particle energy levels $\hat{\eta}_j$ and η_j can be determined numerically for a given N and Λ , and in fact one finds that they rapidly converge with increasing N .

The important implication of this is that for sufficiently large N , H_N^0 is an FP of the RG transformation $\hat{\mathcal{R}}^2$, since for either even or odd N , adding more sites onto the chain does not result in further renormalization of the level energies.

Thus, if an effective Hamiltonian can be written as the sum of a dot part and a completely decoupled conduction band (or pair of conduction bands, in the case of the 2CK model), then it must be an FP Hamiltonian. The dot part is of course unaffected by adding extra sites onto the Wilson chain if it is disconnected from that chain, while the free conduction band part itself is invariant under the action of $\hat{\mathcal{R}}^2$. Thus we see that in general there are two classes of FP obtained in this way: one set for even N and one set for odd N , and FPs of this type are in general defined by

$$H^\star = \hat{\mathcal{R}}^2(H^\star). \quad (3.40)$$

Such FPs describe so-called ‘Fermi liquid’ behaviour⁶, where the system can be interpreted in terms of a model where the dot is removed, but with modified boundary conditions [8] (*ie.* at the Fermi level, the system can be described in terms of non-interacting quasiparticles [8]).

In the next section, we consider the concrete example of the 1CK model, determining the FPs and examining the RG flow as calculated from the NRG. In Sec. 3.4.3 we go on to study the 2CK model relevant to the work of Chapters 4–8, where a richer array of physics is found to arise.

3.4.2 FPs and flows of the 1CK model

In this section we consider the 1CK model Eq. 2.10, and determine its FPs using the approach outlined above [12, 13]. We will then use the NRG to study these FPs and examine the RG flows themselves.

⁶Certain FPs, such as the ‘local moment’ FP (discussed further below), are in fact referred to as ‘singular’ Fermi-liquids due to the marginally irrelevant logarithmic corrections to the FP [127, 134]. Thus, the behaviour can be understood in terms of the non-interacting limit only when precisely *at* the Fermi level.

As the 1CK model has a single parameter — the dot-lead Kondo coupling J_K — two FPs arise by setting $J_K = 0$ and $J_K = \infty$ in Eq. 2.10. We consider first the ‘local moment’ (LM) FP, which is obtained for $J_K = 0$. Here, the dot is decoupled from the lead, and so the dot spin remains free under the application of the RG transformation $\hat{\mathcal{R}}$. The conduction band is invariant under $\hat{\mathcal{R}}^2$ (see Sec.3.4.1), and so $H_{N+2,\text{LM}}^* = \hat{\mathcal{R}}^2(H_{N,\text{LM}}^*)$, where

$$H_{N,\text{LM}}^* = H_N^0 + \tau, \quad (3.41)$$

and τ represents the dot spin- $\frac{1}{2}$ degree of freedom. Thus the LM FP is simply the free conduction band chain, with a double degeneracy corresponding to the free, decoupled dot spin.

The ‘strong coupling’ (SC) FP is obtained for $J_K = \infty$: this case is a little more subtle than the LM FP, as the dot is still coupled to the conduction band. The dot spin forms a singlet state with the ‘0’-orbital of the Wilson chain (the exchange coupling being antiferromagnetic), but because the coupling is infinitely strong, the excited triplet state is inaccessible and so the “Kondo singlet” decouples completely from the rest of the chain. This leaves a free conduction band chain of length $(N-1)$, and hence the SC FP Hamiltonian is simply

$$H_{N,\text{SC}}^* = H_{N-1}^0, \quad (3.42)$$

which is again an FP of the RG transformation $\hat{\mathcal{R}}^2$. The SC FP is thus wholly equivalent to the free conduction band described by a chain with one fewer site: the dot spin is ‘quenched’ or ‘screened’ by coupling to the lead conduction electrons. From the above arguments, we would expect the spectrum of energy levels at the SC FP for a given iteration N to be exactly that of the LM FP for iteration $N+1$. We will show that this is indeed the case shortly when we calculate the lowest energy levels of the 1CK model directly with NRG.

Using the approach of Sec. 3.4, the stability of these FPs can be established. It is found [12,13] that the SC FP is stable (ΔH_N containing only irrelevant corrections to the FP), while the LM FP is marginal. A more sophisticated analysis of the LM FP could be attempted, but it is simpler to examine the numerical results of the NRG itself. In fact, as we shall see below, the LM FP is *unstable*.

First however, we pause to make contact between this approach, developed by Wilson [12], and Anderson’s poor man’s scaling analysis [19], and demonstrate that the latter can also be used to classify the stability of certain FPs. In Sec. 2.3 of Chapter 2 we applied the poor man’s scaling technique to the 1CK model. Within this approach, the trajectory of the effective coupling $\tilde{J}_K$ on successive reduction of the bandwidth/energy scale was calculated perturbatively (and as such, is only

strictly valid for small $\tilde{J}_K$). The existence of the LM FP was established from this analysis: successive reduction in bandwidth causes no renormalization of the effective coupling if the bare coupling is itself zero. Moreover, it was found [19] that for any small finite bare coupling $J_K > 0$, reducing the bandwidth results in an *increase* in the effective coupling (see Eq. 2.18), which implies that the LM FP is unstable.

The existence of the SC FP was also surmised from the results of poor man's scaling. The renormalization of the effective coupling to progressively larger values suggests that the RG flow is tending toward a $\tilde{J}_K = \infty$ FP, although this could not be definitively established since the approach breaks down as $\tilde{J}_K$ becomes large. Wilson's NRG approach does not of course fall foul of this limitation: the SC FP is an FP of the RG transformation $\hat{\mathcal{R}}^2$, and indeed can be shown [12, 13] to be the only stable FP of the 1CK model. As discussed above, this in itself implies that all antiferromagnetically-coupled 1CK systems are fundamentally alike when viewed on the lowest energy scales.

While the approximate treatment of the 1CK model with poor man's scaling leads to an ultimately incomplete description, in the perturbative regime the RG flow can still be simply and usefully understood as the trajectory of the effective Kondo coupling. The essentially-exact solution using NRG cannot be formulated in terms of fixed Hamiltonians with effective parameters however, and so we characterize the evolution of H_N , and hence the RG flow, directly from the many-body energy levels of the system, $E_{Q,S^z,r}^N$, defined at a given iteration by

$$H_N|Q, S^z, r\rangle_N = E_{Q,S^z,r}^N|Q, S^z, r\rangle_N, \quad (3.43)$$

where Q labels the total charge of the system and S^z the total z -component of the spin (*cf.* Eq. 3.18). The Hamiltonian H_N (defined for the 1CK model [12] in an exactly analogous fashion to that of the 2CK model, Eq. 3.13) is rescaled at each iteration, and the energies are always given with respect to the ground state energy of that iteration. Thus, the energy levels of H_N always span approximately the same range. This permits a direct comparison of the lowest energy levels of the system from iteration to iteration. However, for a single-channel model, subspaces with particular quantum numbers (Q, S^z) exist only for even or odd iteration numbers (but not both): at each iteration, a new site of the Wilson chain is added, and must change either Q or S^z . Indeed in Sec. 3.4.1 we discussed how two FPs of the model (the SC and LM FPs) are in fact FPs of the transformation $\hat{\mathcal{R}}^2$ instead of $\hat{\mathcal{R}}$ itself. Thus, we will consider below the cases of even and odd N separately.

In Fig. 3.5, we show how the lowest energy levels of the NRG renormalize with iteration number N for a system with $\rho J_K = 0.056$ (chosen arbitrarily), and we use a discretization parameter $\Lambda = 3$ (the choice of which is discussed in more detail in

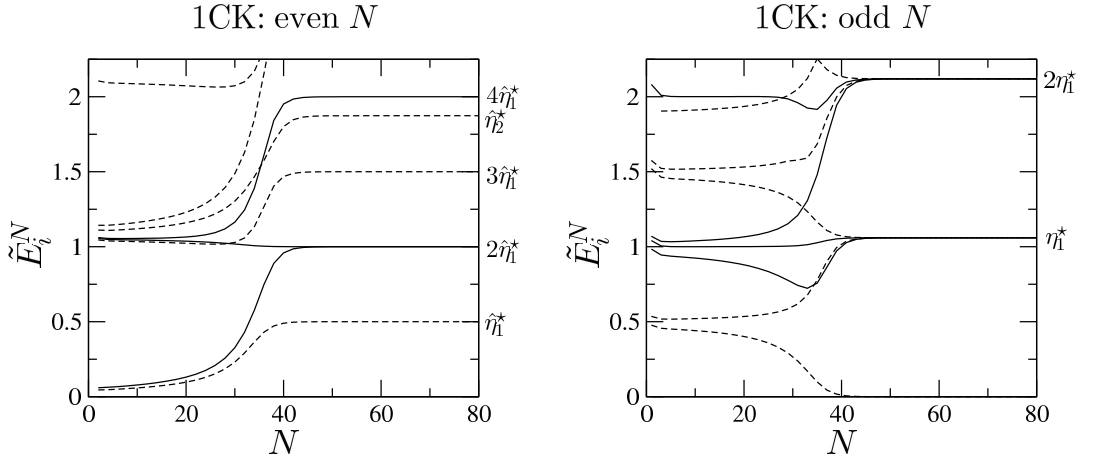


Figure 3.5: NRG energy level flows $\tilde{E}_i^N$ vs iteration number N , for a 1CK model with $\rho J_K = 0.056$. Shown in the left panel for *even* iterations only are the lowest five levels in subspaces with $(Q, S^z) = (0, 0)$ [solid lines] and $(\pm 1, \pm \frac{1}{2})$ [dashed lines]. These subspaces only exist for even N in the 1CK model. In the right panel we plot the levels for *odd* iterations only, again showing the lowest five levels, but now for subspaces $(0, \pm \frac{1}{2})$ [solid] and $(\pm 1, 0)$ [dashed]. The labels on the vertical axes are the SC FP level energies.

Sec. 3.5). In the left panel we consider only even iterations, plotting the lowest five levels in the subspaces with $(Q, S^z) = (0, 0)$ [solid lines] and $(\pm 1, \pm \frac{1}{2})$ [dashed lines]. The right panel is for odd iterations; we again plot the lowest five energy levels, but in the subspaces $(0, \pm \frac{1}{2})$ [solid] and $(\pm 1, 0)$ [dashed]. The energies themselves (as obtained from Eq. 3.43) have been rescaled by a trivial factor, $\tilde{E}_{Q,S^z,r}^N = 0.625 \times E_{Q,S^z,r}^N$ (discussed further below). We also comment that the levels shown in the figure are the lowest levels of the system across all subspaces (not counting degeneracies).

Several general points are apparent from cursory inspection of Fig. 3.5. Firstly, the behaviour of the energy levels (and their overall structure) is rather different for even and odd iterations as expected from the above analysis. Thus, there can be *no* FPs of the transformation $\hat{\mathcal{R}}$ (see Eq. 3.28). However, a given level evolves smoothly with $2N$ (left panel) or $2N + 1$ (right panel), and *two* FPs of the transformation $\hat{\mathcal{R}}^2$ (see Eq. 3.40) can be identified from Fig. 3.5 for both even and odd iterations, which are of course the LM and SC FPs discussed above.

For the very early iterations (with N either even or odd), the energy levels exhibit a certain structure, which changes only slightly with N . As there is only modest renormalization of the levels, H_N and H_{N+2} must be rather similar, and hence H_N must itself be close to an FP. This is the LM FP, characterized by a free (decoupled) dot spin. That the LM FP is unstable is obvious from Fig. 3.5, since as N is increased, the levels begin to move substantially, and cross over rapidly to a new characteristic structure for $N \approx 40$. The levels then remain essentially fixed from $N = 50$ and do not undergo further renormalization (having thus converged to

the $N \rightarrow \infty$ limit). This is the stable SC FP to which all flows ultimately tend.

As mentioned above, these FPs are the only FPs of the isotropic 1CK model, Eq. 2.10, and so below some characteristic low-energy scale, all systems must be described by the SC FP [8, 12, 13]. The bare parameters of the model thus only affect this scale, rather than the ultimate nature of the ground state itself.

An important implication of the flows shown in Fig. 3.5 is that the NRG calculation has essentially converged to the $N \rightarrow \infty$ limit for *finite* N , meaning that the nature of the ground state and low-lying excitations can be definitively determined in practice. Indeed, we can also identify a distinct scale for the crossover to the SC FP from the evolution of the levels with N . This corresponds to an exponentially-small energy scale, since at a given iteration, the characteristic energies on an absolute scale are of order $\sim \Lambda^{-N/2}$. We discuss this in more detail in Sec. 3.5, but here we comment that the scale is the ‘Kondo scale’ T_K^{1CK} , which we derived as the poor man’s scaling invariant in Sec. 2.3.

To confirm the physical picture presented above, we can also calculate directly the expected single-particle energy levels one should obtain at the SC FP for even and odd iterations, using Eqs. 3.42 and 3.39. We have labelled the vertical axis of Fig. 3.5 with these levels (for $\Lambda = 3$), which agree perfectly with the converged NRG levels. Indeed, a duality between the SC FP levels and the LM FP levels is also apparent from Fig. 3.5. We argued above that the SC FP levels for odd iterations should be the same as the levels for the LM FP at even iterations. Comparison of the level structure for *early* iterations (where the system is well-described by the LM FP) in the right panel (odd N), and the *final* iterations (where the system has flowed to the stable SC FP) in the left panel (even N) confirms this prediction.

We will describe how physical properties of the system can be calculated from the NRG energy levels in Sec. 3.5, but first we consider the FP structure and RG flows for the 2CK model.

3.4.3 FPs and flows of the 2CK model

In this section, we consider first the FPs which may arise in the 2CK model Eq. 2.20, and then go on to study the actual NRG energy level flows. As the dot spin- $\frac{1}{2}$ is connected now to *two* leads by distinct exchange couplings J_{KL} and J_{KR} , we expect to obtain *four* FPs by setting either to zero or infinity (adopting the approach of Ref. [13], described above in Sec. 3.4.1). We examine each of these in turn below:

- $J_{KL} = J_{KR} = 0$: both leads are decoupled from the dot spin- $\frac{1}{2}$. The FP Hamiltonian is simply that of two free conduction bands, plus the dot degree of freedom. This is the 2CK local moment FP: $H_{N,LM}^* = H_{LN}^0 + H_{RN}^0 + \tau$.
- $J_{KL} = 0, J_{KR} = \infty$: the left lead is decoupled, while the dot spin- $\frac{1}{2}$ locks

up into a singlet state with the ‘0’-orbital of the right Wilson chain. The FP Hamiltonian is thus $H_{N,SC:R}^* = H_{LN}^0 + H_{R(N-1)}^0$, and can be thought of as the usual SC FP, with an extra free conduction band.

- $J_{KL} = \infty, J_{KR} = 0$: the dot now couples to the left lead, while the right lead is decoupled. The FP Hamiltonian here is then $H_{N,SC:L}^* = H_{L(N-1)}^0 + H_{RN}^0$.
- $J_{KL} = J_{KR} = \infty$: the dot spin- $\frac{1}{2}$ forms a trimer with the ‘0’-orbitals of the left and right Wilson chains. The ground state of this trimer is a doublet state, which is decoupled from the rest of the leads. The FP Hamiltonian is thus $H_{N,SC}^* = H_{L(N-1)}^0 + H_{R(N-1)}^0 + \tau$.

In Sec. 2.4 of Chapter 2, we examined the 2CK model using poor man’s scaling [19], following the approach of Nozières and Blandin [40]. The analysis demonstrates the presence of the LM FP, and it is again straightforward to show that the FP is unstable from the trajectories of the effective parameters. In particular, for finite positive bare couplings to either lead, the effective coupling grows as the bandwidth/energy scale is reduced. The FPs corresponding to strong coupling with *one* of the leads ($H_{N,SC:L}^*$ or $H_{N,SC:R}^*$) are also implicit, but as with the 1CK model, the perturbative approach breaks down as the effective couplings renormalize to large values, so their existence or stability cannot be definitively established from this approach.

The stability of the $H_{N,SC}^*$ FP (which corresponds to strong coupling with both leads) can however be determined by considering the *effective* coupling which is generated between the ground state of the trimer formed from the dot and the two ‘0’-orbitals, and the rest of the lead states. This residual coupling can be calculated perturbatively, and is found to be antiferromagnetic [49]. Such a coupling flows under renormalization and represents a *relevant* correction to the FP, which renders it unstable.

In fact, the poor man’s scaling technique does indicate the presence of another FP at *intermediate coupling* (see Sec. 2.4 and Ref. [40]). We will denote this FP $H_{N,2CK}^*$, as it is unique to the 2CK model. In fact, it was shown in Ref. [125] that at the 2CK FP itself, the effective coupling is $\rho J_K^* \approx 0.35$. Before considering the NRG energy levels themselves, we point out that if the bare model has overall left/right symmetry (Eq. 2.20 with $J_{KL} = J_{KR} \equiv J_K$), then this symmetry must be respected at the FPs of the model. Thus, $H_{N,SC:L}^*$ and $H_{N,SC:R}^*$ are forbidden in this case. As the LM FP is certainly unstable [12, 13, 40], this suggests that the intermediate coupling FP $H_{N,2CK}^*$ is in fact stable here. This is indeed found to be the case, and gives rise to some novel new Kondo physics, as shown below. As the FP cannot be written as a decoupled dot part and a pair of free conduction band leads (as with the other FPs), this FP is a more subtle object, and has no simple description (for

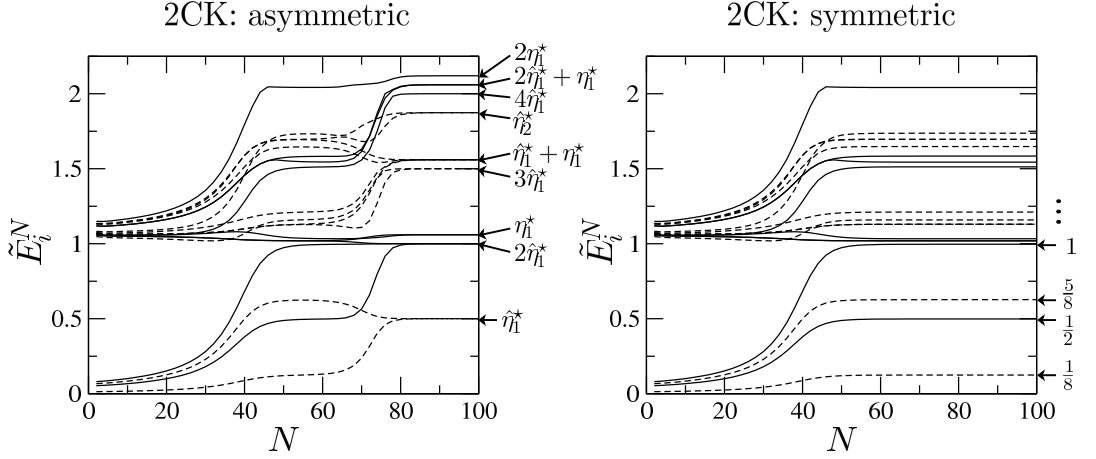


Figure 3.6: NRG energy level flows $\tilde{E}_i^N$ vs (even) iteration number N , for the 2CK model. *Left*: the dot is asymmetrically coupled to the leads; specifically we show results for $\rho J_{KL} = 0.05 + \delta$ and $\rho J_{KR} = 0.05 - \delta$ with $\delta = 10^{-6}$. *Right*: the dot is coupled symmetrically to the leads, with $\rho J_{KL} = \rho J_{KR} = 0.05$ (i.e. $\delta = 0$). Shown are the lowest ten levels of the subspaces $(Q_L, Q_R, S_{tot}^z) = (0, 0, \pm \frac{1}{2})$ [solid lines] and $(\pm 1, 0, 0)$ [dashed lines].

example, in terms of the free conduction band Hamiltonians $H_{\alpha N}^0$). The FP is known as a ‘non-Fermi liquid’ state, because even at the Fermi energy, the system cannot be described simply in terms of non-interacting conduction electron quasiparticles.

Having considered the above FPs and their expected structure, we will study the 2CK model Eq. 2.20 directly with NRG (as in the original work in Refs. [41, 45]), focusing here on the evolution of lowest energy levels of H_N , defined by

$$H_N |Q_L, Q_R, S_{tot}^z, r\rangle_N = E_{Q_L, Q_R, S_{tot}^z, r}^N |Q_L, Q_R, S_{tot}^z, r\rangle_N. \quad (3.44)$$

In Fig. 3.6 we plot the lowest ten levels of the subspaces $(Q_L, Q_R, S_{tot}^z) = (0, 0, \pm \frac{1}{2})$ [solid lines] and $(\pm 1, 0, 0)$ [dashed lines] vs (even) iteration number N . We show results for systems with $\rho J_{KL} = 0.05 + \delta$ and $\rho J_{KR} = 0.05 - \delta$, where in the left panel, we consider the asymmetrically-coupled system where $\delta = 10^{-6}$, while in the right panel we show the left/right mirror symmetric case $\delta = 0$.

At early iterations in both systems, the energy level structure is typical of the LM FP H_{LM}^* (for even N). There is an extra degeneracy in the levels compared with the 1CK model because the left and right chains are both free, but the level energies themselves are given by $\hat{\eta}_j$ (as calculated directly from Eqs. 3.38 and 3.39a). The situation is thus similar to the local moment behaviour of the 1CK model (left panel of Fig. 3.5). At higher iterations, the levels become characteristic of a new FP, not described by the free-chain single-particle levels of Eq. 3.39. For both asymmetric and symmetric systems, at $N \approx 50$ the systems are close to the 2CK FP H_{2CK}^* . For the mirror symmetric model, there are no other FPs, and the system is described

by this stable 2CK FP as $N \rightarrow \infty$. The levels themselves are characteristic of this FP; the conformal field theory (CFT) analysis of the 2CK model by Affleck and Ludwig [46] predicts that the lowest lying levels of the symmetric model are described by the fractions $0, \frac{1}{8}, \frac{1}{2}, \frac{5}{8}, 1, \dots$. We have rescaled the energies in Figs 3.5 and 3.6 by a trivial factor which depends on the NRG discretization parameter Λ ($\tilde{E}_i^N = 0.625 \times E_i^N$ for $\Lambda = 3$, as used here) in order to make direct comparison with the CFT results. Fig. 3.6 shows that the agreement is essentially perfect.

Considering now the asymmetrically-coupled case in the left panel of Fig. 3.6, we see that the 2CK FP is *destabilised* [40, 45, 46, 124]. While the system is well-described by H_{2CK}^* between $N = 45$ – 65 , the levels move away from the characteristic level structure of the 2CK FP, and flow toward a different FP. The levels for $N \approx 80$ are typical of the converged $N \rightarrow \infty$ levels, and thus describe the stable FP of the asymmetric model. Poor man's scaling arguments would suggest that here the stable FP is $H_{SC:L}^*$, as the bare exchange coupling was strongest between the dot and the left lead. This can be confirmed directly from the energy level structure at the FP. We have labelled the levels at $N = 100$ with the free-chain single-particle level energies of Eq. 3.39, which are seen to comprise both $\hat{\eta}_j$ and η_j levels typical of free conduction band chains of length $2N$ and $(2N + 1)$ respectively. This is natural as $H_{N,SC:L}^* = H_{L(N-1)}^0 + H_{RN}^0$, and so the lowest levels of the system comprise a combination of both the levels for even and odd chains. In fact, $H_{SC:R}^*$ would exhibit the same overall level structure at the FP, but the lowest levels would be associated with quantum numbers with left and right labels swapped.

Indeed, neither FP shows an alternation in the lowest levels of the system going from even to odd iteration, as the FP contains levels for both $H_{\alpha N}^0$ and $H_{\alpha(N-1)}^0$ simultaneously, although again, the quantum numbers associated with the levels must alternate. By contrast, at the 2CK FP, there is no alternation between even and odd iterations for *any given level*, which indicates that the interactions at the 2CK FP are long range [8].

Finally, we comment that the asymmetric system (left panel of Fig. 3.6) shows *two* distinct energy scales: one for the flow to the 2CK FP (which is essentially the same as that in the right panel for the symmetric system), and another scale for the flow from this FP to the stable $H_{SC:L}^*$ FP. In fact, the symmetric 2CK model (with $\delta = 0$) is a critical point of Eq. 2.20, separating two phases described by $H_{SC:L}^*$ (for $\delta > 0$) and $H_{SC:R}^*$ (for $\delta < 0$), and has been studied extensively [40, 45, 46, 124]. For small $|\delta|$ it is found that this scale goes as $|\delta|^\nu$ with $\nu = 2$ being characteristic of the transition [45, 46, 124].

As discussed above, the exact RG transformation Eq. 3.28 for the 2CK model prevents a faithful quantitative representation of the RG flow in terms of the renormalization of effective parameters. However, it is often helpful to regard the NRG Hamiltonians H_N as being *approximately* dependent on a few effective parameters,

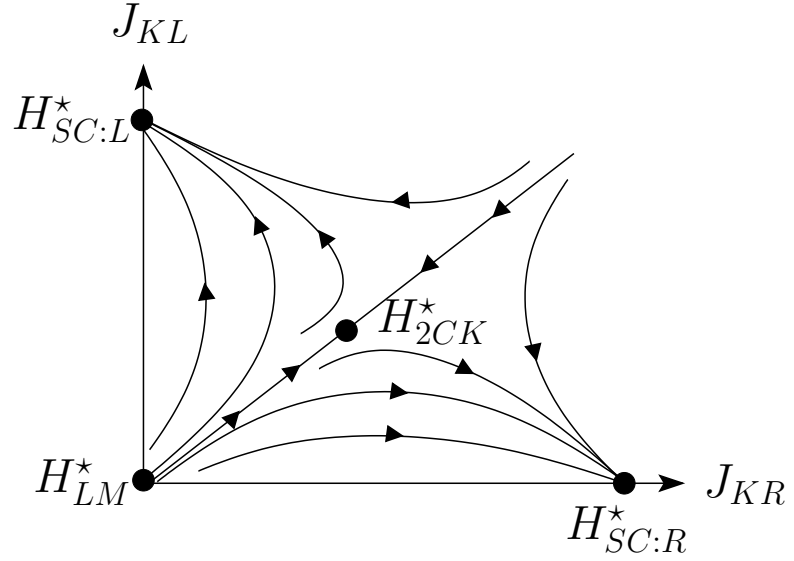


Figure 3.7: Flow diagram for the 2CK model. The FPs are shown as circles, with the RG flow between them in the effective parameter space of J_{KL} and J_{KR} represented by arrows, which approximates qualitatively the energy level flow between FPs as calculated from the NRG. For mirror symmetric systems ($J_{KL} = J_{KR}$) the stable FP is H_{2CK}^* , which is always reached under renormalization as $N \rightarrow \infty$. By contrast, for any $J_{KL} \neq J_{KR}$, the 2CK FP is destabilised, and $H_{SC:\alpha}^*$ is the stable FP (with $J_{K\alpha}$ the stronger bare coupling). However, RG flow may still approach the 2CK FP before eventually being ‘repelled’ (see Fig. 3.6).

which we can use to visualize qualitatively the energy level flow between FPs. For the 2CK model, we show the approximate flow of J_{KL} and J_{KR} , as deduced from the exact numerical data of the NRG in Fig. 3.7.

While it is only the stable FPs which determine the ground state properties of a system, the unstable FPs of a model do affect the RG flow; the route taken to arrive at a stable FP (and hence the underlying low-energy scale for flow to that FP) may be very different from system to system. Indeed, what is less clear is that the unstable FPs, and hence the RG flow, strongly influences the *temperature-dependent* behaviour of a system, as discussed below.

In the next sections, we describe how the physical properties of a system can be calculated within NRG, and show in particular that thermodynamics can be calculated at *each* iteration, progressively building up information about the system on all temperature scales.

3.5 Calculation of thermodynamic properties

In the previous sections we have described how ‘impurity’ problems such as the 1CK and 2CK models can be formulated within NRG, and how a convergent solution for the ground state and low-lying excitations can be obtained. However, the NRG technique is much more powerful than this alone. We shall see in this section that a

connection can be made between the iteration number and an effective temperature, so that thermodynamics can be calculated accurately on essentially all temperature scales. The beauty of the method is then that the concepts of FPs, RG flows and universality discussed in Sec. 3.4 have a fundamental interpretation in terms of the temperature-dependence of physical properties.

We follow the arguments in Refs. [12,13] below, then go on to use the results to calculate thermodynamics for the 1CK and 2CK models. The starting point for the calculation of thermodynamic quantities is the expression for the thermal average of some operator $\hat{A}$, which as usual is given by

$$\langle \hat{A} \rangle = \frac{\text{Tr} \hat{A} \exp(-\beta H)}{\text{Tr} \exp(-\beta H)}, \quad (3.45)$$

where Tr denotes a trace over the states of the system and $1/\beta = k_B T$, with T the temperature and k_B the Boltzmann constant. It is conventional in the NRG to focus on the dot contribution to the thermodynamics rather than bulk quantities. These are defined simply as the difference between the calculated thermodynamics when the dot is present and when it is removed:

$$\langle \hat{A} \rangle_{\text{imp}} = \langle \hat{A} \rangle - \langle \hat{A}^0 \rangle = \frac{\text{Tr} \hat{A} \exp(-\beta H)}{\text{Tr} \exp(-\beta H)} - \frac{\text{Tr} \hat{A}^0 \exp(-\beta H^0)}{\text{Tr} \exp(-\beta H^0)}, \quad (3.46)$$

where H^0 is the Hamiltonian of the system with the dot removed, and A^0 is an operator which acts on that system. The subscript “imp” used for the dot contribution to a thermodynamic quantity is historical in origin, but we shall retain this notation in the current work as is conventional.

To understand how this standard machinery can be used to calculate thermodynamics within the NRG we note that, for sufficiently low temperatures, the contribution to a thermodynamic quantity from the high energy states truncated at previous iterations is exponentially suppressed by the Boltzmann factor (Eq. 3.46). Thus, these states can indeed be safely ignored in the calculation of physical properties at these temperatures. However, the temperature cannot be so low that the splitting of retained levels at later iterations would introduce large errors. Due to the exponential separation of energy scales going from one iteration to the next, it is plausible that there exists a small temperature window at each iteration inside which thermodynamics could be accurately calculated. This is illustrated in Fig. 3.8 where we show that at a given iteration M , there are two energy scales: E_{max} is a cutoff above which high-energy states are discarded, while E_{min} is the splitting of levels which results at the next iteration (and which is exponentially smaller than E_{max}). At a characteristic temperature for this iteration, defined such that $E_{\text{min}} \ll T_M \ll E_{\text{max}}$, thermodynamics calculated for H_M are essentially those

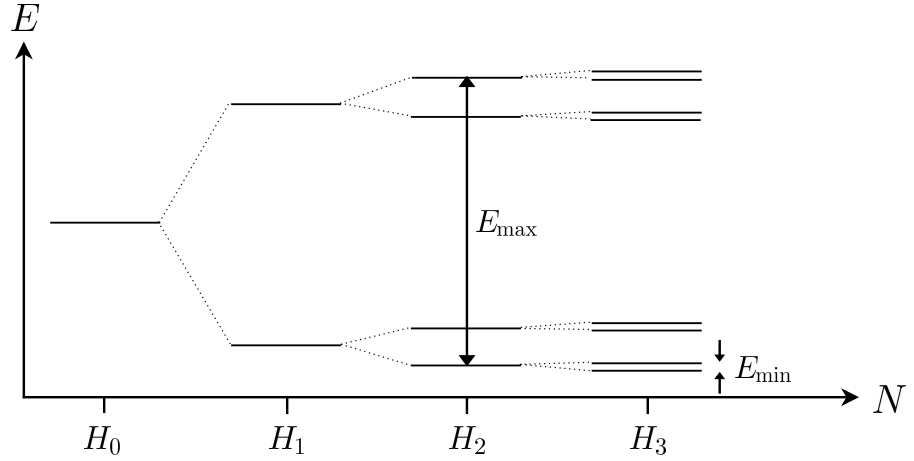


Figure 3.8: Illustration of how the exponential separation of energy scales going from one iteration to the next permits thermodynamics to be calculated at each iteration. For example, at iteration 2, an effective temperature can be defined such that $E_{\min} \ll T_2 \ll E_{\max}$, where thermodynamics of H_2 calculated at T_2 accurately approximate those of the full H .

calculated for H_N , where all states are retained and $N \rightarrow \infty$. Thus thermodynamics calculated at T_M using H_M accurately approximate the thermodynamics which would in principle be calculated for the full Hamiltonian H . This can be shown formally, and the error in the approximation quantified, as described below.

We begin by rewriting Eq. 3.15 in the form

$$\beta H = \lim_{M \rightarrow \infty} \bar{\beta}_M H_M, \quad (3.47)$$

where $\bar{\beta}_M$ follows as

$$\bar{\beta}_M = \frac{1}{2}(1 + \Lambda^{-1})\Lambda^{-(M-1)/2} \left(\frac{D}{k_B T} \right). \quad (3.48)$$

As H_M is in a linear chain form, the full Hamiltonian can be partitioned as follows:

$$\beta H = \bar{\beta}_N H_N + \lim_{M \rightarrow \infty} \bar{\beta}_M R_{M,(N+1)} + \bar{\beta}_N H_I, \quad (3.49)$$

where $N < M$, such that H_N describes a system with shorter chains of length N , while the rest of the chains are described by a remainder term $R_{M,(N+1)}$ given by

$$R_{M,(N+1)} = \Lambda^{(M-1)/2} \sum_{\alpha=L,R} \sum_{n=N+1}^{M-1} \Lambda^{-n/2} \xi_n \left(f_{\alpha n \sigma}^\dagger f_{\alpha(n+1)\sigma} + f_{\alpha(n+1)\sigma}^\dagger f_{\alpha n \sigma} \right), \quad (3.50)$$

which is coupled to the subsystem H_N by the term

$$H_I = \Lambda^{-1/2} \sum_{\alpha=L,R} \xi_N \left(f_{\alpha N \sigma}^\dagger f_{\alpha(N+1)\sigma} + f_{\alpha(N+1)\sigma}^\dagger f_{\alpha N \sigma} \right). \quad (3.51)$$

The approximation made now is to neglect H_I , which was shown in Ref. [13] to give rise to an error formally $\mathcal{O}(\bar{\beta}_N/\Lambda)$.

The key step now is to note that $R_{M,(N+1)} = R_{M,(N+1)}^0$, since the presence or absence of the dot makes no difference to the remainder term if it is disconnected from the rest of the system by setting $H_I = 0$. Thus, using Eq. 3.49 in Eq. 3.46 we obtain

$$\langle \hat{A} \rangle_{\text{imp}} = \frac{\text{Tr} \hat{A}_N \exp(-\bar{\beta}_N H_N)}{\text{Tr} \exp(-\bar{\beta}_N H_N)} - \frac{\text{Tr} \hat{A}_N^0 \exp(-\bar{\beta}_N H_N^0)}{\text{Tr} \exp(-\bar{\beta}_N H_N^0)}, \quad (3.52)$$

where $\hat{A}_N$ is the operator which acts on the reduced space of H_N . This result demonstrates that thermodynamics can be calculated at finite N , provided H_I can be neglected. This is a good approximation [13] only when $\bar{\beta}_N \ll \Lambda$, and so for a given temperature we can use Eq. 3.48 to determine which iteration numbers will yield accurate thermodynamics from Eq. 3.52. In fact, the usual approach is to use a small fixed $\bar{\beta}_N \equiv \bar{\beta} \ll \Lambda$, and instead define an effective temperature T_N for a given iteration N given by

$$\frac{k_B T_N}{D} = \frac{1}{2} (1 + \Lambda^{-1}) \Lambda^{-(N-1)/2} / \bar{\beta}. \quad (3.53)$$

A choice of $\bar{\beta} = 0.7$ gives good results, ensuring that states near the truncation limit are not thermally populated sufficiently to introduce significant errors.

Thus we can calculate thermodynamics accurately at *each* iteration, starting at $T \sim D$ for $N = 1$ and becoming exponentially smaller as N is increased. As arbitrarily many iterations may be performed⁷ and the system always converges to its stable FP after a finite number of iterations, $T = 0$ results can essentially be calculated in this way. The NRG therefore allows calculation of thermodynamics on all temperature scales of interest.

However, an important implication of this result is that the RG flow diagrams presented in the previous section can now be understood in terms of the temperature-dependence of physical properties. For $N \rightarrow \infty$, the system is described by a stable FP, which can now be thought of as the $T = 0$ ground state of the system. However, at intermediate iterations, RG flow may approach quite closely one of the unstable FPs (see for example, Figs. 3.5–3.7), which from Eqs. 3.52 and 3.53 imply that at certain *temperatures*, the system is well-described by these FPs.

As such, the temperature-dependence of thermodynamic quantities provides

⁷The complexity of the numerical calculation remains essentially fixed with N since we retain the same number of states N_s at each iteration.

clear signatures of the underlying FPs reached under renormalization on progressive reduction of the temperature. We will focus in this thesis on the dot contribution to the entropy, $S_{\text{imp}}(T)$ and the uniform magnetic spin susceptibility $\chi_{\text{imp}}(T)$. From the standard relation for the total entropy $S = \partial k_B T \ln(Z)/\partial T$, where $Z = \text{Tr} \exp(-\beta H)$ is the partition function, it follows [13] that

$$S_{\text{imp}}(T_N)/k_B = \bar{\beta} \langle H_N \rangle_{\text{imp}} + \ln(Z_N/Z_N^0) \quad (3.54)$$

where Z_N^0 is the partition function calculated without the dot, and $\langle H_N \rangle_{\text{imp}}$ is easily obtained from Eq. 3.52. Similarly, to calculate the magnetic susceptibility [13] we use $\chi = \partial M / \partial B|_0$, where $M = \langle S_{\text{tot}}^z \rangle$ is the magnetization and B is an infinitesimal test magnetic field, which yields

$$\chi_{\text{imp}}(T_N) = \frac{(g\mu_B)^2}{k_B T_N} \langle (S_{N,\text{tot}}^z)^2 \rangle_{\text{imp}}. \quad (3.55)$$

Hereafter, we will set $k_B = g\mu_B \equiv 1$ for convenience.

These quantities were originally calculated for the single-channel Kondo model by Wilson [12], and for the single impurity Anderson model by Krishnamurthy *et al* [13]. Later, thermodynamics of the two-channel Kondo model were studied with the NRG by Cragg *et al* [41] and Pang and Cox [42], confirming the Bethe *ansatz* predictions made earlier by Sacramento *et al* [45]. As the LM, SC and 2CK FPs will be important in Chapters 4–8, where we study chains and rings of dots connected to two leads, we survey briefly the behaviour of the entropy and susceptibility in the 1CK and 2CK models, and highlight the universality which arises in each case.

In Fig. 3.9 we show for comparison the dot contribution to the entropy $S_{\text{imp}}(T)$ [top panels] and the uniform spin susceptibility $T\chi_{\text{imp}}(T)$ [bottom panels] *vs* T/D for both the 1CK model [left panels] and the (symmetric) 2CK model [right panels]. In each case we have used Kondo coupling strengths $\rho J_K = 0.075$ (dotted lines), 0.05 (dashed lines) and 0.025 (solid lines), where $\rho = 1/(2D)$ is the density of states per orbital and $2D$ is the width of the conduction band, as usual. We have also used three different values of the NRG discretization parameter $\Lambda = 2, 3$ and 4, with the numerical results for each coinciding essentially perfectly⁸.

We consider first the 1CK systems [left panels], and note that the high-temperature (early iteration number) behaviour of all three systems is basically the same. All systems are described at high temperature by the LM FP, where the dot is essentially decoupled from the lead. The dot is modelled as a spin- $\frac{1}{2}$ object in the Kondo model, so at the LM FP [12, 13] the entropy is simply $S_{\text{imp}} = \ln(2)$, and the susceptibility follows the Curie law for a free spin, $T\chi_{\text{imp}} = \frac{1}{4}$, both of which are shown

⁸We have also averaged the thermodynamic data for even and odd iterations. While there are different fixed points associated with odd and even iteration numbers, the thermodynamics calculated for each are the same [13].

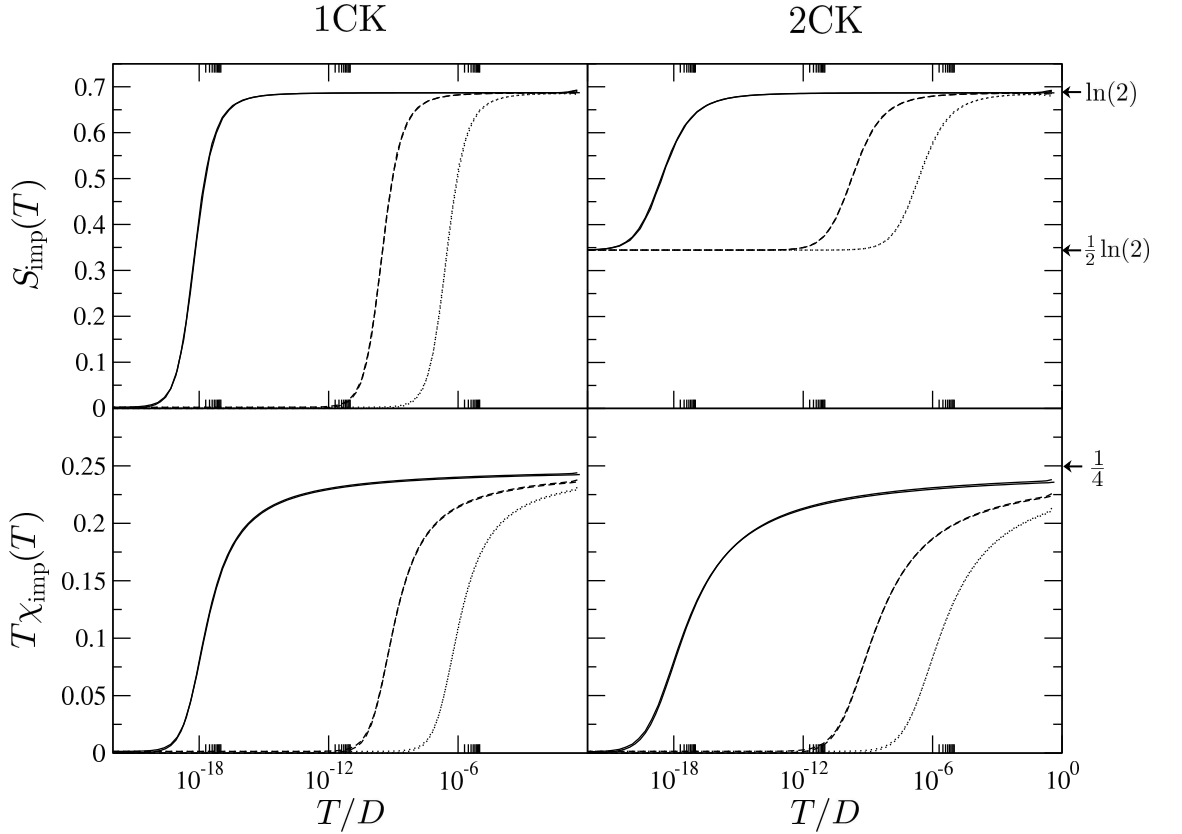


Figure 3.9: Thermodynamics for the 1CK model [left panels] and the (symmetric) 2CK model [right panels], shown for systems with $\rho J_K = 0.075$ (dotted lines), 0.05 (dashed lines) and 0.025 (solid lines). *Top panels*: dot contribution to the entropy $S_{\text{imp}}(T)$; *bottom panels*: dot contribution to the uniform spin susceptibility $T\chi_{\text{imp}}(T)$, both *vs* T/D . We have used three different values of the NRG discretization parameter $\Lambda = 2, 3$ and 4, with the results coinciding essentially perfectly in every case.

to be well-satisfied for $T \sim D$ in Fig. 3.9. By contrast, as $T \rightarrow 0$ (or equivalently $N \rightarrow \infty$), it is found that $S_{\text{imp}} = 0$ and $T\chi_{\text{imp}} = 0$, characteristic [12,13] of the SC FP, where the dot spin has been screened by antiferromagnetic coupling to the conduction band electrons. Thus, all systems show the flow from the LM FP to the SC FP (which are the only FPs of the model). Importantly, the temperature scale for the crossover between these FPs is seen to vary widely as the bare coupling ρJ_K is varied, and we will return to this shortly.

Turning now to the thermodynamics of the 2CK model [right panels of Fig. 3.9], we see exactly the same behaviour as the 1CK model at high temperatures. The dot spin is free, being now decoupled from *both* leads. The characteristic [43–45] $S_{\text{imp}} = \ln(2)$ entropy and Curie law $T\chi_{\text{imp}} = \frac{1}{4}$ susceptibility are seen for all systems. As the temperature is lowered, however, the leads ‘compete’ to screen the spin [49]. All systems ultimately flow to the stable 2CK FP at low temperatures, with

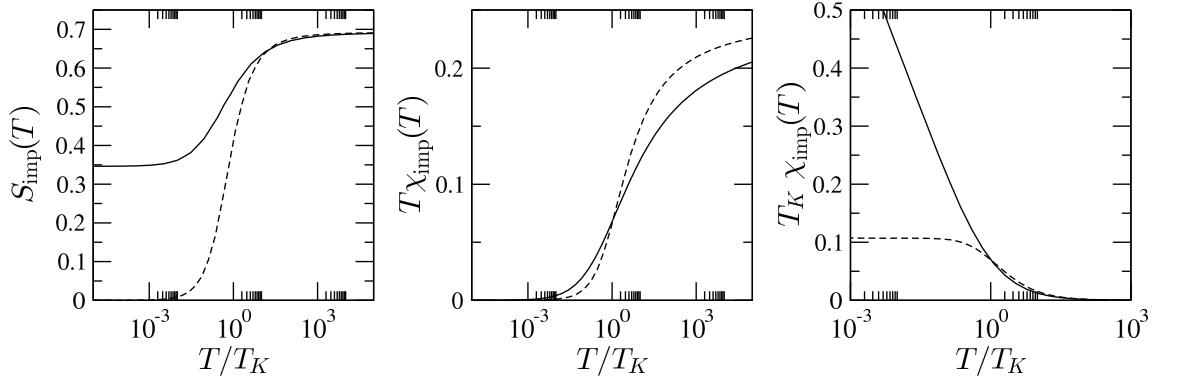


Figure 3.10: Universal scaling curves for the entropy, $S_{\text{imp}}(T)$ [left panel] and spin susceptibility $T\chi_{\text{imp}}(T)$ [middle panel], also shown as $T_K\chi_{\text{imp}}(T)$ [right panel], all *vs* T/T_K , where T_K is the Kondo scale for either the 1CK model (dashed lines) or the 2CK model (solid lines), in either case defined through $T_K\chi_{\text{imp}}(T_K) = 0.07$ [13].

the overscreened dot spin giving the characteristic [43–45] and unusual entropy of $S_{\text{imp}} = \frac{1}{2}\ln(2)$, which remains the residual entropy down to $T = 0$. On the same low-energy scale for each system, the magnetic susceptibility crosses over to its 2CK FP value [43–45] of $T\chi_{\text{imp}} = 0$.

While the temperature scale for the crossover to the stable FP is rather different for each case in Fig. 3.9, the form of the crossover manifest in either entropy or susceptibility appears to be similar for all of the 1CK systems, as indeed it does for the 2CK systems. In Sec. 2.3 we used Anderson’s poor man’s scaling technique [19, 40] to analyse these models, and a ‘scaling invariant’ — an exponentially low-energy scale, referred to as the Kondo temperature — for each model was determined. The existence of such a scale implies that all physical properties at low-temperature must be universal functions of it [19]. The Kondo temperature corresponds to the crossover to the stable FP (the SC FP for the 1CK model, or the 2CK FP for the 2CK model), and thus can be measured directly from the thermodynamics calculated from NRG. The definition is somewhat arbitrary, but is commonly given by [13]

$$T_K\chi_{\text{imp}}(T_K) = 0.07. \quad (3.56)$$

In both 1CK and 2CK models, $T_K\chi_{\text{imp}}$ crosses over from $\frac{1}{4}$ to 0 as the temperature is lowered, and as such is a measure of the flow to the ultimate stable FP of the model (see Fig. 3.9). Thus, we shall adopt the definition in Eq. 3.56 for both T_K^{1CK} and T_K^{2CK} . In fact, we can define the scale equivalently though any physical property. Specifically, using $S_{\text{imp}}(T_K^{1CK}) = 0.4$ for the 1CK model and $S_{\text{imp}}(T_K^{2CK}) = 0.55$ for the 2CK model gives the same numerical value for the Kondo scale as obtained through Eq. 3.56.

In Fig. 3.10, we plot all the data in Fig. 3.9 *vs* T/T_K , where the 1CK systems

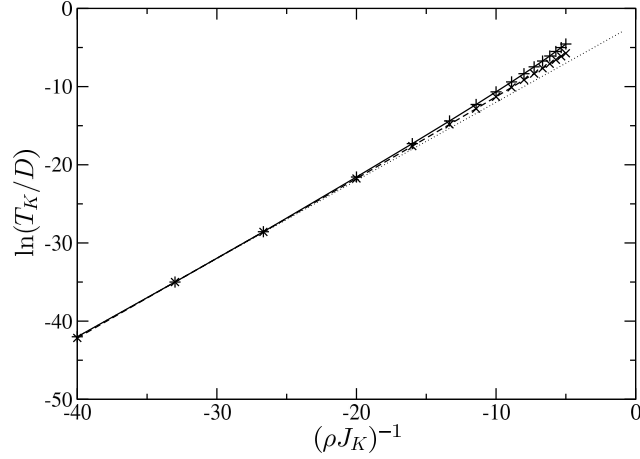


Figure 3.11: Evolution of the Kondo scale determined from the thermodynamics calculated with NRG for the 1CK model, T_K^{1CK} (dashed line) and the Kondo scale for the 2CK model, T_K^{2CK} (solid line) as a function of the bare Kondo coupling ρJ_K . Specifically, we plot $\ln(T_K/D)$ vs $(\rho J_K)^{-1}$, where T_K should be understood to mean either T_K^{1CK} or T_K^{2CK} depending on the model used. The poor man's scaling result to second order in either case is $\ln(T_K/D) = A(\rho J_K)^{-1}$, as indicated by the dotted line.

(dashed lines) are rescaled in terms of T_K^{1CK} while the 2CK systems (solid lines) are rescaled in terms of T_K^{2CK} (both being determined from Eq. 3.56). In the left panel we show the entropy $S_{\text{imp}}(T)$, while in the middle panel we show the susceptibility $T\chi_{\text{imp}}(T)$, which we plot again as $T_K\chi_{\text{imp}}(T)$ in the right panel.

Considering first in Fig. 3.10 the 1CK systems (dashed lines), we see that all data ‘collapse’ onto a single common curve in each panel when scaled in terms of T/T_K^{1CK} , the forms of which being characteristic [12, 13] of the flow from the LM FP to the SC FP. Indeed, when scaled in terms of T/T_K^{2CK} , all of the 2CK results collapse to common curves [43–45] for each thermodynamic quantity, although obviously the 1CK and 2CK forms are themselves very different.

As such, the curves in Fig. 3.10 represent the universal scaling forms for the 1CK and 2CK models for $S_{\text{imp}}(T)$ (left panel), $T\chi_{\text{imp}}(T)$ (middle panel) and $T_K\chi_{\text{imp}}(T)$ (right panel). The important result of this is that all one needs to know is the Kondo temperature, and then all the low-temperature properties of a system can be established from these universal curves.

We briefly comment that while $T\chi_{\text{imp}}(T)$ behaves somewhat similarly in both 1CK and 2CK models (with the spin in both cases being ‘quenched’ in the sense that $T\chi_{\text{imp}}(T) \rightarrow 0$ as $T \rightarrow 0$), the form of the universal curve is rather different. Indeed, for the 1CK model, $\chi_{\text{imp}}(T)$ itself remains constant [8, 12, 13], while it diverges logarithmically in the 2CK model [43–45] (see right panel of Fig. 3.10).

To complete this short survey of the 1CK and 2CK models, we finally examine the evolution of the Kondo scale itself. It is clear from Fig. 3.9 that T_K^{1CK} and

T_K^{2CK} vary exponentially with the bare dimensionless Kondo coupling ρJ_K . In Fig. 3.11, we plot $\ln(T_K^{1CK}/D)$ [dashed line] and $\ln(T_K^{2CK}/D)$ [solid line] both *vs* $(\rho J_K)^{-1}$. We find that (especially for small ρJ_K), the relationship is linear. This is of course in agreement of the calculation of the Kondo scale from poor man's scaling which (to second order) gives for both models $T_K/D \sim \exp(-1/\rho J_K)$, and is shown as the dotted line in Fig. 3.11 for comparison. Indeed, the agreement is rather more precise if we use the poor man's scaling results to third order, which we recap again here for convenience:

$$T_K^{1CK}/D \sim \sqrt{\rho J_K} \exp(-1/\rho J_K) \quad (3.57a)$$

$$T_K^{2CK}/D \sim \rho J_K \exp(-1/\rho J_K) \quad (3.57b)$$

While the above discussion has focused on the calculation of static properties, in fact the NRG technique has been more recently adapted to the calculation of range of dynamic quantities. In particular a formulation of the NRG in terms of the full density matrix [20,21] has permitted the accurate and systematic calculation of such quantities at arbitrary temperatures, and it is to this that we now turn.

3.6 Calculation of Dynamical properties

In this section, we describe briefly the recent developments and extensions of the NRG technique, which allow the accurate calculation of dynamical properties such as the single-particle spectrum.

As discussed in Chapters 1 and 2, single quantum dots are commonly described by the single-impurity Anderson model, Eq. 2.4, since at equilibrium the ‘source’ and ‘drain’ leads can be combined into a *single* lead (see Fig. 2.1). Meir and Wingreen [56] pointed out that the zero-bias conductance through such a dot is

$$\frac{G_c(T)}{G_0} = \int_{-\infty}^{\infty} -\frac{\partial f(\omega)}{\partial \omega} \pi \Gamma D(\omega; T) d\omega \quad (3.58)$$

where $f(\omega) = [e^{\omega/T} + 1]^{-1}$ is the Fermi function (with $\omega = 0$ the Fermi level) and $G_0 = 2e^2/h$ the (spin-summed) conductance quantum, and $D(\omega; T)$ is the single-particle spectrum of the dot. It is defined [8] as $D(\omega) = -\frac{1}{\pi} \text{Im}\{G(\omega)\}$, where the local dot Green function itself is given by $G(\omega) = \langle\langle d_\sigma; d_\sigma^\dagger \rangle\rangle_\omega$ and in general we will define $\langle\langle \hat{A}; \hat{B} \rangle\rangle_\omega$ as the Fourier transform of the retarded correlator $\langle\langle \hat{A}(t_1); \hat{B}(t_2) \rangle\rangle = -i\theta(t_1 - t_2)\langle\{\hat{A}(t_1), \hat{B}(t_2)\}\rangle$.

The (ω, T) -dependence of $D(\omega; T)$ thus controls the conductance, and for $T = 0$ in particular $G_c(T = 0)/G_0 = \pi \Gamma D(\omega = 0; T = 0)$. As the conductance through a quantum dot is commonly measured in experimental setups (see Chapter 1), this provides motivation for the study of the single-particle spectrum.

However, dynamical properties of the Anderson and related models also provide key insights into the underlying physics of the Kondo effect. Lehmann resolving the spectrum [8], one obtains

$$D(\omega) = \sum_{a,b} \langle b | d_\sigma | a \rangle \frac{\exp(-\beta E_a)}{Z} \langle a | d_\sigma^\dagger | b \rangle \delta(\omega + E_a - E_b) \quad (3.59)$$

where $Z = \sum_i \exp(-\beta E_i)$ is the partition function, and E_i is the energy of state $|i\rangle$. The spectrum thus contains information about dynamical processes involving electron ‘hops’ between the dot and the attached metallic lead. At $T = 0$, the spectrum describes excitations made from the many-body ground state alone, while for non-zero temperatures, excitations to and from all states must be considered. Matrix elements of the type in Eq. 3.59 can be calculated directly using the NRG states generated at a given iteration, and so it seems plausible that the spectrum could be built up from the Lehmann sum [26]. However, due to the logarithmic discretization employed in the NRG, the characteristic energy scale at a given iteration n is $\Lambda^{-n/2}$ (see Eq. 3.13), where $1 \geq n \geq N$ and $N \rightarrow \infty$ is the total number of iterations performed. Thus, there must be a contribution to $D(\omega)$ from iteration n , where $\omega \sim \Lambda^{-n/2}$.

But this strategy is problematical for two reasons. Firstly, there are double-counting ambiguities [135] associated with combining spectral information from different iterations. Fundamentally, the problem is that the states from all NRG iterations do not form a *complete* set, so one cannot expect to build up reliable spectral information from the Lehmann sum, Eq. 3.59 [20, 136]. Secondly, high-energy features of the spectrum are constructed from matrix elements involving states of early iterations. Since the correct ground state of the system is only determined after many iterations N , the calculation of such features may be very inaccurate [137] since the ultimate stable fixed point of the problem has not been determined. This is perhaps most pronounced in the calculation of the spectrum for a system in a magnetic field. The magnetization (as calculated as the sum of spectral weight) is particularly poorly determined, since most of the spectral weight arises at high energies where the wrong ground state is used [137]. Only at later iterations is the effect of the symmetry breaking correctly captured by the NRG. Thus, the accurate calculation of the spectrum naturally necessitates starting from the true ground state, as determined from the *last* NRG iteration, and using a complete set of NRG states.

Anders and Schiller (AS) showed recently in Ref. [136] that a complete set of states can in fact be defined within the NRG. The key idea is to reconceptualize the Wilson chain as being of constant fixed length N (where N is the total number of iterations performed in the calculation to obtain a converged solution for the true ground state of the system). Each iteration then corresponds simply to ‘switching

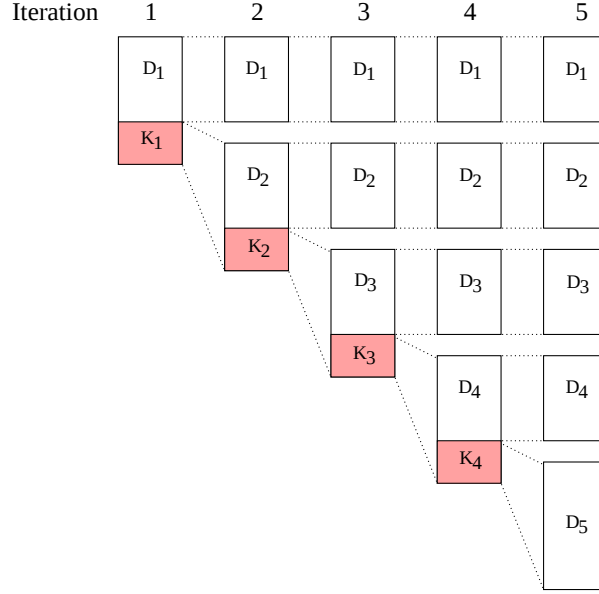


Figure 3.12: Construction of the Anders-Schiller (AS) basis. The states of each NRG iteration are labelled as being either ‘kept’ (K) or ‘discarded’ (D). The AS basis forms a complete set of states, built up from the discarded states of each iteration (and one regards all states of the final iteration as discarded).

on’ the coupling to the next site in this chain. The full chain thus comprises a direct product of a ‘system’ block and an ‘environment’ block. The environment is itself simply a matrix product state of the individual uncoupled chain sites; and the system block is the usual diagonalized NRG states for that iteration. For a Wilson chain of total length N , we will denote the basis states $|r; \mathbf{e}\rangle_n^N$, with n a given iteration $n \leq N$. Thus ‘ $\mathbf{e}$ ’ labels the environment degrees of freedom in the free $(N - n)$ -length chain and r indexes the diagonalized NRG states at iteration n . It follows that

$$H_n |r; \mathbf{e}\rangle_n^N = E_n^r |r; \mathbf{e}\rangle_n^N \quad (3.60)$$

and as such the AS basis states $|r; \mathbf{e}\rangle_n^N$ are exact eigenstates of the approximate NRG Hamiltonian H_n . One assumes further that

$$H |r; \mathbf{e}\rangle_n^N \approx E_n^r |r; \mathbf{e}\rangle_n^N \quad (3.61)$$

thereby regarding the coupling between the system and the remaining environment states as a small perturbation.

Anders and Schiller realised [136] that a *complete* set of states can now be constructed from the basis states $|r; \mathbf{e}\rangle_n^N$. Those states of NRG iteration n which are ‘kept’ and used to construct the states of the next iteration $(n + 1)$ cannot be orthogonal to any of these states (and thus cannot comprise a complete set of states).

However, the ‘discarded’ states of iteration n are of course orthogonal to the kept states of the *same* iteration — and therefore must be orthogonal to the states of all iterations $m > n$. It is then straightforward to show that a complete set of states can be built up from the discarded states of all NRG iterations (and one regards all of the states of the final iteration N as being discarded). The construction of the ‘AS basis’ in this fashion is illustrated in Fig. 3.12.

Dynamics can then be calculated by using the AS basis — which comprise a complete but approximate set of states — in the Lehmann sum, Eq. 3.59. The complication is that matrix elements of local dot operators such as $\langle b|d_\sigma^\dagger|a\rangle$ used in Eq. 3.59 are calculated iteratively within NRG and so are known in the standard NRG basis, rather than the AS basis. This means that only elements ${}_n^N \langle r; \mathbf{e}|d_\sigma^\dagger|r'; \mathbf{e}\rangle_n^N$ involving AS states of the *same iteration* are known, whereas contributions to the spectrum also arise from elements ${}_n^N \langle r; \mathbf{e}|d_\sigma^\dagger|r'; \mathbf{e}'\rangle_m^N$ which connect states of *different* NRG iterations.

The solution proposed in Ref. [20, 21] is to recast the problem in terms of the full density matrix (FDM) defined in the AS basis by

$$\hat{\rho}^{\text{tot}} = \sum_n^N w_n \hat{\rho}_n^{\text{AS}}, \quad (3.62a)$$

$$w_n = d^{N-n} \frac{Z^n}{Z^{\text{tot}}}, \quad (3.62b)$$

which follow naturally since the density matrix is of course diagonal in the AS basis: $[\hat{\rho}_n^{\text{AS}}]_{rr'} = \exp(-\beta E_n^r)/Z^{\text{tot}} \times \delta_{rr'}$, with the total partition function $Z^{\text{tot}} = \sum_n Z^n$ and $Z^n = \sum_r \exp(-\beta E_n^r)$. Thus, w_n corresponds to a weighting function, arising from the d -fold degeneracy of each of the $(N - n)$ environment orbitals.

To utilise the local dot matrix elements calculated in the NRG basis however, we wish to obtain the full density matrix in the same basis. Thus one defines [20, 21]

$$\hat{\rho}^{\text{tot}} = \sum_n^N \hat{\rho}_n^{\text{red}} \quad (3.63)$$

with $\hat{\rho}_n^{\text{red}}$ the ‘reduced density matrix’, which contains contributions from both ‘kept’ and ‘discarded’ states of iteration n . We will not provide a full derivation of the structure of the reduced density matrix here, but rather direct the reader to the original work of Ref. [21]. However, we will sketch briefly the approach used to calculate $\hat{\rho}_n^{\text{red}}$ iteratively.

We note first that the part of $\hat{\rho}_n^{\text{red}}$ connecting discarded states of NRG iteration n is simply $w_n \hat{\rho}_n^{\text{AS}}$, as above. Thus, $\hat{\rho}_N^{\text{red}} = \hat{\rho}_N^{\text{AS}}$ for the last iteration. But what about the part of $\hat{\rho}_n^{\text{red}}$ which connects kept states? Since the kept states of iteration n are used to construct the new states of iteration $(n + 1)$, performing a unitary

transformation⁹ on the entire matrix $\hat{\rho}_{n+1}^{\text{red}}$ yields the part of $\hat{\rho}_n^{\text{red}}$ which connects only the kept states in the basis of NRG states for iteration n . This is equivalent to tracing out the environment degrees of freedom for orbital $(n+1)$. As we know $\hat{\rho}_N^{\text{red}}$, all other $\hat{\rho}_n^{\text{red}}$ for $n < N$ can now be calculated (starting from the last iteration), and thus building up the full $\hat{\rho}^{\text{tot}}$ iteratively.

It was shown in Ref. [21] that using these reduced density matrices, the spectrum can be calculated via

$$D(\omega) = \sum_n \sum_{r,r'} \left[[d_\sigma]_n^n \times [\hat{\rho}_n^{\text{red}}] \right]_{rr'} \times [d_\sigma^\dagger]_{r'r}^n \times \delta(\omega - E_n^r + E_n^{r'}), \quad (3.64)$$

where $[d_\sigma^\dagger]_{r'r}^n = {}_n\langle r' | d_\sigma^\dagger | r \rangle_n$ are local dot matrix elements which connect NRG states $|r\rangle_n$ and $|r'\rangle_n$ (both kept and discarded) of the same iteration n .

In fact, determination of the full density matrix allows access to various spectral functions (not just the single-particle spectrum, as illustrated here) at any temperature. However, the data generated by the above scheme inevitably comprise discrete δ -functions (from Eq. 3.59 or Eq. 3.64), since the conduction band has been discretized in the NRG process. To obtain a smooth spectrum, one needs to broaden these poles. This is typically done by replacing each pole by a log-gaussian of the same weight (exact details on the approach used to obtain the spectra presented in this thesis can be found in Ref. [138]).

In the next section, we apply the above FDM technique to the calculation of some dynamical properties of the Anderson model, and describe how the self-energy can also be determined from NRG.

3.6.1 Dynamics of the Anderson model

In the previous section, we described how the full density matrix [20, 21, 27] can be calculated within the NRG, and how this allows access to frequency- and temperature-dependent dynamics. We now consider two concrete examples for the single-channel Anderson model (Eq. 2.4): the local single-particle spectrum, $D(\omega)$, and the local dynamic susceptibility $\chi(\omega)$.

We examine first the spectral density $D(\omega) = -\frac{1}{\pi} \text{Im}\{G(\omega)\}$, obtained by employing the AS basis in the Lehmann sum Eq. 3.59 via Eq. 3.64, as described above. We can obtain $D(\omega)$ directly from the NRG, but it has been shown [126] that rather more accurate results can be obtained if it is calculated through the Dyson equation,

$$[G(\omega)]^{-1} = [G^0(\omega)]^{-1} - \Sigma(\omega), \quad (3.65)$$

⁹Such unitary transformations are performed using matrices generated in the forward NRG run, and which must be retained at each iteration. This makes the calculation of spectra using the FDM rather more computationally demanding than simply calculating thermodynamic properties.

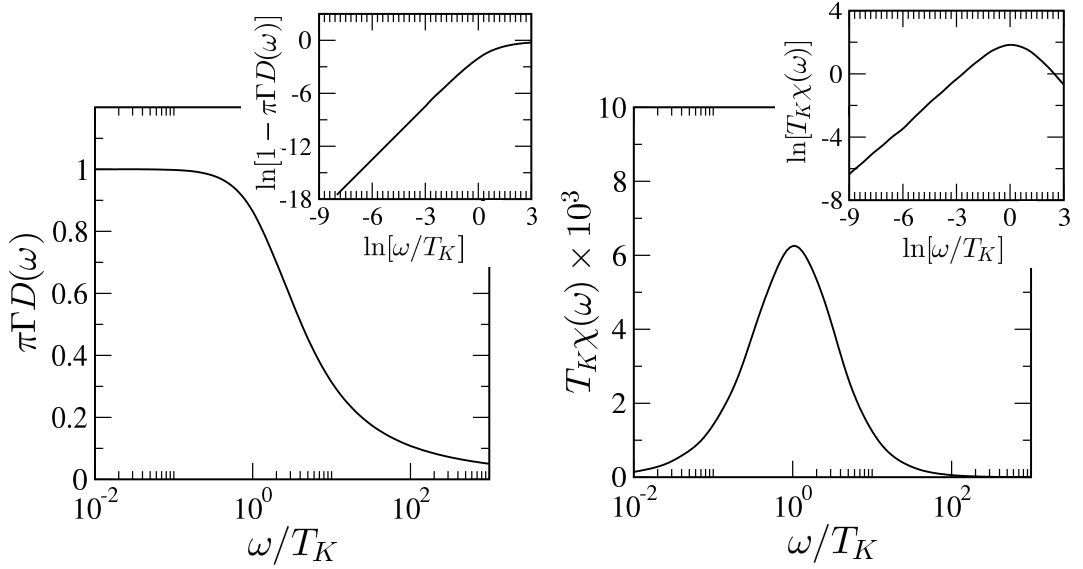


Figure 3.13: Dynamics of the Anderson model. In the left panel we show the local single-particle scaling spectrum $\pi\Gamma D(\omega)$, while in the right panel we show the local dynamic susceptibility $T_K\chi(\omega) \times 10^3$, both *vs.* ω/T_K . The Kondo scale T_K is determined in practice from the thermodynamics as usual. The insets show the low- ω asymptotic forms: we plot $\ln[1 - \pi\Gamma D(\omega)]$ (left) and $\ln[T_K\chi(\omega)]$ (right) both *vs.* $\ln[\omega/T_K]$, which for $\omega/T_K \ll 1$ demonstrates the characteristic Fermi-liquid behaviour described by Eqs. 3.67 and 3.68.

where $G^0(\omega)$ is the non-interacting propagator (obtained for $U = 0$), and $\Sigma(\omega)$ is the proper electron self-energy, with $\Sigma(\omega) \equiv \Sigma^R(\omega) - i\Sigma^I(\omega)$ (such that $\Sigma^I(\omega) \geq 0$). The non-interacting $G^0(\omega)$ is given [8] trivially by $[G^0(\omega)]^{-1} = \omega^+ - \epsilon - \Gamma(\omega)$ (with $\omega^+ = \omega + i0^+$), where $\Gamma(\omega) = \sum_{\mathbf{k}} V^2[\omega^+ - \epsilon_{\mathbf{k}}]^{-1}$ is the usual one-electron hybridization function for coupling of the dot to the lead: $\Gamma(\omega) \equiv \Gamma^R(\omega) - i\Gamma^I(\omega)$, with $\Gamma^I(\omega) = \Gamma (= \pi V^2 \rho_T)$ for all $|\omega| < D$ inside the band, and $\Gamma^R(\omega = 0) = 0$.

The electron self-energy $\Sigma(\omega)$ is itself readily obtained (from the interacting part of H_D in the Anderson model Eq. 2.4) using equation of motion methods [8, 139], and is given by

$$\Sigma(\omega) = U[G(\omega)]^{-1} \langle \langle d_{\uparrow} \hat{n}_{d\downarrow}; d_{\uparrow}^{\dagger} \rangle \rangle_{\omega} \quad (3.66)$$

and $\Sigma(\omega)$ is independent of spin σ in the absence of a magnetic field.

$D(\omega)$ then follows from the Green function calculated by combining Eqs. 3.65 and 3.66, and is highly accurate, eliminating many of the systematic errors known to occur from the NRG due to the discretization [126]. The high-frequency behaviour has been shown to be more accurately described using this self-energy formulation, and low-frequency oscillations in the spectrum are effectively ‘cancelled’ by the quotient of correlators in Eq. 3.66.

We mention briefly that other dynamical quantities can be straightforwardly calculated in the NRG. In particular the local (dot) dynamic susceptibility may

be similarly determined. It is defined as $\chi(\omega) = -\frac{1}{\pi} \text{Im}\{\langle\langle \hat{S}^z; \hat{S}^z \rangle\rangle_\omega\}$, where $\hat{S}^z = \frac{1}{2}(\hat{n}_{d\uparrow} - \hat{n}_{d\downarrow})$ is a spin- $\frac{1}{2}$ operator for the dot.

In Fig. 3.13 we show dynamics for the Anderson model calculated from the NRG using the machinery described above. In the left panel we show the scaling spectrum $\pi\Gamma D(\omega)$ while in the right panel we show the scaling curve $T_K\chi(\omega)$, both *vs.* ω/T_K . The Kondo scale T_K is itself determined as usual [13] from the thermodynamics (via $T_K\chi_{\text{imp}}(T_K) = 0.07$). In the Anderson model, the single-particle spectrum is known [8] to be described at low frequencies by

$$\pi\Gamma D(\omega) \stackrel{\frac{T}{T_K} \ll 1}{\sim} 1 - a(\omega/T_K)^2, \quad (3.67)$$

so that the resonance has a characteristic width $\mathcal{O}(T_K)$. At low frequencies, the dynamic susceptibility is described [8, 140] by

$$T_K\chi(\omega) \stackrel{\frac{T}{T_K} \ll 1}{\sim} \omega, \quad (3.68)$$

with a peak centred on $\omega \sim T_K$.

In the inset to the left panel of Fig. 3.13, we plot $\ln[1 - \pi\Gamma D(\omega)]$ *vs.* $\ln[\omega/T_K]$. At low- ω , the resulting straight line has a slope of 2, as expected from Eq. 3.67. The inset to the right panel shows $\ln[T_K\chi(\omega)]$ *vs.* $\ln[\omega/T_K]$, and is found to have a slope of 1 at low- ω , likewise confirming Eq. 3.68. These exact results for the Anderson model (obtained from Fermi liquid theory [8]) are thus extremely well satisfied at low- ω , demonstrating the power and accuracy of the FDM-NRG technique.

In the next section we consider how such dynamical quantities can be determined for the 1CK model.

3.6.2 Spectra of the 1CK model

In the previous section we described how the single-particle spectrum $D(\omega)$ and the local dynamic susceptibility $\chi(\omega)$ can be calculated for the Anderson model via NRG. We now consider the single-channel Kondo model, which we will write in the form $H^{1CK} = H'_L + H_K^{1CK}$, where

$$\begin{aligned} H'_L &= \sum_{\mathbf{k}} \epsilon_{\mathbf{k}} \hat{n}_{\mathbf{k}} \\ H_K^{1CK} &= \frac{J_K}{2N} \sum_{\mathbf{k}, \mathbf{k}'} \left[\hat{S}^z (a_{\mathbf{k}\uparrow}^\dagger a_{\mathbf{k}'\uparrow} - a_{\mathbf{k}\downarrow}^\dagger a_{\mathbf{k}'\downarrow}) + \hat{S}^+ a_{\mathbf{k}\downarrow}^\dagger a_{\mathbf{k}'\uparrow} + \hat{S}^- a_{\mathbf{k}\uparrow}^\dagger a_{\mathbf{k}'\downarrow} \right]. \end{aligned} \quad (3.69)$$

Clearly, the dynamic susceptibility $\chi(\omega) = -\frac{1}{\pi} \text{Im}\{\langle\langle \hat{S}^z; \hat{S}^z \rangle\rangle_\omega\}$ may be calculated for the 1CK model in exactly the same way as for the Anderson model. However, a natural question arises: to what dynamical property of the pure 1CK model should

the spectral density of the Anderson model, $\pi\Gamma D(\omega)$, be compared? No single-particle propagator can be defined *per se* for the Kondo model, since the dot is a strict *spin*. However, both models are described on the lowest energy scales by the SC FP [13], and so some quantitative comparison should be possible.

Koller, Hewson and Meyer [127] showed that this quandary can be answered by considering the scattering t-matrix of both systems. The t-matrix, $t(\omega)$, is defined in the usual way [8] in terms of scattering of electron states in the attached lead, via

$$G_{\mathbf{k},\mathbf{k}'}(\omega) = \frac{\delta_{\mathbf{k}\mathbf{k}'}}{\omega^+ - \epsilon_{\mathbf{k}}} + \frac{1}{\omega^+ - \epsilon_{\mathbf{k}}} t(\omega) \frac{1}{\omega^+ - \epsilon_{\mathbf{k}'}} \quad (3.70)$$

where $G_{\mathbf{k},\mathbf{k}'}(\omega) = \langle\langle a_{\mathbf{k}\sigma}; a_{\mathbf{k}'\sigma}^\dagger \rangle\rangle_\omega$ is the propagator for the lead states. Using equations of motion [8, 139] methods to obtain an expression for this propagator, it is straightforward to show that for the Anderson model (Eq. 2.4) the t-matrix follows as

$$\begin{aligned} t^{\text{And}}(\omega) &= \langle\langle [a_{\mathbf{k}\sigma}, H_{\text{hyb}}]; [H_{\text{hyb}}, a_{\mathbf{k}'\sigma}^\dagger] \rangle\rangle_\omega \\ &= V^2 G(\omega), \end{aligned} \quad (3.71)$$

where $G(\omega) = \langle\langle d_\sigma; d_\sigma^\dagger \rangle\rangle_\omega$ is the standard dot Green function. The particularly simple form of Eq. 3.71 is obtained since the dot part of the Anderson Hamiltonian, H_D contains only *pairs* of fermionic dot operators, and hence $[a_{\mathbf{k}\sigma}, H_D] = 0$. Similarly, for the Kondo model (Eq. 3.69) one obtains

$$\begin{aligned} t^{1\text{CK}}(\omega) &= \langle\langle [a_{\mathbf{k}\sigma}, H_K^{1\text{CK}}]; [H_K^{1\text{CK}}, a_{\mathbf{k}'\sigma}^\dagger] \rangle\rangle_\omega \\ &= \frac{J_K^2}{4N} G^{1\text{CK}}(\omega), \end{aligned} \quad (3.72)$$

where

$$G^{1\text{CK}}(\omega) = \langle\langle \hat{S}^- f_{0\downarrow} + \hat{S}^z f_{0\uparrow}; \hat{S}^+ f_{0\downarrow}^\dagger + \hat{S}^z f_{0\uparrow}^\dagger \rangle\rangle_\omega, \quad (3.73)$$

and $f_{0\sigma}^\dagger$ is an operator for the ‘0’-orbital of the Wilson chain, as defined in Eq. 2.9

The single-particle spectrum for the Anderson model can be written in terms of the t-matrix: $\pi\Gamma D(\omega) = -\pi\rho_T \text{Im}\{t^{\text{And}}(\omega)\}$ (recall that $\Gamma = \pi V^2 \rho_T$ is the hybridization). Comparison of $-\pi\rho_T \text{Im}\{t^{\text{And}}\}$ for the Anderson model to its pure 1CK counterpart (and using $\rho_T/N = \rho = 1/(2D)$) gives the desired correspondence

$$\pi\Gamma D(\omega) \leftrightarrow D \rho^{1\text{CK}}(\omega) \quad (3.74)$$

with spectral density

$$\rho^{1\text{CK}}(\omega) = -\frac{\pi}{2} (\rho J_K)^2 \text{Im}\{G^{1\text{CK}}(\omega)\} \quad (3.75)$$

for the single-spin 1CK model [127].

$G^{1CK}(\omega)$, as given in Eq. 3.73, can be calculated directly with NRG, and hence the spectrum $D\rho^{1CK}(\omega)$ is readily obtained. We have also developed, however, a scheme for a more accurate determination of this quantity in the spirit of Ref. [126]. We outline this briefly below as a technical aside.

For the 1CK model, dividing Eq. 3.70 by N and summing over $\mathbf{k}$ and $\mathbf{k}'$ immediately yields an expression for the Green function of the ‘0’-orbital of the Wilson chain, $G_0(\omega) = \langle\langle f_{0\sigma}; f_{0\sigma}^\dagger \rangle\rangle_\omega$, viz:

$$G_0(\omega) = G_0^0(\omega) + G_0^0(\omega) N t^{1CK}(\omega) G_0^0(\omega), \quad (3.76)$$

where $G_0^0(\omega) = \frac{1}{N} \sum_{\mathbf{k}} (\omega^+ - \epsilon_{\mathbf{k}})^{-1}$ is the non-interacting propagator. There is in fact no non-interacting limit of $G^{1CK}(\omega)$ itself, as the dot spin is inherently correlated, and so there is no dot self-energy *per se*. However, a self-energy of the ‘0’-orbital can readily be defined by rearranging Eq. 3.76 into the form of the Dyson equation, $[G_0(\omega)]^{-1} = [G_0^0(\omega)]^{-1} - \Sigma_0(\omega)$. In the wide flat band limit, $G_0^0(\omega) = -i\pi\rho$, and using this with Eqs. 3.72 and 3.76 we now obtain

$$\Sigma_0(\omega) = -\frac{1}{4}i\pi\rho J_K^2 \left(\frac{G^{1CK}(\omega)}{G_0(\omega)} \right). \quad (3.77)$$

Both $G^{1CK}(\omega)$ and $G_0(\omega)$ can be calculated with NRG, and hence highly accurate determination of the self-energy $\Sigma_0(\omega)$ follows from Eq. 3.77. $G_0(\omega)$ can then be obtained using the Dyson equation, and so access to $G^{1CK}(\omega)$ and hence $D\rho^{1CK}(\omega)$ straightforwardly follows through Eqs. 3.76 and 3.72.

We put this technique into use, plotting in Fig. 3.14 the $T = 0$ local spectrum of the 1CK model $D\rho^{1CK}(\omega)$ *vs.* ω/D for a system with $\rho J_K = 0.08$ (solid line). We also plot for comparison the single-particle spectrum $\pi\Gamma D(\omega)$ of an Anderson model (dashed line) with $U/(\pi\Gamma) \simeq 10$, $\epsilon = -\frac{1}{2}U$ and $\Gamma/D = 10^{-2}$ (the parameters of the latter chosen so that both systems have the same Kondo scale, T_K^{1CK}).

In panel (A) of Fig. 3.14 we show the spectra on a logarithmic frequency scale, exhibiting thereby both the high- and low- ω behaviour. For the Anderson model (dashed line), the high-energy spectral features (the so-called ‘Hubbard satellites’) reflect simple one-electron addition to the isolated dot ground state (*cf.* Eq. 3.59). Such an excitation incurs an energy cost $U - |\epsilon|$. On tunnel-coupling to the leads, this pole is naturally broadened, as seen in panels (A) and (B). For $\omega < 0$, the Hubbard satellite corresponds to one-electron removal from the singly-occupied isolated dot ground state, which incurs an energy cost $|\epsilon|$. As the system shown in Fig. 3.14 is particle hole symmetric ($\epsilon = -\frac{1}{2}U$), it follows that $\pi\Gamma D(\omega) = \pi\Gamma D(-\omega)$, as seen explicitly for example in panel (B).

The Hubbard satellites are of course absent in $D\rho^{1CK}(\omega)$ by construction, as

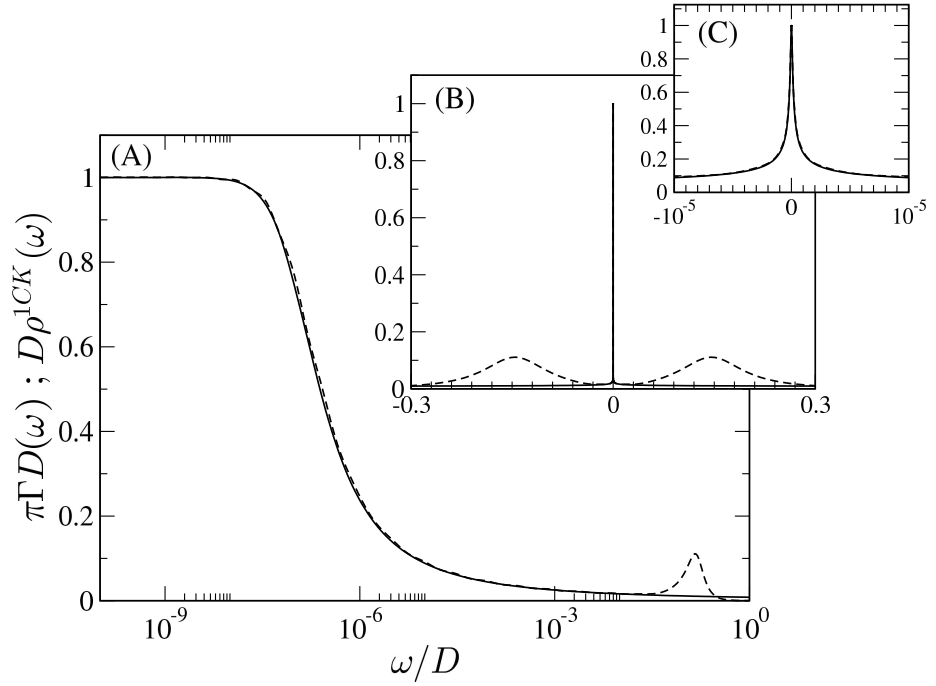


Figure 3.14: $T = 0$ local spectrum $D \rho^{1CK}(\omega)$ for the Kondo model (solid line) *vs.* ω/D for a system with $\rho J_K = 0.08$. Also plotted is the $T = 0$ spectrum of an Anderson model (dashed line) with $U/(\pi\Gamma) \simeq 10$, $\epsilon = -\frac{1}{2}U$ and $\Gamma/D = 10^{-2}$. Panel (A) shows the data on a logarithmic frequency scale while panels (B) and (C) show the spectra on a linear frequency scale.

the dot is modelled as a strict spin.

The most important feature of the spectra in Fig. 3.14 is the low-energy Kondo resonance, the form of which reflects RG flow in the vicinity of the stable SC FP for both Anderson and Kondo models. In particular, at the Fermi level $\omega = 0$, $\pi\Gamma D(0) = D \rho^{1CK}(0) = 1 - ie$, the unitarity limit characteristic [8] of the SC FP, which is itself guaranteed for the Anderson model in the singly-occupied Kondo limit by the Friedel sum rule [8]. Indeed, for $|\omega| < 10^{-3}$, the behaviour of $\pi\Gamma D(\omega)$ and $D \rho^{1CK}(\omega)$ is essentially indistinguishable, demonstrating the common universal scaling form for both models (see left panel of Fig. 3.13). This is also shown clearly in the zoomed view on a linear scale for $-10^{-5} < \omega < +10^{-5}$ (panel (C)). The agreement indicates that the low- ω asymptotic behaviour of $\pi\Gamma D(\omega)$ described by Eq. 3.67 for the Anderson model also applies as expected to $D \rho^{1CK}(\omega)$ for the Kondo model.

In the next section, we extend this work to the two-channel Kondo model, and calculate the equivalent spectrum with NRG.

3.6.3 Spectra of the 2CK model

In the previous sections, we used the full density matrix formulation [20, 21, 27] of the NRG to calculate the single-particle spectrum $\pi\Gamma D(\omega)$ of the Anderson model, and derived an equivalent dynamical quantity [127] $D\rho^{1CK}(\omega)$ for the 1CK model. We confirmed by explicit calculation that the spectra exhibit common, universal behaviour at low-frequencies. Here we consider the single-spin 2CK model of relevance to the work of Chapters 4–8.

We will identify the desired spectrum through the t-matrix of the 2CK model (as for the 1CK model considered in Sec. 3.6.2 and Ref. [127]). However, *two* such t-matrices can be defined: $t_\alpha(\omega)$ describes the scattering of electron states in lead $\alpha = L$ or R . Thus two distinct spectra must in general arise. This is of course physically natural: for example, when $J_{KL} > J_{KR}$ (see Eq. 2.20 for the channel-anisotropic 2CK Hamiltonian), on the lowest energy scales the dot spin forms a Kondo singlet by strong-coupling to the left lead, while the right lead decouples. The spectra for spin scattering in the left and right leads must therefore be very different. Specifically, the spectrum for the left lead is expected to be characteristic of the 1CK spectrum (Fig. 3.14), while the spectrum for the right lead should be that of a decoupled lead.

However, we stress that for mirror-symmetric systems (where the stable FP is the 2CK FP), obviously $t_L(\omega) = t_R(\omega) \equiv t^{2CK}(\omega)$, and hence there is a single spectrum characteristic of the 2CK FP.

Equation of motion methods [8, 139] yield the t-matrix for the $\alpha = L, R$ lead of the 2CK model Eq. 2.20, which follow as

$$\begin{aligned} t_\alpha(\omega) &= \langle\langle [a_{\alpha\mathbf{k}\sigma}, H_{2CK}]; [H_{2CK}, a_{\alpha\mathbf{k}'\sigma}^\dagger] \rangle\rangle_\omega \\ &= \frac{J_{K\alpha}^2}{4N} G_\alpha^{2CK}(\omega), \end{aligned} \quad (3.78)$$

where

$$G_\alpha^{2CK}(\omega) = \langle\langle \hat{S}^- f_{\alpha 0\downarrow} + \hat{S}^z f_{\alpha 0\uparrow}; \hat{S}^+ f_{\alpha 0\downarrow}^\dagger + \hat{S}^z f_{\alpha 0\uparrow}^\dagger \rangle\rangle_\omega. \quad (3.79)$$

and $f_{\alpha 0\sigma}^\dagger$ is an operator for the ‘0’-orbital of the $\alpha = L, R$ Wilson chain, as defined in Eq. 3.2.

Following the approach outlined in Sec. 3.6.2, we now define $D\rho_\alpha^{2CK}(\omega) = -\pi\rho_T \text{Im}\{t_\alpha(\omega)\}$ with spectral density

$$\rho_\alpha^{2CK}(\omega) = -\frac{\pi}{2}(\rho J_{K\alpha})^2 \text{Im}\{G_\alpha^{2CK}(\omega)\} \quad (3.80)$$

for the single-spin 2CK model.

In Fig. 3.15 we plot $D\rho_L^{2CK}(\omega) = D\rho_R^{2CK}(\omega) \equiv D\rho^{2CK}(\omega)$ vs. ω/D for a mirror symmetric 2CK system with $\rho J_{KL} = \rho J_{KR} \equiv \rho J_K = 0.08$. Notably, at the Fermi-

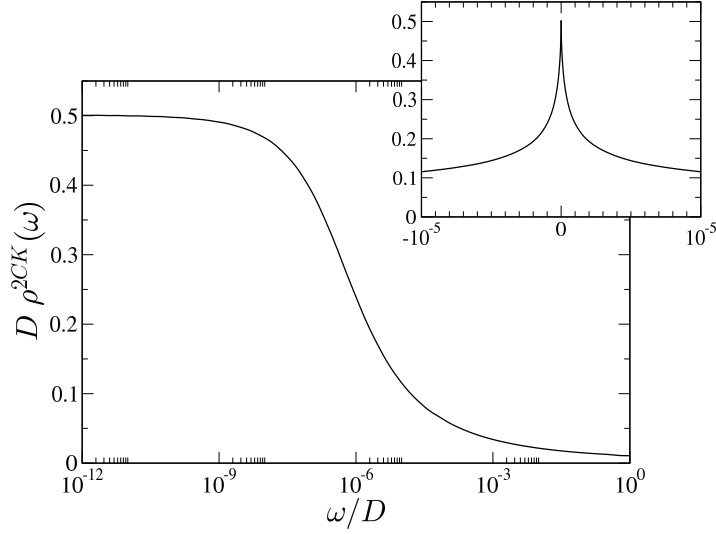


Figure 3.15: $T = 0$ local spectrum $D\rho_L^{2CK}(\omega) = D\rho_R^{2CK}(\omega) \equiv D\rho^{2CK}(\omega)$ vs. ω/D for a mirror-symmetric 2CK model with $\rho J_{KL} = \rho J_{KR} \equiv \rho J_K = 0.08$. The inset shows the low- ω behaviour on a linear scale.

level $\omega = 0$, $D\rho^{2CK}(\omega) = \frac{1}{2}$ (see also, inset), which is *half* of the unitarity limit. This is a hallmark of the 2CK FP, likewise known from study of the two-channel quadrupolar single-impurity Anderson model [108, 141] and the large U limit of the $O(3)$ symmetric Anderson model [106, 107]. We will discuss the behaviour of the 2CK spectrum more fully in Sec. 4.2.2 of the next chapter, where we consider chains of dots coupled to two leads. It is again studied in Sec. 6.2.2 of Chapter 6, where we compare it to the single-particle spectrum of a system of three mutually exchange-coupled dots, tunnel-coupled to two leads in a 2CK phase.

Having discussed in detail the NRG technique — both as a tool to solve numerically models of quantum dot systems which exhibit complex many-body behaviour; and as an underlying conceptual framework for understanding such problems — in the next chapter we apply it to systems of chains of quantum dots, connected to two metallic leads.

CHAPTER 4

Coupled quantum dot chains

In Chapter 2 we introduced the single-spin two-channel Kondo (2CK) model Eq. 2.10 which, in the spirit of the work by Nozières and Blandin [40], we analysed using poor man’s scaling [19]. This approach was used to show that an intermediate-coupling fixed point (FP) arises in the model, and that a scaling invariant — the Kondo temperature, T_K^{2CK} — governs the low-energy physics. However, as this scale depends non-analytically on the exchange coupling between the dot spin and the conduction electrons of the leads, a fundamentally non-perturbative approach is required.

In Chapter 3, we described how the powerful non-perturbative numerical renormalization group (NRG) technique of Wilson [12] could be used to solve the 2CK model, and showed that essentially-exact results for thermodynamics [12,13,45] and dynamics [20,21] can be obtained on all temperature/energy scales of interest.

As we discussed in the Introduction, the development of nanofabrication techniques over the last decade [50,59,88,90–94] together with atomic-scale manipulation using scanning tunneling microscopy [95,96], has sparked intense interest in novel mesoscopic devices where strong electron correlation and many-body effects play a central role [142]. In particular, the elusive 2CK effect has recently been observed experimentally in quantum dots for the first time by Potok *et al* [52].

In *coupled* quantum dot devices — the “molecular” analogue of single quantum dots viewed as artificial atoms [59] — exquisite experimental control is now available over the geometry, capacitance and couplings of the dots [90,92]. Both spin and internal, orbital degrees of freedom are now important, and the subtle interplay between the two gives rise to a great diversity in the resulting correlated electron behaviour. Coupled quantum dots connected to a single metallic lead have been widely studied theoretically (*eg.* double quantum dots in Refs. [61,63,66,73–78] and triple dots in Refs. [60,62,65,79–84]), and have been shown to exhibit quite different low-temperature behaviour from their single-dot counterparts [60].

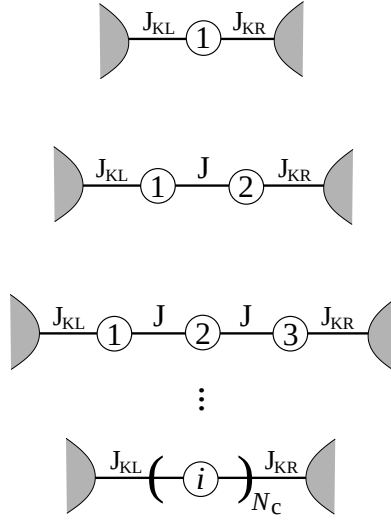


Figure 4.1: Schematic illustration of quantum dot chains connected to two leads.

Considerable theoretical interest has been generated by the prospect of realizing systems of coupled quantum dots in *two-channel* environments [36, 37, 65, 67, 68, 71, 85, 109–111, 114]. Here, the unusual non-Fermi liquid behaviour of the single-spin 2CK model competes with the local degrees of freedom of the nanodevice itself, and has been shown to give rise to a rich array of physical behaviour.

In this chapter, we consider a general class of 2CK models, in which leads are connected to both ends of a chain of quantum dots. We examine a range of different chain lengths, focusing here on the case of large interdot coupling, and demonstrate that the resulting behaviour can be understood in terms of the universal low-temperature/energy properties of simpler paradigmatic models, such as the single-spin 2CK model and the two-channel two-impurity (2IK) model. We use the NRG technique together with physical arguments to study these systems in detail.

4.1 Models of quantum dot chains coupled to two leads

The models we consider here are chains of spins, coupled together by a common (antiferromagnetic) Heisenberg exchange interaction, J . Each end of the chain is coupled to its own metallic lead, as illustrated schematically in Fig. 4.1. The class of Hamiltonians we study are thus of the form $H = H_L + H_{\text{chain}} + H_K$. As usual, $H_L = \sum_{\alpha, \mathbf{k}, \sigma} \epsilon_{\mathbf{k}} a_{\alpha \mathbf{k} \sigma}^\dagger a_{\alpha \mathbf{k} \sigma}$ refers to the two equivalent non-interacting leads ($\alpha = L, R$), and

$$H_{\text{chain}}^{N_c} = J \left(\sum_{i=1}^{N_c-1} \hat{\mathbf{S}}_i \cdot \hat{\mathbf{S}}_{i+1} \right), \quad (4.1)$$

$$H_K = J_{KL} \hat{\mathbf{S}}_1 \cdot \hat{\mathbf{S}}_{L0} + J_{KR} \hat{\mathbf{S}}_{N_c} \cdot \hat{\mathbf{S}}_{R0},$$

where $\hat{\mathbf{S}}_i$ is a spin- $\frac{1}{2}$ operator for dot i and N_c is the total number of dots in the chain. $\hat{\mathbf{S}}_{L0}$ is the spin density of the left lead at dot 1, and similarly $\hat{\mathbf{S}}_{R0}$ is the spin density of the right lead at dot N_c , as defined previously in Eq. 3.2. For generality we have allowed at this stage for a distinct coupling to each lead, noting that the system has full left $\leftrightarrow$ right mirror symmetry at the special point $J_{KL} = J_{KR}$.

For $N_c = 1$, Eq. 4.1 is simply the standard single-spin 2CK model, Eq. 2.20 (or Eq. 2.24 in the channel-isotropic case), while for $N_c = 2$, we recover the celebrated 2IK model [36, 37, 78, 109]. The latter represents a classic paradigm where the tendency to form a local singlet state on the two dots competes with the formation of a state where the dots are decoupled, generating in effect two separated single-channel Kondo (1CK) models. Analysis of the 2IK model with NRG [36, 37, 78, 109] and conformal field theory (CFT) [48, 112, 113] has shown that the critical point separating these phases is the 2CK FP. The physical origin of this is somewhat obscure [71], but can in fact be understood from simple scaling arguments in the asymmetric case [78], as discussed further in Sec. 5.2.1.

In the next chapter we study the full model Eq. 4.1 in the small interdot coupling limit. In this Chapter however, we consider the opposite limit, focusing specifically on the case where the interdot couplings are large compared with the dot-lead couplings: $J > J_{K\alpha}$ for $\alpha = L, R$. In the following section, we consider the behaviour of the *isolated* chains which, while somewhat trivial, will give an insight into the expected behaviour of the full system when the leads are attached.

4.1.1 Properties of isolated chains

We consider first the properties of isolated spin chains, and thus set $J_{KL} = J_{KR} = 0$ in Eq. 4.1. Diagonalization of $H_{\text{chain}}^{N_c}$ yields the exact eigenstates and energies of the chains, which naturally depends on the chain length N_c .

We will denote the lowest (ground) state of an isolated chain $|N_c; S^z\rangle_{g.s.}$, and consider the form of these states explicitly below. For $N_c = 1$, the ‘chain’ is of course a single spin- $\frac{1}{2}$, which can be written trivially as $|N_c = 1; S^z\rangle_{g.s.} = |S_1^z\rangle$ with $|S_1^z\rangle$ the state of the dot and $S^z \equiv S_1^z = \pm\frac{1}{2}$ for spins $\uparrow / \downarrow$. For $N_c = 2$, we obviously obtain singlet and triplet states, separated by an energy J . For antiferromagnetic J (considered here throughout), the lowest state is the singlet, $|N_c = 2; S^z = 0\rangle_{g.s.} = \frac{1}{\sqrt{2}} (|\uparrow, \downarrow\rangle - |\downarrow, \uparrow\rangle)$, where $|S_1^z, S_2^z\rangle \equiv |S_1^z\rangle \otimes |S_2^z\rangle$ are the basis states which span the

4-dimensional Hilbert space of the two dots.

We note that for $N_c = 3$, we can write $H_{\text{chain}}^{N_c=3} = J\hat{\mathbf{S}}_2 \cdot \hat{\mathbf{S}}_{13} = \frac{1}{2}J(\hat{\mathbf{S}}^2 - \hat{\mathbf{S}}_{13}^2 - \frac{3}{4})$ where $\hat{\mathbf{S}}_{13} = (\hat{\mathbf{S}}_1 + \hat{\mathbf{S}}_3)$ is the combined spin of dots 1 and 3, and $\hat{\mathbf{S}} = (\hat{\mathbf{S}}_2 + \hat{\mathbf{S}}_{13})$ is the total spin of the trimer. Two doublet states and one quartet result from coupling three spins; it is now clear that the lowest-lying of these is the doublet state in which spins 1 and 3 are found in a *triplet* combination. As will be seen in the next section, this has important implications for the behaviour of the system when the leads are reattached. The other states of the trimer are $\mathcal{O}(J)$ higher in energy.

As both $\hat{\mathbf{S}}$ and $\hat{\mathbf{S}}_{13}$ are conserved quantities of $H_{\text{chain}}^{N_c=3}$, all eigenstates can be classified according to them. The states themselves can be generated straightforwardly by the vector coupling of $\hat{\mathbf{S}}_{13}$ (which can either be a singlet or a triplet) with $\hat{\mathbf{S}}_2$ (which is a spin- $\frac{1}{2}$ object by construction), viz

$$|S, S^z; S_{13}\rangle = \sum_{S_1^z, S_2^z, S_3^z} C_{\frac{1}{2}, S_2^z, S_{13}, \mu}^{S, S^z} C_{\frac{1}{2}, S_1^z, \frac{1}{2}, S_3^z}^{S_{13}, \mu} |S_1^z, S_2^z, S_3^z\rangle, \quad (4.2)$$

where $C_{j_1, m_1, j_2, m_2}^{J, M} \equiv \langle j_1, j_2, m_1, m_2 | J, M \rangle$ are the standard Clebsch-Gordon coefficients. The composition of the states is thus independent of the coupling J , and using $S = \frac{1}{2}$ and $S_{13} = 1$ we obtain the ground trimer state,

$$|N_c = 3; S^z\rangle_{g.s.} = \frac{2S^z}{\sqrt{6}} \left(|S^z, S^z, -S^z\rangle + | -S^z, S^z, S^z\rangle - 2|S^z, -S^z, S^z\rangle \right), \quad (4.3)$$

with $S^z = \pm\frac{1}{2}$ for the two components of the doublet ground state.

The situation becomes rapidly more complex with increasing N_c , but for anti-ferromagnetic J it is physically obvious that for *even* N_c the lowest chain state is a spin-singlet, while for *odd* N_c it is a doublet state. While one can always write the states of a spin chain using a vector coupling scheme similar to Eq. 4.2, such states cannot be eigenstates of $H_{\text{chain}}^{N_c}$ for $N_c > 3$ because in general, only the total spin $\hat{\mathbf{S}}$ is conserved. With $N_c = 4$ for example, $\hat{\mathbf{S}}_{14}$ and $\hat{\mathbf{S}}_{23}$ are not conserved, and so states generated using a vector coupling of these combined spins cannot be eigenstates of $H_{\text{chain}}^{N_c=4}$. This implies that for $N_c > 3$, the terminal dots 1 and N_c are not going to be found in a pure singlet or triplet configuration, but rather will comprise a mixture of the two.

For $N_c > 3$, therefore, we must resort to numerical diagonalization of $H_{\text{chain}}^{N_c}$. We note here that for even chains, $|N_c; S^z\rangle_{g.s.}$ is indeed always found to be a spin-singlet, while for odd chains, $|N_c; S^z\rangle_{g.s.}$ is always a *doublet* state, with all other states being $\mathcal{O}(J/N_c)$ higher in energy.

The terminal dots (1 and N_c) are connected to the leads in the full model, and we will see below that the configuration of these spins is crucial in determining the low-energy behaviour of such systems. In Table 4.1 we show the variation of the

N_c	$\langle N_c; S^z \hat{\mathbf{S}}_1 \cdot \hat{\mathbf{S}}_{N_c} N_c; S^z \rangle_{g.s.}$	$\langle N_c; S^z \hat{S}_1^z + \hat{S}_{N_c}^z N_c; S^z \rangle_{g.s.}$
2	$-\frac{3}{4}$	0
3	$+\frac{1}{4}$	$S^z \times \frac{4}{3}$
4	-0.5399...	0
5	+0.2280...	$S^z \times 1.0234...$
6	-0.2341...	0
7	+0.1482...	$S^z \times 0.8404...$
8	-0.1553...	0

Table 4.1: Variation of $T = 0$ spin-spin correlators $\langle \hat{\mathbf{S}}_1 \cdot \hat{\mathbf{S}}_{N_c} \rangle \equiv \langle N_c; S^z | \hat{\mathbf{S}}_1 \cdot \hat{\mathbf{S}}_{N_c} | N_c; S^z \rangle_{g.s.}$ and matrix elements $\langle N_c; S^z | \hat{S}_1^z + \hat{S}_{N_c}^z | N_c; S^z \rangle_{g.s.}$ as a function of N_c for isolated chains.

spin-spin correlation functions $\langle \hat{\mathbf{S}}_1 \cdot \hat{\mathbf{S}}_{N_c} \rangle \equiv \langle N_c; S^z | \hat{\mathbf{S}}_1 \cdot \hat{\mathbf{S}}_{N_c} | N_c; S^z \rangle_{g.s.}$ with chain length N_c , calculated directly from the exact ground states¹ of $H_{\text{chain}}^{N_c}$.

As $\hat{\mathbf{S}}_{1N_c}$ is a conserved quantity in isolated chains for $N_c = 2$ and 3, we obtain $\langle N_c = 2; S^z | \hat{\mathbf{S}}_1 \cdot \hat{\mathbf{S}}_2 | N_c = 2; S^z \rangle_{g.s.} = -\frac{3}{4}$, which characterizes the singlet configuration of dots 1 and 2 for $N_c = 2$, while $\langle N_c = 3; S^z | \hat{\mathbf{S}}_1 \cdot \hat{\mathbf{S}}_3 | N_c = 3; S^z \rangle_{g.s.} = +\frac{1}{4}$ as expected for the triplet combination of terminal spins in the trimer.

As N_c increases for even chains, $\langle N_c; S^z | \hat{\mathbf{S}}_1 \cdot \hat{\mathbf{S}}_{N_c} | N_c; S^z \rangle_{g.s.}$ remains negative (indicating the dominant singlet character of the configuration) but decreases in magnitude. As such, the correlators quantify the increasing degree of triplet character in the configuration of the terminal spins as N_c increases for even chains. By contrast, for odd chains, the degree of triplet character *decreases* with N_c , with $\langle N_c; S^z | \hat{\mathbf{S}}_1 \cdot \hat{\mathbf{S}}_{N_c} | N_c; S^z \rangle_{g.s.}$ remaining positive, but decreasing in magnitude.

That the magnitude of the correlators decrease with N_c (for either even or odd chains) is of course physically natural. One would expect the correlations between the terminal spins to decrease as the length of the chain increases, such that $\langle N_c; S^z | \hat{\mathbf{S}}_1 \cdot \hat{\mathbf{S}}_{N_c} | N_c; S^z \rangle_{g.s.} \rightarrow 0$ as $N_c \rightarrow \infty$.

Also shown in Table 4.1 is the variation with N_c of matrix elements of the type $\langle N_c; S^z | \hat{S}_1^z + \hat{S}_{N_c}^z | N_c; S^z \rangle_{g.s.}$. Strikingly, such elements are identically zero for all even chains. In fact, this is a general result of the $SU(2)$ spin symmetry of the model, as we now show. In Appendix A, we derive an operator $\hat{P}_{i,\uparrow\downarrow} = \hat{S}_i^+ + \hat{S}_i^-$ which permutes ‘up’ and ‘down’ spins on a given dot i . The chain Hamiltonian $H_{\text{chain}}^{N_c}$ is invariant under simultaneous exchange of $\uparrow$ and $\downarrow$ spins on all dots (as the model

¹Correlators and matrix elements are calculated at $T = 0$, as we retain only the lowest (ground) states of $H_{\text{chain}}^{N_c}$.

has full $SU(2)$ symmetry in the absence of a magnetic field), and so we define

$$\hat{P}_{\uparrow\downarrow}^{N_c} = \prod_{i=1}^{N_c} \hat{P}_{i,\uparrow\downarrow} \quad (4.4)$$

such that $[H_{\text{chain}}^{N_c}, \hat{P}_{\uparrow\downarrow}^{N_c}] = 0$. From Eq. A.7 in Appendix A it now follows that $\hat{P}_{\uparrow\downarrow}^{N_c} |N_c; S^z\rangle_{g.s.} = \mu |N_c; -S^z\rangle_{g.s.}$. In fact, $\mu = \pm 1$ only, as the permutation operator is involutory (*ie.* it is self-inverse: $(\hat{P}_{\uparrow\downarrow}^{N_c})^2 = 1$). Using $\hat{P}_{i,\uparrow\downarrow} S_i^z = -S_i^z \hat{P}_{i,\uparrow\downarrow}$, we obtain

$$\begin{aligned} \langle N_c; S^z | \hat{S}_1^z + \hat{S}_{N_c}^z | N_c; S^z \rangle_{g.s.} &= \langle N_c; S^z | \hat{P}_{\uparrow\downarrow}^{N_c} \hat{P}_{\uparrow\downarrow}^{N_c} (\hat{S}_1^z + \hat{S}_{N_c}^z) \hat{P}_{\uparrow\downarrow}^{N_c} \hat{P}_{\uparrow\downarrow}^{N_c} | N_c; S^z \rangle_{g.s.} \\ &= \mu^2 \langle N_c; -S^z | \hat{P}_{\uparrow\downarrow}^{N_c} (\hat{S}_1^z + \hat{S}_{N_c}^z) \hat{P}_{\uparrow\downarrow}^{N_c} | N_c; -S^z \rangle_{g.s.} \\ &= -\langle N_c; -S^z | \hat{S}_1^z + \hat{S}_{N_c}^z | N_c; -S^z \rangle_{g.s.} \end{aligned} \quad (4.5)$$

The last line implies that $\langle N_c; S^z | \hat{S}_1^z + \hat{S}_{N_c}^z | N_c; S^z \rangle_{g.s.} = 0$ for *even* chains, where the lowest state is a spin-singlet ($S^z = -S^z = 0$). However, by contrast we obtain the key result that $\langle N_c; S^z | \hat{S}_1^z + \hat{S}_{N_c}^z | N_c; S^z \rangle_{g.s.} \propto S^z$ for *odd* chains, where the lowest state is a doublet ($|S^z| = \frac{1}{2}$). This is indeed shown to be the case in Table 4.1, where we evaluate these matrix elements for the ground state of chains up to length $N_c = 8$. We will see in the next section that the properties of these elements play an important role in determining the *effective* coupling between the lowest chain state and the leads, and hence the resulting physical behaviour at low temperatures.

4.1.2 Effective models

The interesting and nontrivial behaviour of Eq. 4.1 of course arises on coupling to the leads. To understand the low-temperature/energy properties of systems in the large interdot coupling regime, we will treat the coupling to the leads (described by H_K in Eq. 4.1) as a perturbation to the states of $H_{\text{chain}}^{N_c}$ (considered above), and derive a low-energy effective model. We show below that the underlying physical behaviour can then be simply understood in terms of this effective model. In Secs. 4.2.1–4.3.2 we go on to study the full model with NRG, analyzing in detail both thermodynamic and dynamical properties of such systems, confirming the physical picture discussed in this section.

We begin by rewriting H_K in the form

$$H_K = (J_K + \delta) \hat{\mathbf{S}}_1 \cdot \hat{\mathbf{s}}_{L0} + (J_K - \delta) \hat{\mathbf{S}}_{N_c} \cdot \hat{\mathbf{s}}_{R0} \quad (4.6)$$

where $J_K = \frac{1}{2}(J_{KL} + J_{KR})$ and $\delta = \frac{1}{2}(J_{KL} - J_{KR})$, such that the mirror-symmetric case is recovered for $J_{KL} = J_{KR} \equiv J_K$, where $\delta = 0$. Provided the states of $H_{\text{chain}}^{N_c}$ are not near-degenerate, only the lowest state $|N_c; S^z\rangle_{g.s.}$ need be retained. As all

other states are $\mathcal{O}(J/N_c)$ higher in energy (see Sec.4.1.1), and we consider here the regime where $J > \max(J_{KL}, J_{KR})$, a low-energy effective model is obtained simply by projecting onto the reduced Hilbert space of this state, using

$$\hat{1}_{N_c} = \sum_{S^z} |N_c; S^z\rangle_{g.s.} \langle N_c; S^z|. \quad (4.7)$$

The resultant Hamiltonian $H_{\text{eff}}^{N_c} = \hat{1}_{N_c} H_K \hat{1}_{N_c}$ then follows as

$$\begin{aligned} H_{\text{eff}}^{N_c} &= (J_K + \delta) \hat{1}_{N_c} \hat{\mathbf{S}}_1 \hat{1}_{N_c} \cdot \hat{\mathbf{s}}_{L0} + (J_K - \delta) \hat{1}_{N_c} \hat{\mathbf{S}}_{N_c} \hat{1}_{N_c} \cdot \hat{\mathbf{s}}_{R0}, \\ &= \frac{1}{2} J_K \hat{1}_{N_c} (\hat{\mathbf{S}}_1 + \hat{\mathbf{S}}_{N_c}) \hat{1}_{N_c} \cdot (\hat{\mathbf{s}}_{L0} + \hat{\mathbf{s}}_{R0}) + \frac{1}{2} \delta \hat{1}_{N_c} (\hat{\mathbf{S}}_1 + \hat{\mathbf{S}}_{N_c}) \hat{1}_{N_c} \cdot (\hat{\mathbf{s}}_{L0} - \hat{\mathbf{s}}_{R0}), \end{aligned} \quad (4.8)$$

where the last line is obtained using the symmetry $\hat{1}_{N_c} \hat{\mathbf{S}}_1 \hat{1}_{N_c} = \hat{1}_{N_c} \hat{\mathbf{S}}_{N_c} \hat{1}_{N_c} = \frac{1}{2} \hat{1}_{N_c} (\hat{\mathbf{S}}_1 + \hat{\mathbf{S}}_{N_c}) \hat{1}_{N_c}$. The latter can be shown formally (see Sec. A.2 of Appendix A), but the result is physically obvious, since the isolated chains themselves have strict mirror symmetry (it is only the coupling to left and right leads which may break this symmetry in the full model).

Considering the z -component of the term $\hat{1}_{N_c} (\hat{\mathbf{S}}_1 + \hat{\mathbf{S}}_{N_c}) \hat{1}_{N_c}$, one obtains²

$$\sum_{S^z} |N_c; S^z\rangle_{g.s.} \langle N_c; S^z| (\hat{S}_1^z + \hat{S}_{N_c}^z) |N_c; S^z\rangle_{g.s.} \langle N_c; S^z|.$$

For even chains, we showed in Sec. 4.1.1 that due to the $SU(2)$ spin symmetry of the model, matrix elements of the type $\langle N_c; S^z | (\hat{S}_1^z + \hat{S}_{N_c}^z) | N_c; S^z \rangle_{g.s.}$ must vanish. In fact, as the lowest state of an isolated even-length chain is always a spin-singlet, it is straightforward to show that all components of $\hat{1}_{N_c} (\hat{\mathbf{S}}_1 + \hat{\mathbf{S}}_{N_c}) \hat{1}_{N_c}$ vanish. This is of course physically natural, as there can be no spin exchange coupling between a *singlet* state and the leads. Thus, when the temperature is reduced so that $T \ll J$, all states of the chain are projected out except the lowest singlet state, which must be decoupled from the leads.

However, for *odd* chains, markedly different physics arises. As $|N_c; S^z\rangle_{g.s.}$ is now a doublet, we obtain $\langle N_c; S^z | (\hat{S}_1^z + \hat{S}_{N_c}^z) | N_c; S^z \rangle_{g.s.} \propto S^z$ (see Sec. 4.1.1 and Table 4.1). In the absence of a magnetic field, the z -direction of the spin is arbitrary. Thus, the other components of Eq. 4.8 follow from the $SU(2)$ spin symmetry of the problem and it can be shown that

$$H_{\text{eff}}^{N_c} = J_{K,\text{eff}}^{N_c} \hat{\mathbf{S}} \cdot (\hat{\mathbf{s}}_{L0} + \hat{\mathbf{s}}_{R0}) + \delta_{\text{eff}}^{N_c} \hat{\mathbf{S}} \cdot (\hat{\mathbf{s}}_{L0} - \hat{\mathbf{s}}_{R0}) \quad : \text{ odd } N_c \quad (4.9)$$

where $\hat{\mathbf{S}}$ is a spin- $\frac{1}{2}$ operator representing the lowest doublet of the isolated chain,

²Terms connecting S^z and $S^{z'}$ (where $S^z \neq S^{z'}$) vanish, since $\hat{S}_i^z$ cannot change the z -component of the spin.

with components $\hat{S}_z = \sum_{S^z} |N_c; S^z\rangle_{g.s.} S^z_{g.s.} \langle N_c; S^z|$ and $\hat{S}^\pm = |N_c; \pm \frac{1}{2}\rangle_{g.s.} \langle N_c; \mp \frac{1}{2}|$. Eq. 4.9 is a model of 2CK form, with effective couplings given by

$$J_{K,\text{eff}}^{N_c} = \langle N_c; \frac{1}{2} | (\hat{S}_1^z + \hat{S}_{N_c}^z) | N_c; \frac{1}{2} \rangle_{g.s.} J_K, \quad (4.10a)$$

$$\delta_{\text{eff}}^{N_c} = \langle N_c; \frac{1}{2} | (\hat{S}_1^z + \hat{S}_{N_c}^z) | N_c; \frac{1}{2} \rangle_{g.s.} \delta, \quad (4.10b)$$

with the matrix elements themselves given in Table 4.1.

Considering first the mirror-symmetric case $J_{KL} = J_{KR} \equiv J_K$ and $\delta = 0$, the low-energy effective model for odd chains is the familiar channel-isotropic 2CK model, discussed in Sec. 2.4 and Chapter 3. The lowest spin- $\frac{1}{2}$ state of these chains is thus overscreened by conduction electrons in the two leads, embodied in the infrared 2CK FP which describes the non-Fermi liquid ground state [40, 47, 49], where the partially quenched spin is characterised by a residual entropy of $S_{\text{imp}} = \frac{1}{2} \ln 2$. This overscreening sets in below the characteristic symmetric 2CK scale T_K^{2CK} , which can be determined from perturbative scaling (see Eq. 2.25 and Ref. [40]):

$$T_K^{2CK} \sim J_{K,\text{eff}}^{N_c} \exp\left(-1/\rho J_{K,\text{eff}}^{N_c}\right), \quad (4.11)$$

where $\rho = 1/(2D)$ is the density of states per orbital and $2D$ is the conduction bandwidth as usual. The 2CK scale thus depends on the chain length N_c through the effective coupling $J_{K,\text{eff}}^{N_c}$ given in Eq. 4.10a.

By contrast, the 2CK FP is destabilised by the left/right (L/R) symmetry-breaking second term of the low-energy effective model Eq. 4.9. For $J_{KL} \neq J_{KR}$ (*ie.* $\delta \neq 0$), the lowest spin- $\frac{1}{2}$ of the (odd) chain forms a Kondo singlet with the lead to which it is initially more strongly coupled [40, 45, 46, 124]. Below a characteristic scale T_K^{SC} , the dot spin is thus fully screened by conduction electrons in that lead, while the other lead decouples completely [40, 45, 46, 124].

Specifically, the ‘SC:L’ FP describes the lowest-energy behaviour for $\delta > 0$, where the system flows to *strong coupling* with the left lead ($J_{KL} \rightarrow \infty$) while the right lead decouples ($J_{KR} \rightarrow 0$), and for $\delta < 0$, the system flows to the ‘SC:R’ FP, where the situation is reversed (see Secs. 2.4 and 3.4.3). Thus the *sign* of δ dictates which FP is stable, and hence the phase.

For large $|\delta|$, the Kondo scale for flow to the stable FP (SC:L for $\delta \gg 0$ and SC:R for $\delta \ll 0$) is again obtained from poor man’s scaling, and is given by

$$T_K^{SC} \sim J_{>}^{N_c} \exp\left(-1/\rho J_{>}^{N_c}\right). \quad (4.12)$$

where $J_{>}^{N_c} = J_{K,\text{eff}}^{N_c} + |\delta_{\text{eff}}^{N_c}|$ is the effective coupling between the lowest chain doublet state and the more strongly-coupled lead.

For very small $|\delta_{\text{eff}}^{N_c}|$, RG flow is expected in the vicinity of the 2CK FP, which

is stable only at the point $\delta = 0$, and thus represents a critical point of the channel-anisotropic model. The T_K^{SC} scale must therefore vanish as the transition is approached, but the characteristic way in which this occurs cannot be established from these simple perturbative arguments. We will consider this case again in detail using NRG in Sec. 4.3.1.

In the following sections, we use NRG to study the full model Eq. 4.1 in the ‘large’ J regime, considering first the thermodynamics of the mirror symmetric case, $\delta = 0$.

4.2 Mirror symmetric case

The physical picture is thus clear from the above discussion. In the following sections, we consider explicitly the mirror-symmetric case $\delta = 0$, and use the NRG to calculate thermodynamic and dynamical properties of the full model Eq. 4.1.

4.2.1 Thermodynamics

In this section, we focus on the ‘impurity’ (chain) contribution [13, 27] to the thermodynamics. Specifically, we consider chiefly the entropy $S_{\text{imp}}(T)$ and the uniform spin susceptibility, $\chi_{\text{imp}}(T) = \langle (\hat{S}^z)^2 \rangle_{\text{imp}} / T$ (here $\hat{S}^z$ refers to the spin of the entire system and $\langle \hat{\Omega} \rangle_{\text{imp}} = \langle \hat{\Omega} \rangle - \langle \hat{\Omega} \rangle_0$ with $\langle \hat{\Omega} \rangle_0$ denoting a thermal average in the absence of the chain, as discussed in Sec. 3.5). As we will see, the temperature dependence of these quantities provides clear signatures of the underlying FPs reached under renormalization on progressive reduction of the temperature/energy scale [13, 27].

The numerical calculations presented in this chapter were performed using an NRG discretization parameter $\Lambda = 3$, and we retain typically $N_s = 4000$ states at each iteration.

In Fig. 4.2 we show the entropy $S_{\text{imp}}(T)/\ln(2)$ (left panel) and susceptibility $4T\chi_{\text{imp}}(T)$ (right panel) both *vs.* T/D , for chains with common fixed $\rho J_K = 0.075$ and $\rho J = 0.15$ (and $\delta = 0$, giving as desired a bare model with strict mirror symmetry). In the main panels we show odd- N_c only (with solid, dotted, dashed and dot-dashed lines corresponding to $N_c = 1, 3, 5, 7$), while the insets show even- N_c only (now solid, dotted, dashed and dot-dashed lines refer to $N_c = 2, 4, 6, 8$).

Considering first the variation of the entropy in the left panel of Fig. 4.2, one finds as expected that at ‘high’ temperatures $T > J$, all states of the chain are thermally accessible, and so we obtain $S_{\text{imp}}(T) = N_c \ln(2)$ ($k_B \equiv 1$). For $N_c = 1$, there is of course only a single spin, and so the behaviour at the highest temperatures is governed simply by the local moment (LM) FP. For $N_c > 1$ however, all spins of the chain are essentially free, the FP being Eq. 4.1 with $J = J_{KL} = J_{KR} = 0$. As the temperature is lowered, the higher-lying states are depopulated, and for $T < J$, only the lowest state of the chain is accessible. For odd chains (main panels)

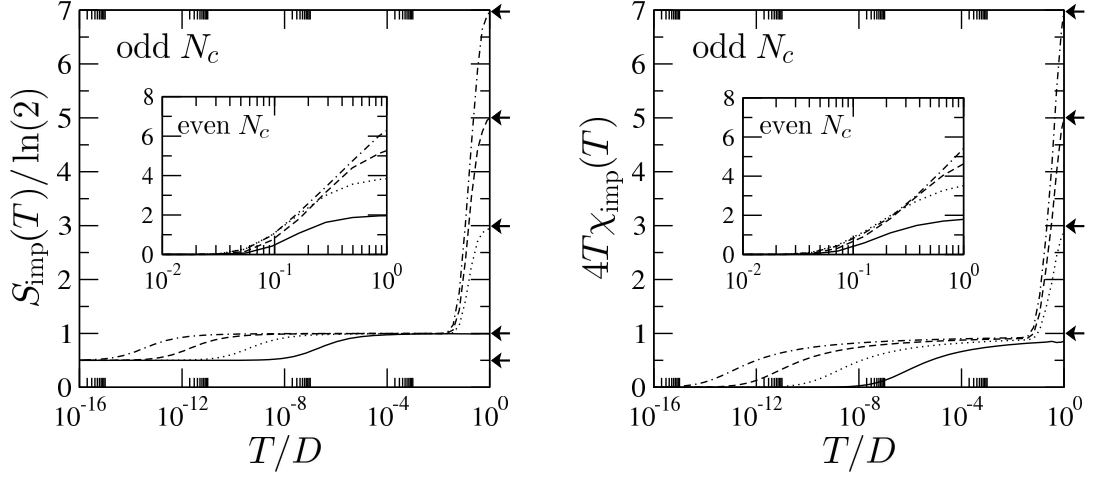


Figure 4.2: Thermodynamics in the ‘large’ J regime for L/R mirror symmetric systems ($\delta = 0$), calculated for the full model via NRG. Plotted are results for fixed $\rho J_K = 0.075$ and $\rho J = 0.15$, varying the chain length N_c . In the left panel we show $S_{\text{imp}}(T)/\ln(2)$, while the right panel shows $4T\chi_{\text{imp}}(T)$, both *vs.* T/D . In the main panels, we plot odd- N_c only: specifically $N_c = 1, 3, 5, 7$ correspond respectively to solid, dotted, dashed and dot-dashed lines, while even- N_c are shown in the insets ($N_c = 2, 4, 6, 8$ correspond here to the solid, dotted, dashed and dot-dashed lines). The horizontal arrows indicate the FP values.

the lowest state is of course a doublet state, and so the LM FP is reached, with the characteristic entropy $S_{\text{imp}}(T) = \ln(2)$ for all odd N_c . By contrast, for even chains, the lowest chain state is a *singlet*, which is decoupled from the leads, and $S_{\text{imp}}(T) = 0$ results. This ‘decoupled singlet’ (DS) FP and the LM FP are both described by Eq. 4.1 with $J_{KL} = J_{KR} = 0$ but $J = \infty$.

In the inset to the left panel, we see that for even chains, the DS FP describes the behaviour of the system down to $T = 0$ as expected, and the only scale in the problem is the non-universal high-energy scale of J . However for odd chains (main panel), residual correlations between the lowest doublet state of the chain and the leads drives the system away from the unstable LM FP, and toward the 2CK FP below the characteristic Kondo scale T_K^{2CK} . At the lowest temperatures, we find for all odd N_c that $S_{\text{imp}} = \frac{1}{2} \ln(2)$, which is characteristic [43–45] of the overscreened non-Fermi liquid (NFL) ground state.

This behaviour is likewise evident in the evolution of $4T\chi_{\text{imp}}(T)$, shown in the right panel of Fig. 4.2. At the highest temperatures, the spins of the chain are essentially decoupled, and each makes a Curie law contribution to the susceptibility, giving $T\chi_{\text{imp}}(T) = \frac{1}{4}N_c$. For $T \lesssim J$, all but the lowest chain state is projected out, leaving thereby a free spin- $\frac{1}{2}$ object for the odd chains (main panel). The susceptibility of $T\chi_{\text{imp}}(T) = \frac{1}{4}$ is characteristic [12, 13] of the LM FP, and describes the behaviour of each system for $T_K^{2CK} \ll T \ll J$. Below T_K^{2CK} , the local moment is ‘quenched’, in the sense that $T\chi_{\text{imp}}(T) \rightarrow 0$ as $T \rightarrow 0$ (although $\chi_{\text{imp}}(T)$ itself

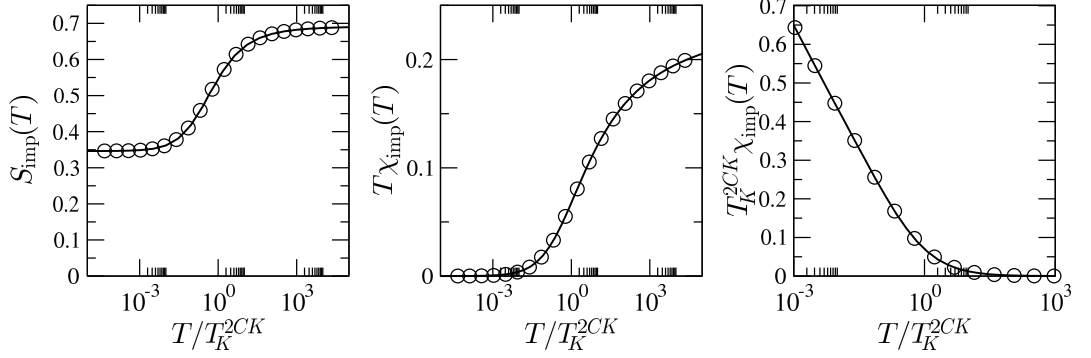


Figure 4.3: Thermodynamics for odd chains with the same parameters as Fig. 4.2, rescaled in terms of their Kondo scales. In the left panel we show $S_{\text{imp}}(T)$, in the middle panel we show $T\chi_{\text{imp}}(T)$ and in the right panel we show $T_K^{2CK}\chi_{\text{imp}}(T)$, all *vs.* T/T_K^{2CK} . In each panel, all data collapse onto a common universal scaling curve characteristic of the standard single-spin 2CK model ($N_c = 1$, shown with circles).

diverges logarithmically [43–45] as $T \rightarrow 0$, as we show shortly). This is again characteristic of the 2CK FP, which describes the ground state of all odd chains. By contrast, for even chains (see inset of the right panel), the DS FP describes the behaviour of all systems for $T \ll J$.

We will not discuss the behaviour of even chains further here, since below the scale of J , all states of the chain except the lowest singlet are projected out; and the singlet itself is trivially decoupled from the leads. Only for odd- N_c do we see the emergence of a low-energy scale, T_K^{2CK} . For any odd N_c , all systems flow to the LM FP for $T \lesssim J$, then crossover to the 2CK FP for $T \lesssim T_K^{2CK}$. While this scale inevitably depends on the bare parameters (and the chain length N_c , see Eq. 4.11), the FPs themselves are always the same, and hence universality is expected to arise on rescaling in terms of T_K^{2CK} . This is demonstrated in Fig. 4.3, where we present the same systems as Fig. 4.2 (for odd N_c), but rescale them in terms of their Kondo scales. In the left panel we show $S_{\text{imp}}(T)$, while in the middle and right panels we show $T\chi_{\text{imp}}(T)$ and $T_K^{2CK}\chi_{\text{imp}}(T)$ respectively, all *vs.* T/T_K^{2CK} . The collapse to the 2CK scaling curves ($N_c = 1$, shown with circles) confirms the mapping onto an effective single-spin 2CK model (Eq. 4.9), and that that the properties of all such systems are fundamentally alike when viewed at low temperatures. In particular, the NFL behaviour [43–45] is evident in the residual entropy $S_{\text{imp}}(T = 0) = \frac{1}{2} \ln(2)$ and the susceptibility which diverges as $T_K^{2CK}\chi_{\text{imp}}(T) = \alpha \ln(T_K^{2CK}/T)$.

As the Kondo scale characterizes the flow from the LM FP to the 2CK FP, it can be identified directly from the evolution of the thermodynamics in Fig. 4.2. As mentioned in Sec. 3.5, we can define T_K^{2CK} as the temperature where $T_K^{2CK}\chi_{\text{imp}}(T_K^{2CK}) = 0.07$ (chosen suitably between the limiting LM FP value of $\frac{1}{4}$ and the 2CK value of 0). Equivalently, we can define the scale through the entropy: $S_{\text{imp}}(T_K^{2CK}) = 0.55$

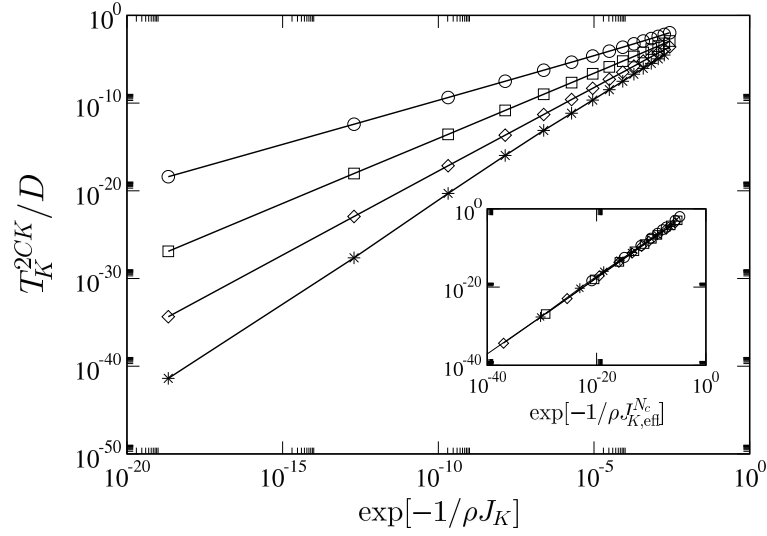


Figure 4.4: Evolution of the 2CK scale as determined from the thermodynamics (defined such that $T_K^{2CK} \chi_{\text{imp}}(T_K^{2CK}) = 0.07$), varying ρJ_K for common fixed $\rho J = 0.15$ in the mirror-symmetric case ($\delta = 0$). Shown are results for odd chains: $N_c = 1, 3, 5, 7$ correspond to circles, squares, diamonds and stars respectively. Specifically, we plot T_K^{2CK}/D vs. $(\rho J_K) \exp(-1/\rho J_K)$, the latter being the expected form of the Kondo scale for a single-spin 2CK model, as derived from poor man's scaling. The inset shows T_K^{2CK}/D vs. $(\rho J_{K,\text{eff}}^{N_c}) \exp(-1/\rho J_{K,\text{eff}}^{N_c})$; the collapse to a single line demonstrates the mapping of all odd chains onto an effective single-spin 2CK model, Eq. 4.9.

(which corresponds to a value between $\ln(2)$ and $\frac{1}{2} \ln(2)$). It is clear from Fig. 4.2 that T_K^{2CK} varies exponentially with N_c , and it is also found to change widely with the bare coupling J_K for a given N_c . It is known from poor man's scaling (see Ref. [40] and Sec. 2.4) that the Kondo scale for a (symmetric) single-spin 2CK model has the form $T_K^{2CK}/D \sim \exp(-1/\rho J_K)$ to second order. In Fig. 4.4 we plot T_K^{2CK}/D (as measured from the thermodynamics) vs. $\exp(-1/\rho J_K)$ for a wide range of bare couplings ρJ_K and for odd chains of length $N_c = 1, 3, 5, 7$, shown with circles, squares, diamonds and stars, respectively.

For $N_c = 1$ (circles), the familiar poor man's scaling result is confirmed (the gradient of the log-log plot being precisely 1). For $N_c > 1$, the functional form remains the same, but the different slopes of the lines indicate that the effective dot-lead coupling is renormalized. This is of course the result expected from the discussion of Sec. 4.1.2, where we derived a low-temperature effective model of 2CK form (see Eq. 4.9), with an effective Kondo coupling $J_{K,\text{eff}}^{N_c}$. The Kondo scale for odd chains is thus expected to have the generic form of Eq. 4.11 which (to second order³) is simply $T_K^{2CK}/D \sim \exp(-1/\rho J_{K,\text{eff}}^{N_c})$, where $\rho J_{K,\text{eff}}^{N_c}$ is itself given by Eq. 4.10a. In the inset to Fig. 4.4 we plot T_K^{2CK}/D vs. $\exp(-1/\rho J_{K,\text{eff}}^{N_c})$; the collapse to a single

³We have used the second order poor man's scaling result here for simplicity. The third order result [40] given in Eq. 4.11 gives rather more accurate results, especially for large ρJ_K .

line (of gradient 1) confirms the physical picture discussed in Sec. 4.1.2 and the validity of the low-energy effective model. The agreement between the numerics and the analytical result derived from scaling arguments indicates that the value of $\rho J_{K,\text{eff}}^{N_c}$ for other systems may in fact be determined simply from the NRG as the inverse of the gradients in the main panel.

In the next section we consider the dynamical properties of odd chains, focusing on the $T = 0$ local spectrum.

4.2.2 Dynamics

Adopting a similar approach to Ref. [127], we showed in Secs. 3.6.2 and 3.6.3 that two characteristic spectra can be identified for the single-spin 2CK model: $D\rho_L^{2CK}(\omega)$ and $D\rho_R^{2CK}(\omega)$, which correspond to dynamical spin-scattering processes involving the dot and the left or right leads. For the case $J_{KL} = J_{KR} \equiv J_K$, we obviously obtain $D\rho_L^{2CK}(\omega) = D\rho_R^{2CK}(\omega) \equiv D\rho^{2CK}(\omega)$, which trivially follows from the mirror symmetry of the setup. Thus there is a *single characteristic 2CK spectrum* in this case (see Sec. 3.6.3 and Fig. 3.15).

We now turn to systems of chains of dots, first extending this work by identifying the relevant dynamical quantities. We then go on to study the resulting spectra for mirror symmetric systems ($\delta = 0$), and establish the universal scaling spectrum for all odd chains.

For generality, we start by considering the full channel-anisotropic model Eq. 4.1, which can be rewritten using Eq. 3.2 in the form $H = H_L + H_K + H_{\text{chain}}^{N_c}$, where

$$\begin{aligned} H_L &= \sum_{\alpha, \mathbf{k}, \sigma} \epsilon_{\mathbf{k}} a_{\alpha \mathbf{k} \sigma}^\dagger a_{\alpha \mathbf{k} \sigma} \\ H_K &= \sum_{\alpha, \mathbf{k}, \mathbf{k}'} \frac{J_{K\alpha}}{2N} \left[\hat{S}^z (a_{\alpha \mathbf{k} \uparrow}^\dagger a_{\alpha \mathbf{k}' \uparrow} - a_{\alpha \mathbf{k} \downarrow}^\dagger a_{\alpha \mathbf{k}' \downarrow}) + \hat{S}^+ a_{\alpha \mathbf{k} \downarrow}^\dagger a_{\alpha \mathbf{k}' \uparrow} + \hat{S}^- a_{\alpha \mathbf{k} \uparrow}^\dagger a_{\alpha \mathbf{k}' \downarrow} \right] \\ H_{\text{chain}}^{N_c} &= J \left(\sum_{i=1}^{N_c-1} \hat{\mathbf{S}}_i \cdot \hat{\mathbf{S}}_{i+1} \right). \end{aligned} \tag{4.13}$$

The first step (as in Sec. 3.6.3) is to determine the t-matrices for the left and right leads. Using equation of motion methods [8, 139] for the Hamiltonian Eq. 4.13, and comparing to Eq. 3.70, it can readily be shown that

$$\begin{aligned} t_\alpha^{N_c}(\omega) &= \langle \langle [a_{\alpha \mathbf{k} \sigma}, H_K]; [H_K, a_{\alpha \mathbf{k}' \sigma}^\dagger] \rangle \rangle_\omega \\ &= \frac{J_{K\alpha}^2}{4N} G_\alpha^{N_c}(\omega). \end{aligned} \tag{4.14}$$

The above result is independent of the chain part of the Hamiltonian, $H_{\text{chain}}^{N_c}$, since the latter involves only spin-exchange interaction terms between the dots, and hence

$[a_{\alpha\mathbf{k}\sigma}, H_{\text{chain}}^{N_c}] = 0$. The correlators $G_{\alpha}^{N_c}(\omega)$ themselves straightforwardly follow as

$$\begin{aligned} G_L^{N_c}(\omega) &= \langle\langle \hat{S}_1^- f_{L0\downarrow} + \hat{S}_1^z f_{L0\uparrow}; \hat{S}_1^+ f_{L0\downarrow}^\dagger + \hat{S}_1^z f_{L0\uparrow}^\dagger \rangle\rangle_{\omega}, \\ G_R^{N_c}(\omega) &= \langle\langle \hat{S}_{N_c}^- f_{R0\downarrow} + \hat{S}_{N_c}^z f_{R0\uparrow}; \hat{S}_{N_c}^+ f_{R0\downarrow}^\dagger + \hat{S}_{N_c}^z f_{R0\uparrow}^\dagger \rangle\rangle_{\omega}. \end{aligned} \quad (4.15)$$

where $f_{\alpha 0\sigma}^\dagger$ is an operator for the ‘0’-orbital of the $\alpha = L, R$ Wilson chain, as defined in Eq. 3.2, while $\hat{S}_i^z$ and $\hat{S}_i^\pm$ are spin- $\frac{1}{2}$ operators for dot i .

We now define $D\rho_{\alpha}^{N_c}(\omega) = -\pi\rho_T \text{Im}\{t_{\alpha}^{N_c}(\omega)\}$ (as with the spectra of the single-spin 1CK and 2CK models discussed in Secs. 3.6.2 and 3.6.3). The spectral density is thus given by

$$\rho_{\alpha}^{N_c}(\omega) = -\frac{\pi}{2}(\rho J_{K\alpha})^2 \text{Im}\{G_{\alpha}^{N_c}(\omega)\}. \quad (4.16)$$

In the mirror-symmetric cases considered in this section, there is a single characteristic spectral function for chains of any length, and so we drop the $\alpha = L, R$ index: $D\rho_L^{N_c}(\omega) = D\rho_R^{N_c}(\omega) \equiv D\rho^{N_c}(\omega)$. As we discussed in Sec. 4.2.1, the lowest state of an even chain is a singlet, which consequently decouples from the leads at low temperatures/energies. There is no low-energy Kondo scale and no universality. The spectral density of any even-length chain is thus not appreciable at any frequency, but in particular $D\rho^{N_c}(\omega) \simeq 0$ for $|\omega| \ll J$. This has been confirmed directly with NRG, and we do not discuss the dynamical behaviour of even chains here further.

For odd chains, however, the lowest chain state is a doublet which itself undergoes the 2CK effect below $T \sim T_K^{2CK}$ (see Secs. 4.1.2 and 4.2.1). In Fig. 4.5 we plot the $T = 0$ spectrum $D\rho^{N_c}(\omega)$ vs. ω/D for odd chains of length $N_c = 1, 3, 5, 7$ (shown as the solid, dotted, dashed and dot-dashed lines, respectively). All systems have a common $\rho J_K = 0.075$ and $\rho J = 0.15$ (as in Fig. 4.2). The low- ω behaviour is dominated by the 2CK resonance, the form of which reflects RG flow in the vicinity of the stable FP, which is of course the 2CK FP for all odd chains. The resonance is centred on the Fermi level $\omega = 0$ and is of width $\sim T_K^{2CK}$. The 2CK scale itself (given analytically from poor man’s scaling [40] by Eq. 4.11, and confirmed numerically from the thermodynamics in Fig. 4.4), decreases exponentially with increasing (odd) N_c , and this is indeed reflected in the exponential narrowing of the 2CK resonance in Fig. 4.5 (see also, inset). For all odd chains however, at the Fermi level $\omega = 0$ we find that the spectrum reaches *half* the unitarity limit $D\rho^{N_c}(0) = \frac{1}{2}$, which is characteristic of the 2CK FP. As mentioned in Sec. 3.6.3, this result has been similarly established from study of the two-channel quadrupolar single-impurity Anderson model [108, 141], and also from the large U limit of the $O(3)$ symmetric Anderson model [106, 107]. Here we obtain it directly for the single-spin 2CK model ($N_c = 1$, solid line), and furthermore confirm that the same zero-frequency value is a ubiquitous feature of odd chains of dots coupled symmetrically to two leads.

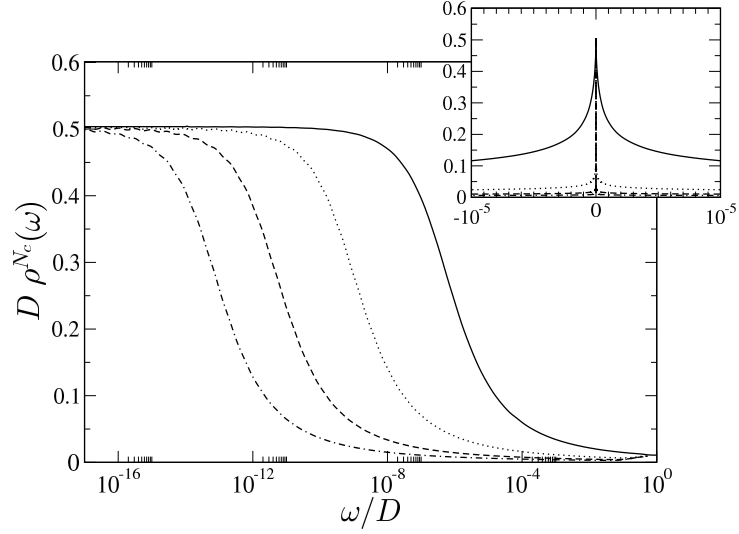


Figure 4.5: $T = 0$ local spectrum $D\rho^{N_c}(\omega)$ vs. ω/D for odd chains with $\rho J_K = 0.075$ and $\rho J = 0.15$ (as in Fig. 4.2); $N_c = 1, 3, 5, 7$ correspond to the solid, dotted, dashed and dot-dashed lines respectively. The inset shows the data on a linear frequency scale.

As the stable FP of all odd chains is the 2CK FP (demonstrated both by thermodynamics in Fig. 4.2 and now the spectra in Fig. 4.5), we expect universal scaling collapse of $D\rho^{N_c}(\omega)$ in terms of ω/T_K^{2CK} , which is demonstrated explicitly in Fig. 4.6. The 2CK scale itself has been determined as usual from the thermodynamics, although a wholly equivalent measure could have been made through *eg.* the half-width at half-maximum of the spectra in Fig. 4.5. The low-frequency asymptotic behaviour of the resulting scaling spectrum in Fig. 4.6 is found to be

$$D\rho^{N_c}(\omega) \stackrel{\frac{|\omega|}{T_K^{2CK}} \ll 1}{\sim} \frac{1}{2} [1 - a (|\omega|/T_K^{2CK})^{\frac{1}{2}}] \quad (4.17)$$

with the constant $a \simeq 0.47$, as consistent with that found for the quadrupolar Anderson impurity model [108]; and in contrast to the $[1 - a(\omega/T_K)^2]$ decay of $\pi\Gamma D(\omega)$ characteristic [8] of the normal Fermi liquid FP in the single-channel Anderson model (see Fig. 3.13), or $D\rho^{1CK}(\omega)$ for the 1CK model (see Fig. 3.14). For $|\omega|/T_K^{2CK} \gg 1$ by contrast, as also shown in Fig. 4.6, the asymptotic behavior is

$$D\rho^{N_c}(\omega) \stackrel{\frac{|\omega|}{T_K^{2CK}} \gg 1}{\sim} A / [\ln^2(|\omega|/T_K^{2CK}) + B] \quad (4.18)$$

with A and B pure constants $\mathcal{O}(1)$. The form of this high-frequency behaviour is also asymptotically common to the single-channel spin- $\frac{1}{2}$ Anderson model [31] and its $SU(2N)$ generalization [33]. This is physically natural, the origin of the ‘high’ energy leading $\sim 1/\ln^2(|\omega|/T_K)$ logarithms being spin-flip scattering [8], which occurs for

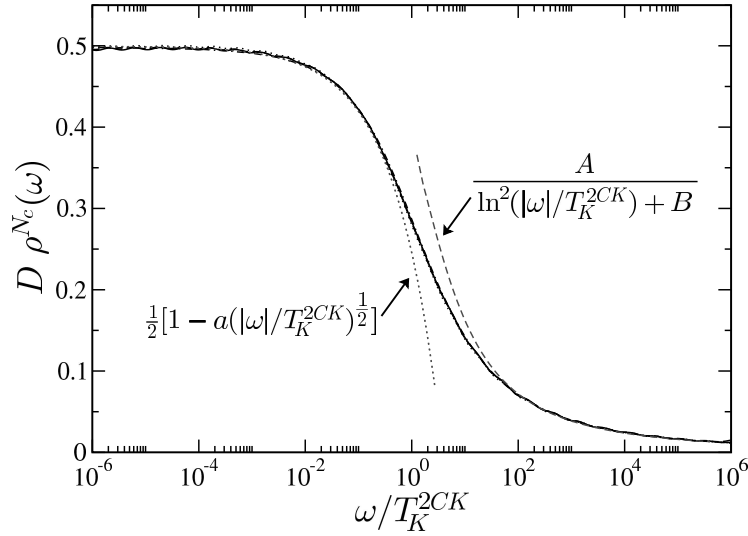


Figure 4.6: $T = 0$ scaling spectrum for odd chains: $D \rho^{N_c}(\omega)$ vs. ω/T_K^{2CK} for the same systems as plotted in Fig. 4.5 (and the 2CK scale T_K^{2CK} is determined as usual from the thermodynamics). All spectra collapse to the same universal form. The dotted line shows the low- $|\omega|/T_K^{2CK}$ asymptotic behaviour $D \rho^{N_c}(\omega) = \frac{1}{2}[1 - a(|\omega|/T_K^{2CK})^{\frac{1}{2}}]$, while the dashed line describes the high- $|\omega|/T_K^{2CK}$ scaling behaviour $D \rho^{N_c}(\omega) = A/[\ln^2(|\omega|/T_K^{2CK}) + B]$.

both single- and two-channel models.

We note that while varying J_K changes the Kondo scale for any odd N_c (see Eq. 4.11), in all cases $D \rho^{N_c}(\omega = 0) = \frac{1}{2}$ still results, and indeed the low-frequency behaviour is a universal function of ω/T_K^{2CK} , as shown Fig. 4.6.

In the next section, we consider the channel-anisotropic case, where the mirror symmetry of the problem is broken by distinct exchange couplings to left and right leads. As discussed in Sec. 4.1.2, this destabilises the 2CK FP [40, 45, 46, 124], although RG flow in its vicinity may still strongly affect the temperature-dependent thermodynamics and the frequency-dependent spectrum, as shown for odd chains below.

4.3 Asymmetric case

Having considered the mirror-symmetric $\delta = 0$ case in the previous sections, we now turn to systems which have distinct exchange couplings to left and right leads. An effective one-channel quenching of the dot spin is known [40, 45, 46, 124] to occur for the single-spin 2CK model. The channel anisotropy drives the system to strong-coupling with the lead with the stronger *bare* coupling below a characteristic low-energy scale T_K^{SC} , while the other lead decouples completely [40, 45, 46, 124]. This situation was discussed for the canonical $N_c = 1$ case in Secs. 2.4 and 3.4.3. In the following sections, we consider the generic behaviour of chains of dots coupled

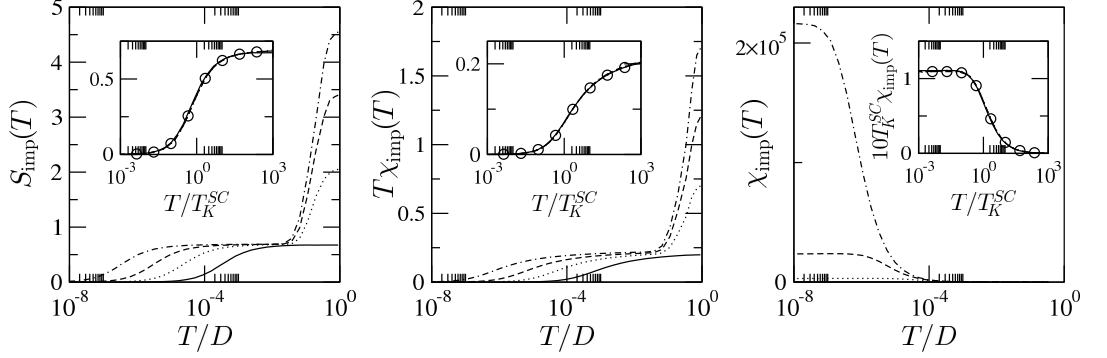


Figure 4.7: Thermodynamics for L/R asymmetric systems with $\rho J_K = 0.1$, $\rho\delta = \pm 0.05$ and $\rho J = 0.15$. In the left panel we show the entropy $S_{\text{imp}}(T)$, while we plot the uniform spin susceptibility $T\chi_{\text{imp}}(T)$ in the middle panel, and $\chi_{\text{imp}}(T)$ itself in the right panel, all *vs.* T/D , for odd chains of length $N_c = 1, 3, 5, 7$ corresponding to the solid, dotted, dashed and dot-dashed lines, respectively. The insets show the universality arising on rescaling in terms of T/T_K^{SC} , and the circles are the universal scaling curves for a single-spin 1CK model.

asymmetrically to two leads, focusing initially on the thermodynamic properties of such systems.

4.3.1 Thermodynamics

We again begin by considering the thermodynamics, since the underlying FP structure and relevant energy scales can be readily identified from the temperature-dependence of such quantities.

In Fig. 4.7 we recap the known thermodynamic behaviour [45] of the standard single-spin 2CK model (*ie.* Eq. 4.1 with $N_c = 1$), shown as the solid lines, for a system with $\rho J_K = 0.1$ and $\rho\delta = \pm 0.05$. In the left panel we show the entropy $S_{\text{imp}}(T)$ while we plot the magnetic susceptibility $T\chi_{\text{imp}}(T)$ in the middle panel and $\chi_{\text{imp}}(T)$ itself in the right panel, all *vs.* T/D . At high temperatures, the systems are described by the LM FP: the dot spin is free and hence yields a characteristic [13,45] entropy $S_{\text{imp}}(T) = \ln(2)$ and a Curie law susceptibility $T\chi_{\text{imp}}(T) = \frac{1}{4}$. As the temperature is lowered below $T \sim T_K^{SC}$, the dot spin is fully compensated by the formation of a Kondo singlet with the left lead conduction electrons for $\rho\delta = +0.05$, or with the right lead electrons for $\rho\delta = -0.05$. In either case, the entropy drops to $S_{\text{imp}}(T) = 0$, and likewise the susceptibility $T\chi_{\text{imp}}(T) = 0$ while $\chi_{\text{imp}}(T)$ itself plateaus to a constant, all being characteristic [13,45] of flow to the stable SC: α FP, where the dot spin is quenched by the $\alpha = L, R$ lead for $T \ll T_K^{SC}$. The functional dependence of T_K^{SC} on the bare system parameters can again be obtained from poor man's scaling [40], given in Eq. 4.11, and we analyse this further in Fig. 4.9, below.

The thermodynamics, reflecting the dot contribution only, are ‘blind’ to the sign of $\rho\delta$: systems with common magnitude $|\rho\delta|$ have precisely the same behaviour, as

shown in Fig. 4.7.

Importantly, we also show in Fig. 4.7 the thermodynamics for other odd chains, with the same $\rho J_K = 0.1$ and $\rho\delta = \pm 0.05$. We use $\rho J = 0.15$ as the interdot exchange couplings, and show results for $N_c = 3, 5, 7$ as the dotted, dashed and dot-dashed lines, respectively.

At the highest temperatures, all of the dot states are quasidegenerate, and the spins are essentially uncoupled. Thus the entropy (as for the symmetric model) is $S_{\text{imp}}(T) = N_c \ln(2)$ and the susceptibility is simply $T\chi_{\text{imp}}(T) = \frac{1}{4}N_c$, as expected for N_c free spins. For $T \lesssim J$ however, all but the lowest chain doublet state is projected out, and all systems flow to the LM FP. Thus all systems are described by $S_{\text{imp}}(T) = \ln(2)$ and $T\chi_{\text{imp}}(T) = \frac{1}{4}$ below a non-universal high-energy scale $\mathcal{O}(J)$. Having discarded the higher lying chain states, the systems behave like a single-spin 2CK model, but with renormalized couplings. The system is then described by the low-energy effective model Eq. 4.9 which we derived perturbatively in Sec. 4.1.2, and which is valid only for $T \ll J$. For $T \lesssim T_K^{SC}$, the effective antiferromagnetic coupling between the lowest doublet and the leads embodied in Eq. 4.9 drives the system to either the SC:L FP for $\delta > 0$ or the SC:R FP for $\delta < 0$ (as for the single-spin 2CK model). The Kondo scale T_K^{SC} depends on J_K and δ as expected, but also of course on the chain length N_c , as discussed in Sec. 4.1.2 (see Eq. 4.11). This is clearly apparent in Fig. 4.7 through the flow from $S_{\text{imp}}(T) = \ln(2) \rightarrow 0$ in the left panel or $T\chi_{\text{imp}}(T) = \frac{1}{4} \rightarrow 0$ in the middle panel, which occurs on a temperature scale which decreases exponentially with increasing (odd) N_c .

In the right panel, we see that in all cases, $\chi_{\text{imp}}(T)$ itself plateaus to a constant, which is found to be inversely proportional [13,45] to the effective one-channel Kondo scale T_K^{SC} . In the insets, we show the data for all odd chains $N_c = 1, 3, 5, 7$ rescaled in terms of T/T_K^{SC} (measured via $T_K^{SC}\chi_{\text{imp}}(T_K^{SC}) = 0.07$ as usual), and in the inset to the right panel we plot $T_K^{SC}\chi_{\text{imp}}(T)$ vs. T/T_K^{SC} . The universality which arises confirms the mapping of the full model Eq. 4.1 onto the effective single-spin channel-anisotropic 2CK model Eq. 4.9 at low temperatures. The circles are the scaling curves for the standard single-spin 1CK model, demonstrating that the residual chain doublet state is indeed quenched in an effective *one*-channel fashion.

In Sec. 4.2.1 we studied the symmetric case $\delta = 0$, where the intermediate-coupling 2CK FP controls the lowest-temperature behaviour. No sign of the 2CK FP is observed in the thermodynamics shown in Fig. 4.7 when the mirror symmetry of the problem is broken. Using a much smaller value of $|\rho\delta|$ is expected to result in RG flow in the vicinity of the 2CK FP however, although for any system lacking strict mirror symmetry, the ultimate stable FP must be either SC:L or SC:R. As the SC:L and SC:R FPs themselves are distinct, there must be a phase transition as a function of δ , with $\delta = 0$ itself being the critical point of the model. The ‘small’ $|\rho\delta|$ regime thus corresponds to the situation close to the transition, and we examine the

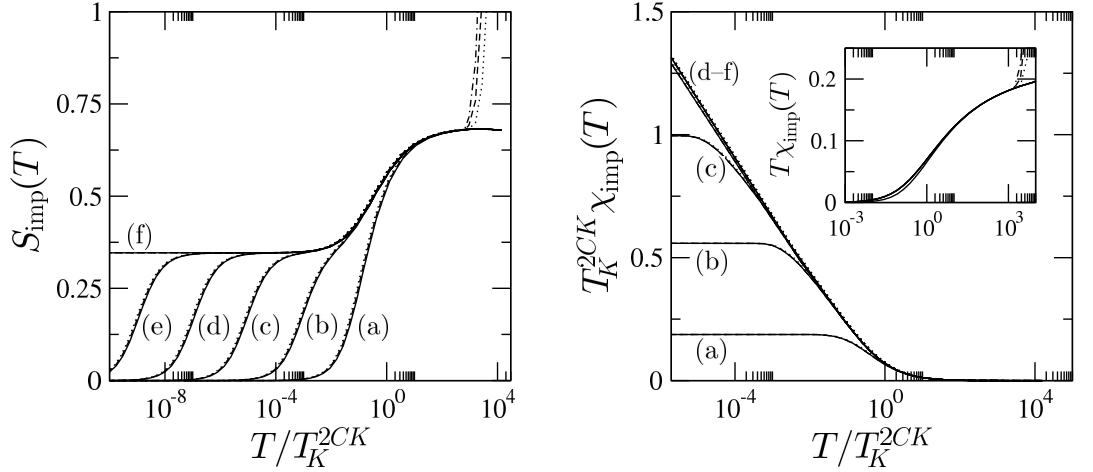


Figure 4.8: Thermodynamics for systems with common $\rho J = 0.15$ and $\rho J_{K,\text{eff}}^{N_c} = 0.1$ for $N_c = 1, 3, 5, 7$ (shown as the solid, dotted, dashed and dot-dashed lines, respectively). We vary the degree of channel asymmetry for each system via $\rho \delta_{\text{eff}}^{N_c} = \pm 5 \times 10^n$ and $n = -3, -4, -5, -6, -7$ [lines (a–e)] approaching the transition $\delta_{\text{eff}}^{N_c} = 0$ [lines (f)], which is the symmetric case studied above. The left panel shows $S_{\text{imp}}(T)$ while the right panel shows $T_K^{2CK} \chi_{\text{imp}}(T)$, both *vs.* T/T_K^{2CK} , where T_K^{2CK} is the Kondo scale for the symmetric case [lines (f)]. The inset to the right panel shows $T \chi_{\text{imp}}(T)$ *vs.* T/T_K^{2CK} .

resulting thermodynamics for odd chains below.

As shown in the preceding sections, at low temperatures the behaviour of odd chains is described by an effective single-spin 2CK model Eq. 4.9, with effective parameters $J_{K,\text{eff}}^{N_c}$ and $\delta_{\text{eff}}^{N_c}$, which we derived perturbatively and gave in Eq. 4.10. Thus, we expect the behaviour of chains of different length N_c to be fundamentally alike at the lowest temperatures.

For $N_c = 1$, the system is of course the standard single-spin 2CK model. In Fig. 4.8 we plot the thermodynamics for this case as the solid lines, showing systems with common $\rho J_K = 0.1$, and varying the degree of channel asymmetry through $\rho \delta = \pm 5 \times 10^n$ and $n = -3, -4, -5, -6, -7$ [lines (a–e)] approaching the transition $\delta = 0$ [line (f)], which is the mirror symmetric case studied above. In the left panel we show the entropy $S_{\text{imp}}(T)$, while in the right panel we show the susceptibility $T_K^{2CK} \chi_{\text{imp}}(T)$, both *vs.* T/T_K^{2CK} , where T_K^{2CK} is the Kondo scale for the symmetric case [line (f)].

To make a quantitative comparison with the canonical $N_c = 1$ case in the critical region approaching the transition, we use the same *effective* parameters $\rho J_{K,\text{eff}}^{N_c}$ and $\rho \delta_{\text{eff}}^{N_c}$ (as calculated through Eq. 4.10) for the other chains, and for each of the lines (a–f). Specifically, we have plotted $N_c = 3, 5, 7$ as the dotted, dashed and dot-dashed lines, respectively in Fig. 4.8.

We study first the variation of the entropy in the left panel of Fig. 4.8, and consider only the universal regime $T \ll J$. At the highest temperatures, systems

with different N_c obviously appear very different. However, viewed on lower energy scales, the same effective 2CK model Eq. 4.9 results in all cases. For $T \lesssim J$, all systems shown in Fig. 4.8 are described by the LM FP, with its characteristic [13,45] $\ln(2)$ entropy. For lines (a) — which correspond to $|\rho\delta_{\text{eff}}^{N_c}| = 5 \times 10^{-3}$ — the entropy drops to its ultimate $T = 0$ value, $S_{\text{imp}} = 0$, on the scale of T_K^{SC} for all N_c , as discussed above. As before, the quenched entropy itself is indicative of the stable SC:L FP in the $\rho\delta_{\text{eff}}^{N_c} > 0$ phase, or the SC:R FP in the $\rho\delta_{\text{eff}}^{N_c} < 0$ phase.

The degree of asymmetry decreases for lines (b–e), which progressively approach the transition, $\rho\delta_{\text{eff}}^{N_c} = 0$ [lines (f)], from either side. The presence of the unstable 2CK FP is clearly evident, with a characteristic [43–45] plateau at $S_{\text{imp}}(T) = \frac{1}{2} \ln(2)$. As systems approach the transition more closely, there is more persistent RG flow in the vicinity of the 2CK FP, with the result that the $\frac{1}{2} \ln(2)$ plateau is extended. As $|\rho\delta_{\text{eff}}^{N_c}|$ is decreased therefore, the systems in Fig. 4.8 ‘fold’ onto the 2CK scaling curve down to lower and lower temperatures. The crossover scale to the stable SC:L or SC:R FP thus depends strongly on $\rho\delta_{\text{eff}}^{N_c}$, and is seen to vanish as $\rho\delta_{\text{eff}}^{N_c} \rightarrow 0 \pm$. Precisely at the critical point (which is of course the symmetric case studied in Sec. 4.2.1) the characteristic residual entropy $S_{\text{imp}}(T) = \frac{1}{2} \ln(2)$ persists down to $T = 0$. The way in which the scale vanishes is characteristic of the transition itself, and we study it below.

First, however, we consider the right panel of Fig. 4.8, where we plot $T_K^{2CK} \chi_{\text{imp}}(T)$ vs. T/T_K^{2CK} . The 2CK scaling curve for the susceptibility is shown by lines (f), where $\rho\delta_{\text{eff}}^{N_c} = 0$. Due to numerical inaccuracies, it is difficult to establish the behaviour of $\chi_{\text{imp}}(T)$ for $T \lesssim 10^{-6} \times T_K^{2CK}$, and we find that over this temperature range, lines (d,e) [corresponding to $\rho\delta_{\text{eff}}^{N_c} = \pm 5 \times 10^{-6}$ and $\pm 5 \times 10^{-7}$] are essentially indistinguishable from the symmetric case [line (f)]. However, lines (a–c) clearly show a departure from the 2CK scaling curve on a temperature scale $T \sim T_K^{SC}$, and can be seen to plateau to a constant value. Indeed, the ultimate $T = 0$ value reached is also related to this scale, $T_K^{2CK} \chi_{\text{imp}}(T = 0) \sim 1/T_K^{SC}$, and therefore is consistent with the chain spin being fully quenched on the lowest temperature scales [13,45].

The behaviour of the magnetic susceptibility in the vicinity of the transition is thus characterized by $T_K^{2CK} \chi_{\text{imp}}(T) \sim a \ln(T_K^{2CK}/T)$ for $T \gg T_K^{SC}$, but by contrast $T_K^{SC} \chi_{\text{imp}}(T) \sim b$ for $T \ll T_K^{SC}$, with a and b constants $\mathcal{O}(1)$. In either case however, $T \chi_{\text{imp}}(T) \simeq 0$ for $T \ll T_K^{2CK}$, as shown explicitly in the inset to Fig. 4.8. Interestingly therefore, as the transition is approached, there is no sign of a vanishing T_K^{SC} scale in the behaviour of $T \chi_{\text{imp}}(T)$, although the form of the curve is characteristic of the flow to the 2CK FP (see Fig. 4.3) rather than the SC FP (shown in Fig. 4.7).

That all odd chains share the same behaviour in the critical region close to the point of mirror symmetry further demonstrates that such systems can be understood in terms of the well-known behaviour of the single-spin channel-anisotropic 2CK model. The low-energy Kondo scale T_K^{SC} is known [42, 45, 46, 124] to decay in a

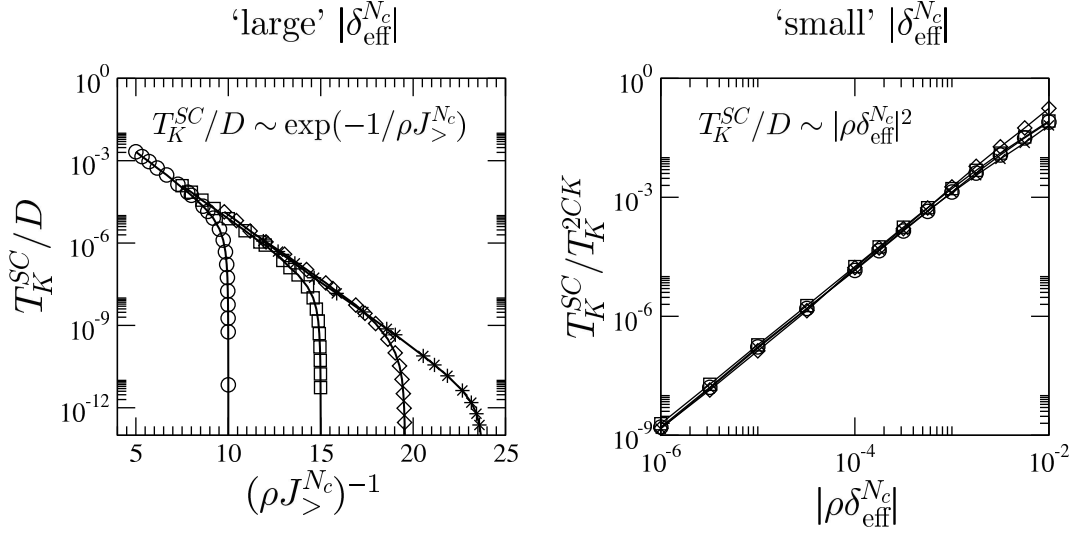


Figure 4.9: Variation of the Kondo scale T_K^{SC} with channel asymmetry $\delta_{\text{eff}}^{N_c}$. Shown for odd chains $N_c = 1, 3, 5, 7$ (using circles, squares, diamonds and stars, respectively), with common fixed $\rho J_K = 0.1$ and $\rho J = 0.15$. In the left panel we consider the behaviour away from the transition which arises for ‘large’ $|\delta_{\text{eff}}^{N_c}|$, and plot T_K^{SC}/D vs. $(\rho J_{>}^{N_c})^{-1}$ with $J_{>}^{N_c} \equiv J_{K,\text{eff}}^{N_c} + |\delta_{\text{eff}}^{N_c}|$. The collapse to a common linear form confirms the poor man’s scaling result $T_K^{SC}/D \sim \exp(-1/\rho J_{>}^{N_c})$, and demonstrates the validity of the low-energy effective 2CK model. In the right panel we consider the ‘small’ $|\delta_{\text{eff}}^{N_c}|$ regime which is therefore close to the transition. Specifically, we plot T_K^{SC}/T_K^{2CK} vs. $|\delta_{\text{eff}}^{N_c}|$, and find that $T_K^{SC}/D \sim |\rho \delta_{\text{eff}}^{N_c}|^2$ for all odd chains approaching the symmetric limit $\delta_{\text{eff}}^{N_c} \rightarrow 0\pm$.

characteristic power-law fashion in the critical region of this model. Thus, from Fig. 4.8 we expect any odd chain to behave similarly. Indeed, when the same effective parameters $\rho J_{K,\text{eff}}^{N_c}$ and $\rho \delta_{\text{eff}}^{N_c}$ are used (as in Fig. 4.8), the physical behaviour for $N_c = 1, 3, 5, 7$ at low temperatures is essentially indistinguishable, and hence we expect

$$T_K^{SC} \xrightarrow{\delta \rightarrow 0\pm} \mathcal{A} |\delta_{\text{eff}}^{N_c}|^\nu \quad : \quad \nu = 2 \quad (4.19)$$

with critical exponent $\nu = 2$ and common amplitudes $\mathcal{A}$ on approaching $\delta_{\text{eff}}^{N_c}$ from either side, for any N_c .

In the right panel of Fig. 4.9 we examine the scale dependence on $|\delta_{\text{eff}}^{N_c}|$ explicitly for different N_c using NRG. We plot T_K^{SC}/T_K^{2CK} vs. $|\delta_{\text{eff}}^{N_c}|$ for odd chains with $N_c = 1, 3, 5, 7$ (shown with circles, squares, diamonds and stars, respectively) and for systems with common fixed $\rho J_K = 0.1$ and $\rho J = 0.15$. The common slope on the log-log plot of $\nu = 2$ agrees with the known critical exponent for the single-spin 2CK model [42, 45, 46, 124], and the collapse to a single line confirms that the amplitude $\mathcal{A}$ is also common for all odd N_c , as expected from Eq. 4.19.

We also consider in Fig. 4.9 the evolution of T_K^{SC} away from the transition, when $|\delta_{\text{eff}}^{N_c}|$ is large. The Kondo scale in this regime is expected to be described by the poor

man's scaling result, Eq. 4.12, which to second order gives $T_K^{SC}/D \sim \exp(-1/\rho J_{>}^{N_c})$, where $J_{>}^{N_c} \equiv J_{K,\text{eff}}^{N_c} + |\delta_{\text{eff}}^{N_c}|$. We plot T_K^{SC}/D (on a logarithmic scale) *vs.* $(\rho J_{>}^{N_c})^{-1}$ (on a linear scale) in the left panel of Fig. 4.9. For systems not close to the transition, the poor man's scaling result is expected to describe accurately the variation of T_K^{SC} , and this is indeed confirmed by the collapse to a common straight line for all odd N_c .

The left and right panels of Fig. 4.9 thus describe the limiting universal regimes for odd chains for dots. For 'large' $|\delta_{\text{eff}}^{N_c}|$, systems of any N_c are not close to the transition, and thus RG flow is not affected by the presence of the 2CK FP. By contrast, for 'small' $|\delta_{\text{eff}}^{N_c}|$, systems flow close to the 2CK FP before ultimately flowing to the stable SC:L or SC:R FPs. The departure from these limiting regimes depicted in Fig. 4.9 allows us to quantify more specifically where this crossover occurs. We find in all cases that evidence of the 2CK FP is first observed in the thermodynamics for $|\rho \delta_{\text{eff}}^{N_c}|^2 \approx T_K^{2CK}/D$, where T_K^{2CK} is the Kondo scale in the $\delta = 0$ symmetric case, as usual.

Finally, we comment briefly on the behaviour of even chains. The fact that the chain is coupled asymmetrically to the left and right leads is irrelevant here: for $T \lesssim J$, all states of an even chain are projected out apart from the lowest singlet state, which obviously decouples from the leads. Thus, there is no low-energy scale which depends on either J_{KL} or J_{KR} in the 'large' J regime⁴. The resulting physical behaviour is thus identical to that presented in the insets to Fig. 4.2, and we do not discuss it further here.

In the next section, we consider the dynamics for odd chains with $\delta \neq 0$, showing that distinct spectra for $D\rho_L^{N_c}(\omega)$ and $D\rho_R^{N_c}(\omega)$ arise, allowing to distinguish the SC:L and SC:R FPs.

4.3.2 Dynamics

In the previous section, we considered the thermodynamics of odd chains, coupled asymmetrically to two leads. We consider the same systems here, focusing now on the spectra $D\rho_L^{N_c}(\omega)$ and $D\rho_R^{N_c}(\omega)$ (see Sec. 4.2.2). In mirror-symmetric systems, $D\rho_L^{N_c}(\omega) = D\rho_R^{N_c}(\omega)$, but when this symmetry is broken by distinct exchange couplings $J_{KL} \neq J_{KR}$ as considered here, one expects the spectra to be different, since they reflect spin-scattering processes in different leads.

We will study the $\delta > 0$ case only here, but note that $D\rho_L^{N_c}(\omega)$ for a system with a given value of δ is of course identical to $D\rho_R^{N_c}(\omega)$ using $-\delta$.

We consider first the inset to Fig. 4.10, where we show the $T = 0$ spectrum $D\rho_L^{N_c}(\omega)$ *vs.* ω/T_K^{SC} for odd chains ($N_c = 1, 3, 5, 7$) with common $\rho J_{K,\text{eff}}^{N_c} = 0.1$,

⁴In fact, we will see in the next chapter that this situation is markedly different when $J \ll T_K^{SC}$, where we show that the terminal spins undergo a standard 1CK effect with their attached lead, while the rest of the chain decouples.

$\rho J = 0.15$ and $\rho \delta_{\text{eff}}^{N_c} = +0.05$. The systems are thus well away from the mirror-symmetric 2CK critical point of the model (see Secs. 4.2.1 and 4.3.1). The collapse to a single universal curve is expected from the discussion of the previous section, where we showed from the thermodynamics that all systems away from the transition for any odd chain length N_c flow at low temperatures/energies from the LM FP to the SC:L FP (for $\delta > 0$ as considered here). The effective 1CK quenching of the lowest chain doublet by strong-coupling to the left lead is thus expected to be characteristic at low-frequencies of the standard *single*-channel Kondo effect. This is confirmed by the precise agreement with the circles in the inset, which represent the scaling spectrum $\pi \Gamma D(\omega)$ for the single-impurity, single-channel Anderson model (see Sec. 3.6.1). That $\pi \Gamma D(\omega = 0) = D \rho_L^{N_c}(\omega = 0) = 1$ is a consequence of the Friedel sum rule [8] for the Anderson model in the singly-occupied Kondo regime.

By contrast, the spectrum $D \rho_R^{N_c}(\omega) \simeq 0$ for all frequencies (not plotted), since the right lead flows under renormalization to *weak*-coupling. In particular, for $|\omega| \ll |\delta_{\text{eff}}^{N_c}|^2$, we find $D \rho_R^{N_c}(\omega) = 0$ away from the transition.

In the main panel of Fig. 4.10 we plot $D \rho_L^{N_c}(\omega)$ [solid lines] and $D \rho_R^{N_c}(\omega)$ [dashed lines] *vs.* ω/T_K^{2CK} , again using $\rho J_{K,\text{eff}}^{N_c} = 0.1$ and $\rho J = 0.15$ for all $N_c = 1, 3, 5, 7$, but now reducing the degree of channel-asymmetry via $\rho \delta_{\text{eff}}^{N_c} = +5 \times 10^n$ where $n = -3, -4, -5, -6, -7$ [lines (a–e)], which progressively approach the transition $\delta_{\text{eff}}^{N_c} = 0$ [dotted lines (f)], and thus correspond to the same systems as plotted for the thermodynamics in Fig. 4.8. The frequency axis is rescaled in terms of the 2CK scale T_K^{2CK} at the transition itself (lines (f) thus corresponding to the 2CK scaling spectrum). Importantly, we show that for each case (a–f), the low- ω behaviour is essentially the same for all odd chains. Again, this is expected from the mapping of all such systems onto the same effective single-spin channel-anisotropic 2CK model, Eq. 4.9. Using the same effective parameters $\rho J_{K,\text{eff}}^{N_c}$ and $\rho \delta_{\text{eff}}^{N_c}$, and rescaling in terms of the T_K^{2CK} scale yields universal scaling behaviour in the vicinity of the transition, as shown in Fig. 4.10.

At the Fermi level $\omega = 0$, we find that $D \rho_L^{N_c}(\omega = 0) = 1$ for each of the solid lines (a–e) and for all odd chains. This is physically natural, since the lowest doublet state of the chain is fully quenched by the left lead, and hence we expect the unitarity limit to be satisfied, characterizing [8] as it does RG flow to strong-coupling with the left lead. At $\omega = 0$, the right lead is completely decoupled and plays no role, as exemplified by the dashed lines (a–e), where $D \rho_R^{N_c}(\omega = 0) = 0$.

However, close to the transition, RG flow in the vicinity of the 2CK FP strongly affects the behaviour of the spectra at *finite* frequencies, and this is manifest in both $D \rho_L^{N_c}(\omega)$ and $D \rho_R^{N_c}(\omega)$. In particular, a plateau at $D \rho_\alpha^{N_c}(\omega) = \frac{1}{2}$ is clearly observed for both $\alpha = L$ and R in lines (d,e) over the frequency range $T_K^{SC} \ll |\omega| \ll T_K^{2CK}$. As T_K^{SC} vanishes as the transition is approached, the length of the plateau increases, and so we naturally recover $D \rho_\alpha^{N_c}(\omega = 0) = \frac{1}{2}$ in the mirror symmetric case [lines (f)].

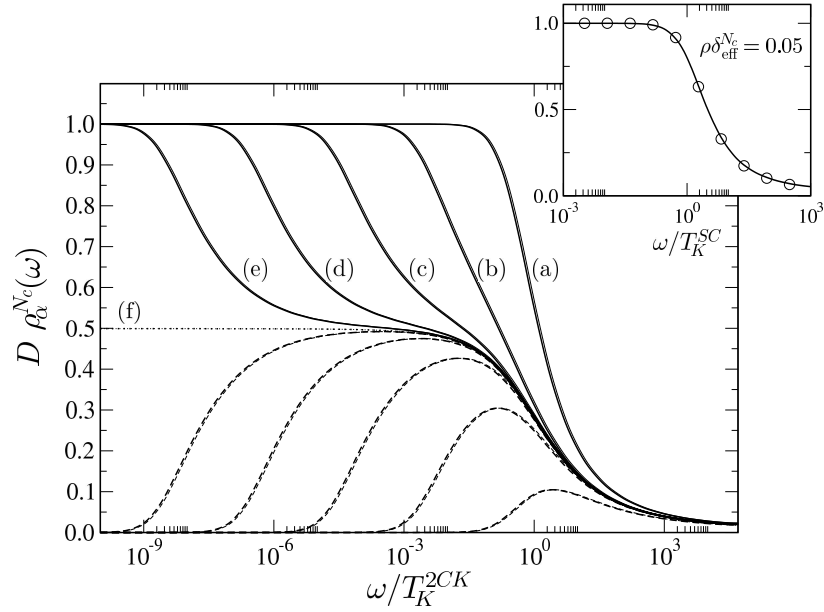


Figure 4.10: $T = 0$ spectrum $D \rho_L^{N_c}(\omega)$ [solid lines] and $D \rho_R^{N_c}(\omega)$ [dashed lines] vs. ω/T_K^{2CK} . As in Fig. 4.8, we use the same $\rho J_{K,\text{eff}}^{N_c} = 0.1$ and $\rho J = 0.15$ for all $N_c = 1, 3, 5, 7$, varying $\rho \delta_{\text{eff}}^{N_c} = +5 \times 10^n$ and $n = -3, -4, -5, -6, -7$ [lines (a–e)] approaching the transition $\delta_{\text{eff}}^{N_c} = 0$ [dotted lines (f)]. The data are rescaled in terms of the 2CK scale in the symmetric case, and as such represent the universal scaling behaviour close to the transition. The inset shows $D \rho_L^{N_c}(\omega)$ away from the transition ($\rho \delta_{\text{eff}}^{N_c} = +0.05$), rescaled in terms of T/T_K^{SC} . The circles show the universal scaling spectrum for the single impurity Anderson model $\pi \Gamma D(\omega)$.

Lines (a,b) are much further from the transition ($\rho \delta_{\text{eff}}^{N_c} = +5 \times 10^{-3}$ and $+5 \times 10^{-4}$ respectively), and correspond to the crossover region where evidence of the 2CK FP is first observed. While there is no plateau at $D \rho_\alpha^{N_c}(\omega) = \frac{1}{2}$ in either case, the shape of these spectra are in fact still affected by the presence of the 2CK FP, and the incipient RG flow in its vicinity. In particular the significant spectral density $D \rho_R^{N_c}(\omega)$ at intermediate frequencies is in stark contrast to the behaviour well away from the transition, where $D \rho_R^{N_c}(\omega) \simeq 0$ for all frequencies, as discussed above.

Thus, for any odd chain, the spectra $D \rho_L^{N_c}(\omega)$ and $D \rho_R^{N_c}(\omega)$ exhibit behaviour characteristic of either the strong-coupling or weak-coupling FPs of a *single*-channel model at $\omega = 0$, but the inherent two-channel nature of the problem is clearly evident at *finite* frequencies close to the point of mirror symmetry. Indeed, for $\delta = 0$ itself [lines (f)], the 2CK FP controls the behaviour of the spectrum on all frequency scales.

In the preceding sections, we have tried to emphasize the universal properties of chains of quantum dots, showing in particular that the behaviour of all odd chains at low temperatures/energies can be understood in terms of the behaviour of the single-spin 2CK model. By contrast, even chains exhibit no such behaviour, since on temperature/energy scales $\mathcal{O}(J)$, all but the lowest singlet state of the chains is

projected out. The observed behaviour at lower temperatures is then the same as if the chain was simply removed from the system completely. As such, the behaviour of even chains corresponds directly to the behaviour of the two-impurity Kondo model [36, 37, 109] in the “large” interdot coupling regime.

In the next section we go on to consider the case when the interdot exchange couplings J are somewhat smaller than the dot-lead couplings J_K .

4.4 Smaller interdot couplings

In Sec. 4.1.2 we derived perturbatively an effective low-energy model of 2CK form for systems of chains of dots in the regime where the interdot exchange coupling J is much larger than the dot-lead couplings J_K . Here we briefly examine the opposite limit: $J/J_K \ll 1$. Clearly for $J = 0$, markedly different physics results, since the dots are completely decoupled from each other. Thus, the system is wholly equivalent to two separated *single*-channel Kondo models (dot 1 connected to the left lead, and dot N_c connected to the right lead), plus $(N_c - 2)$ free spins. As the temperature is lowered, the terminal dots obviously undergo the Kondo effect below a characteristic temperature $T_{K,\alpha}^{1CK}$ which depends on the dot-lead coupling $J_{K\alpha}$ for lead $\alpha = L, R$. The interior spins of course remain free down to $T = 0$.

But what happens for small but finite interdot coupling, J ? This is the situation considered in detail in the next chapter, but here we briefly examine the case where the interdot coupling is smaller than the dot-lead couplings, but is still much greater than the single-channel Kondo scales $T_{K,L}^{1CK}$ and $T_{K,R}^{1CK}$.

The perturbative analysis of Sec. 4.1.2 is clearly invalid here, but on heuristic grounds, one might still expect the underlying FPs to be the same as those studied above. In particular, for odd- N_c , the NRG Hamiltonian H_N (see Sec. 3.3) always comprises an odd number of orbitals for any given N (the total number of orbitals being $2N + N_c$). The lowest state of such a chain is always a doublet, even for $J \ll J_K$. The question then is: what is the effective coupling between this state and the rest of the lead states? If it is antiferromagnetic, 2CK physics should again result on the lowest temperature/energy scales. A similar argument can be applied to the even chains, where the resulting singlet state might be expected to decouple from the rest of the system.

In this case, the essential physics would be unchanged as J is reduced, although the Kondo scales themselves cannot of course be described by Eqs. 4.10–4.12, as these were derived perturbatively in the $J/J_K \gg 1$ regime. In Fig. 4.11 we plot the entropy $S_{\text{imp}}(T)/\ln(2)$ vs. T/D for systems with $\rho J_K = 0.075$, $\rho J = 0.005$ and $\rho\delta = 0$ (noting that $J \approx 1000 \times T_K^{1CK}$, and so is in this sense still large in comparison to the universal single-channel scales). In the left panel we show odd chains (solid, dotted, dashed and dot-dashed lines correspond to $N_c = 1, 3, 5, 7$) while the right

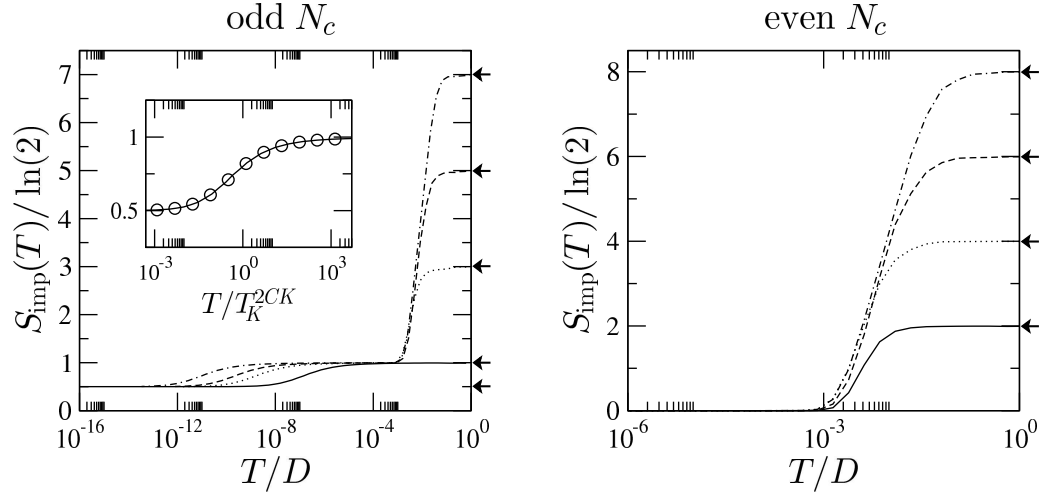


Figure 4.11: Entropy $S_{\text{imp}}(T)/\ln(2)$ vs. T/D for mirror symmetric systems with $\rho J_K = 0.075$, $\rho J = 0.005$ and $\rho \delta = 0$. The left panel shows odd length chains ($N_c = 1, 3, 5, 7$ correspond to the solid, dotted, dashed and dot-dashed lines respectively), while the right panel shows even length chains (the solid, dotted, dashed and dot-dashed lines here refer to $N_c = 2, 4, 6, 8$). The inset to the left panel shows the universality arising when odd chains are rescaled in terms of T/T_K^{2CK} ; there is apparently no low-energy scale for even N_c , and therefore no such universality.

panel shows even chains (solid, dotted, dashed and dot-dashed lines now referring to $N_c = 2, 4, 6, 8$).

In both panels, the behaviour for $T > J$ is that of N_c free spins — hence the entropy of $S_{\text{imp}}(T) = N_c \ln(2)$. While J is small, it is nonetheless a *non-universal* scale; for $T \lesssim J$ the entropy drops to $\ln(2)$ for the odd chains (characteristic of the LM FP) and zero for the even chains (characteristic of the DS FP). Importantly, the residual local moment for the odd chains is overscreened by the conduction electrons of both leads (to which the chain is symmetrically coupled for $\delta = 0$), and the 2CK FP is reached below T_K^{2CK} in all cases. The inset shows the low-temperature behaviour rescaled in terms of T/T_K^{2CK} , with the collapse to the universal 2CK scaling curve (circles) confirming that the effective low-energy description is indeed that of a single-spin 2CK model, even though the systems shown are outside of the regime of validity for Eq. 4.9.

However, qualitatively distinct low-temperature physics might arise if the inter-dot coupling is *less* than the single-channel Kondo scales $T_{K,\alpha}^{1CK}$. In this regime, the preferential formation of a Kondo singlet between the terminal dots and their attached leads is expected. This is the case considered explicitly in the next chapter.

4.5 Summary

In this chapter, we have considered a general class of models in which a chain of N_c quantum dots is coupled to two leads (see Eq. 4.1 and Fig. 4.1). Specifically, we model the system as a Heisenberg chain of *spins*, with an interdot exchange-coupling J . The terminal dots of the chain are each coupled to their own lead, with $J_{K\alpha}$ the exchange coupling to the $\alpha = L, R$ lead (see Fig. 4.1).

Two distinct regimes arise in the model, corresponding to “large” and “small” interdot coupling strengths. In this chapter we have considered chiefly the large J limit, where a low-energy effective model can be derived perturbatively. We showed in Sec. 4.1.2 that the higher lying chain eigenstates become thermally inaccessible at low temperatures $T \ll J$, and so only the ground chain state need be retained in order to describe the physical behaviour of the system on low temperature/energy scales.

The lowest state of an odd-length chain is a *doublet* state (see Sec. 4.1.1). In Sec. 4.1.2 we showed that an effective *antiferromagnetic* Kondo coupling arises between this doublet state and the leads (see Eq. 4.10). An effective model (Eq. 4.9) of 2CK form thus results.

In Sec. 4.2, we considered explicitly the mirror-symmetric case in which the bare dot-lead couplings are equal. This symmetry is of course respected in the low-energy effective model, and so 2CK physics is expected to dominate the behaviour of the system on the lowest temperature/energy scales for all odd chains. Using NRG, we calculated thermodynamic properties of such systems in Sec. 4.2.1, and showed that the 2CK FP does indeed describe the behaviour of all systems for temperatures below the Kondo scale T_K^{2CK} , as is evident in the characteristic residual entropy $S_{\text{imp}} = \frac{1}{2} \ln(2)$ and a logarithmic divergence in the uniform spin susceptibility $\chi_{\text{imp}}(T) \sim \ln(1/T)$.

The effective coupling of the ground chain doublet to the leads in the low-energy model Eq. 4.9 depends on the bare dot-lead coupling J_K and on the chain length N_c , as given by Eq. 4.10. From perturbative scaling, it can then be shown that the underlying Kondo scale, T_K^{2CK} , must also therefore depend on these parameters. The functional dependence of T_K^{2CK} on J_K and N_c derived in Eq. 4.11 is confirmed directly from the thermodynamics calculated with NRG, as shown in Fig. 4.4. Indeed, universality is expected to arise at low temperatures on rescaling in terms of T_K^{2CK} , and this is shown in Fig. 4.3, thus demonstrating the mapping of the full chain model Eq. 4.1 onto the effective single-spin 2CK model Eq. 4.9.

Dynamical results for these systems is also presented in Sec. 4.2.2, where we show that the $T = 0$ spectral density $D \rho^{N_c}(\omega)$ at low- ω is characteristic of the standard single-spin 2CK model (which we discussed in Sec. 3.6.3). In particular, the scaling spectrum is given (which is of course common for all odd N_c), and both the high- ω

and low- ω asymptotic behaviour is established, as given in Eqs. 4.17 and 4.18. In all cases, at the Fermi level $\omega = 0$ the spectrum reaches *half* the unitarity limit.

In Sec. 4.3, we go on to consider the case where the mirror symmetry is broken. The 2CK FP is the critical point of the channel-anisotropic 2CK model, and so in general a strong-coupling Fermi-liquid state is formed on the lowest temperature/energy scales for the single-spin model. We show that the same behaviour results for all odd chains, and again demonstrate the universality arising in such systems on rescaling in terms of an effective *single*-channel Kondo scale.

When the degree of asymmetry is reduced, systems with any N_c flow near the 2CK FP. As with the $N_c = 1$ case, a transition is found to occur between phases where the residual chain spin- $\frac{1}{2}$ doublet state is exactly screened by either the left lead (for $J_{KL} > J_{KR}$) or the right lead (for $J_{KR} > J_{KL}$). We study both thermodynamics (in Sec. 4.3.1) and dynamics (see Sec. 4.3.2) as the transition is crossed.

By contrast, the lowest state of an even chain is a spin-*singlet* (see Sec. 4.1.1), which simply decouples from the rest of the system for $T \ll J$. We comment that this situation is essentially equivalent to the large- J regime of the two-impurity Kondo (2IK) model.

Throughout this chapter, we have focused on the universality which arises in such chain systems on low temperature/energy scales. In particular, we have shown that the behaviour of all odd chains in the large J limit can be understood in terms of an effective single-spin 2CK model, while even chains are characteristic of the 2IK model.

In the next chapter, we examine the behaviour of Eq. 4.1 in the opposite limit, where the interdot couplings are small.

CHAPTER 5

Chains with weak interdot coupling

In the previous chapter, we considered a generic class of models in which a chain of quantum dots is coupled to two metallic leads, as described by Eq. 4.1 and illustrated in Fig. 4.1. We studied the behaviour of such systems in the “large” interdot coupling regime, where a low-energy effective model can be simply derived by projecting the full Hamiltonian onto the lowest chain eigenstate. In this regime, we showed that an effective single-spin 2CK model results for all odd chains. We went on to study the full model directly with NRG and confirmed this physical picture. For even chains by contrast, a local singlet state forms at low temperatures, which decouples from the leads.

As the interdot coupling J is reduced, the perturbative results obtained in Sec. 4.1 of the previous chapter obviously break down, and so the behaviour of the full system cannot be understood in terms of this simple prescription. In Sec. 4.4 we used NRG to show that even for $J = \frac{1}{15} \times J_K$, the low-temperature/energy behaviour of both even and odd chains is fundamentally the same as that studied in the large J limit — despite the fact that the perturbatively derived effective model is clearly inapplicable here.

The obvious question is: what happens as J is decreased still further? Clearly for $J = 0$, the physics is fundamentally different, since the terminal dots must undergo the standard single-channel Kondo effect with their attached metallic lead below T_K^{1CK} , while the other dots of the chain remain free down to $T = 0$.

Indeed, the paradigmatic ‘two-impurity’ Kondo (2IK) model is simply the $N_c = 2$ case of Eq. 4.1, and has been widely studied (*eg.* in Refs. [36, 37, 78, 109, 112, 113]). It is the simplest case in which the tendency of the dots to form a local singlet state driven by the antiferromagnetic interdot exchange J competes with the formation of two separated single-channel Kondo states, and a quantum phase transition is found [37] at very small but *finite* $J \sim T_K^{1CK}$. In Sec. 5.2, we show that the behaviour of all even chains in the small J regime can be understood in terms of the 2IK

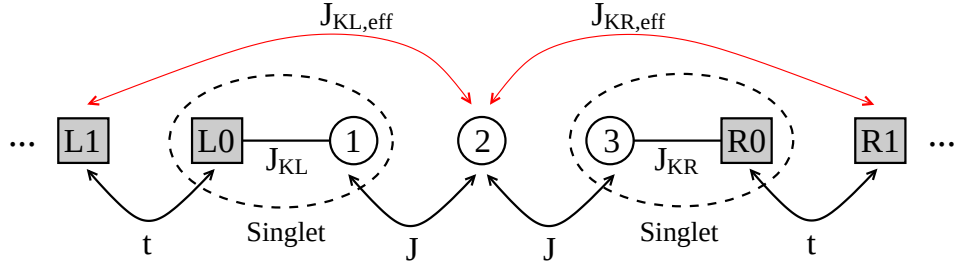


Figure 5.1: Illustration of the $N_c = 3$ case, where J_{KL} and J_{KR} are both $\gg J$. Dot 1 and the ‘L0’-orbital of the left Wilson chain form a singlet state, as do dot 3 and the ‘R0’ orbital of the right Wilson chain. However, there is a residual antiferromagnetic effective coupling between the central dot 2 and the ‘L1’ and ‘R1’ orbitals, which ultimately drives the system to the 2CK FP below T_K^{2CK} for mirror-symmetric systems.

model. We also provide physical arguments which indicate that for any even N_c , the transition itself is characteristic of that found in a channel-anisotropic single-spin 2CK model. We go on to confirm this physical picture directly with NRG.

In the next section however, we examine the case of odd chains, employing simple physical arguments together with NRG to show that 2CK physics ubiquitously arises in these systems for any finite positive interdot coupling J .

5.1 Odd chains

In this section, we consider the generic behaviour of odd chains of spins coupled to two leads (see Fig. 4.1 and Eq. 4.1); focusing specifically on mirror-symmetric systems in the regime where the interdot coupling are small, but the dot-lead couplings are large. In Sec. 5.1.1 we develop an effective low-energy model for the behaviour of the $N_c = 3$ case, and then we go on to study other odd chains directly with NRG, emphasizing the universal behaviour that results.

We first note that recent work in Ref. [85] describes a variant of the $N_c = 3$ case in which dots 1 and 3 are also exchange-coupled to form a ring. The critical point of the $N_c = 2$ model mentioned above is found to be smoothly connected to the 2CK FP as a third dot is weakly coupled into the system [85]. Using NRG it is found [85] that all such systems are described by the 2CK FP on the lowest energy scales¹, as is consistent with our findings presented below.

¹We revisit this ring system in Chapter 6, and show that in fact the magnetic frustration inherent in the model also leads to a quantum phase transition as a function of interdot coupling.

5.1.1 Effective model and physical picture for the trimer

In this section, we examine explicitly the $N_c = 3$ case, and argue that 2CK physics is expected for any non-zero interdot coupling J (and as found from the numerical survey in Ref. [85]). In the following sections, we go on to consider the behaviour of other odd chains in the small J regime, and obtain a universal description of all such systems at low temperature using NRG.

The physical picture when J is much smaller than J_{KL} or J_{KR} is illustrated in Fig. 5.1, and discussed below. When $J_{KL} \gg J$, dot 1 and the ‘L0’-orbital of the left Wilson chain can be thought of as locking up into a singlet state, with the exchange coupling to dot 2 acting as a small perturbation. An effective coupling is then generated between dot 2 and the ‘L1’-orbital, mediated by this singlet state. A similar effect has been studied previously in the context of side-coupled quantum dots [74, 143–149], where it is found that dots not directly coupled to a lead can undergo a second-stage quenching driven by this residual coupling.

Here of course, dot 3 is also coupled to the right lead, and so for $J_{KR} \gg J$, it forms a singlet with the ‘R0’-orbital. An effective coupling between dot 2 and the ‘R1’-orbital results, and so at low temperatures the system is expected to behave like a standard single-spin 2CK model, with dot 2 coupled to two leads (each of which have their zero-orbital removed).

In the following, we formulate the above argument mathematically and confirm this physical picture. We also obtain an expression for the 2CK Kondo scale, which we go on to test with NRG in Sec. 5.1.2. The first step is to write the Hamiltonian Eq. 4.1 for $N_c = 3$ in its dimensionless linear chain form [12, 13] as used in the NRG (see Sec. 3.3, Eq. 3.13). We partition the Hamiltonian as $H_N = H_0 + H_1$, such that

$$\begin{aligned} H_0 &= \mathcal{J}_{KL} \hat{\mathbf{S}}_1 \cdot \hat{\mathbf{S}}_{L0} + \mathcal{J}_{KR} \hat{\mathbf{S}}_3 \cdot \hat{\mathbf{S}}_{R0} \\ H_1 &= \mathcal{J} \hat{\mathbf{S}}_2 \cdot (\hat{\mathbf{S}}_1 + \hat{\mathbf{S}}_3) + \sum_{\sigma, \alpha} \sum_{n=0}^{N-1} t_n \left(f_{\alpha n \sigma}^\dagger f_{\alpha(n+1)\sigma} + f_{\alpha(n+1)\sigma}^\dagger f_{\alpha n \sigma} \right) \end{aligned} \quad (5.1)$$

with $\mathcal{J}_{K\alpha} = 4\rho J_{K\alpha} \Lambda^{(N-1)/2} / (1 + \Lambda^{-1})$ the rescaled coupling to a given lead $\alpha = L, R$, $\mathcal{J} = 4\rho J \Lambda^{(N-1)/2} / (1 + \Lambda^{-1})$ the rescaled interdot coupling, and $t_n = \Lambda^{(N-1)/2} \Lambda^{-n/2} \xi_n$ the tunnel-coupling between lead orbitals, with ξ_n given [12] in Eq. 3.12. Λ is the NRG discretization parameter as usual.

The full Hamiltonian is then recovered in the $N \rightarrow \infty$ limit [12, 13], as described in Sec. 3.3, via

$$H = \lim_{N \rightarrow \infty} \left\{ \frac{1}{2} D (1 + \Lambda^{-1}) \Lambda^{-(N-1)/2} H_N \right\}. \quad (5.2)$$

We will consider now the limit of strong dot-lead coupling: $\mathcal{J}_{K\alpha} \gg \max(\mathcal{J}, t_n)$; so that H_0 in Eq. 5.1 favours the formation of a pair of singlet states between the terminal dots and the ‘0’-orbital of their attached lead. The ground state of H_0 thus

comprises a 1-‘L0’ singlet (which we will denote $|s; L\rangle$) and a 3-‘R1’ singlet (similarly denoted $|s; R\rangle$), as shown schematically in Fig. 5.1.

H_1 now acts as a small perturbation, and we project onto the states of H_0 using the unity operator for the reduced Hilbert space,

$$\hat{1}_s = |s; L\rangle\langle s; R| + |s; R\rangle\langle s; L|. \quad (5.3)$$

An effective Hamiltonian may be obtained using the Brillouin-Wigner perturbation expansion [122] of H_N . The first-order term $\hat{1}_s H_1 \hat{1}_s = \tilde{H}_L$ follows as

$$\tilde{H}_L = \sum_{\sigma, \alpha} \sum_{n=1}^{N-1} t_n \left(f_{\alpha n \sigma}^\dagger f_{\alpha(n+1)\sigma} + f_{\alpha(n+1)\sigma}^\dagger f_{\alpha n \sigma} \right), \quad (5.4)$$

with t_n given above. Eq. 5.4 thus corresponds to a pair of free conduction bands, with the ‘0’-orbital of each removed. The second-order term of the perturbative expansion of H_N contributes only potential scattering [13] in the problem, which we ignore here. An effective coupling between dot 2 and the ‘L1’ and ‘R1’ orbitals is generated only to *third*-order in H_1 , given explicitly [122] by

$$H_N^{\text{III}, \text{eff}} = \hat{1}_s H_1 (E_0 - H_0)^{-1} \hat{P} H_1 (E_0 - H_0)^{-1} \hat{P} H_1 \hat{1}_s \quad (5.5)$$

where $\hat{P} = \hat{1}_{\text{full}} - \hat{1}_s$ is a projection operator for the excited states of the system, and $E_0 = -\frac{3}{4}(\mathcal{J}_{KL} + \mathcal{J}_{KR})$ is the ground state energy of H_0 . Combining Eqs. 5.1, 5.3 and 5.5, and after rather lengthy manipulation, the effective Hamiltonian to third-order follows as

$$H_N^{\text{III}, \text{eff}} = \rho J_{KL, \text{eff}} \hat{\mathbf{S}}_2 \cdot \hat{\mathbf{S}}_{L1} + \rho J_{KR, \text{eff}} \hat{\mathbf{S}}_2 \cdot \hat{\mathbf{S}}_{R1}, \quad (5.6)$$

with the dimensionless effective coupling to the $\alpha = L, R$ lead given by

$$\rho J_{K\alpha, \text{eff}} = \left(\frac{20t_0^2 \mathcal{J}}{9\mathcal{J}_{K\alpha}^2} \right). \quad (5.7)$$

To this level of calculation, and neglecting RG irrelevant potential scattering terms, the overall effective model is then $H_N^{\text{eff}} = \tilde{H}_L + H_N^{\text{III}, \text{eff}}$, which describes the residual antiferromagnetic coupling between dot 2 and the ‘L1’ and ‘R1’ orbitals of a pair of leads (with dots 1 and 3 and lead orbitals ‘L0’ and ‘R0’ removed). This is a model of 2CK form — in particular, for mirror-symmetric systems $J_{KL} = J_{KR} \equiv J_K$ (which of course yields $J_{KL, \text{eff}} = J_{KR, \text{eff}} \equiv J_{K, \text{eff}}$ in the effective model), the 2CK FP should describe the system on the lowest energy scales. This is the regime we now consider explicitly.

The above analysis depends on the formation of a singlet state between the terminal dots and the ‘0’-orbitals of their attached leads, which is only valid in the strong

dot-lead coupling limit. However, we note that in the $J = 0$ limit, the model reduces to two, disconnected single-channel Kondo models, with an additional decoupled free spin on dot 2. The physics of this system is related simply to that of the canonical 1CK model: the spin- $\frac{1}{2}$ on dot 1 is exactly screened by antiferromagnetic coupling to its attached lead below a characteristic Kondo scale $T_K^{1CK}/D \sim \exp(-1/\rho J_K)$. Dot 1 and the ‘L0’-orbital of the left Wilson chain form a Kondo singlet, and are effectively removed from the system. Similarly, dot 3 forms a Kondo singlet with the ‘R0’-orbital of the right Wilson chain below T_K^{1CK} (and dot 2 of course remains free). Thus, for any antiferromagnetic J_K , the terminal dots always form Kondo singlet states with the ‘0’-orbitals of their attached lead on renormalization under progressive reduction of the temperature/energy scale in the case of $J = 0$.

Indeed, for $J \ll T_K^{1CK}$, the same physics is expected down to energy scales $\mathcal{O}(T_K^{1CK})$, and so any such system can be described at low temperatures in terms of singlet-locked 1-‘L0’ and 3-‘R0’ states, as illustrated in Fig. 5.1. While the ‘0’-orbitals are removed from the leads in $\tilde{H}_L$, a local Fermi-liquid description applies, and consequently the remaining states of each lead still act as a ‘bath’ of non-interacting conduction electrons [85] which compete to screen the spin on dot 2. This effective interaction is then described by Eqs. 5.6 and 5.7 for $T \sim T_K^{1CK}$.

In general, for $J \lesssim T_K^{1CK}$ an effective model of 2CK form must therefore arise at low-temperatures $T \sim T_K^{1CK}$:

$$H^{\text{eff}} = \tilde{H}_L + \tilde{J}_{K,\text{eff}} \hat{\mathbf{S}}_2 \cdot (\hat{\mathbf{S}}_{L1} + \hat{\mathbf{S}}_{R1}) \quad (5.8)$$

where $\tilde{J}_{K,\text{eff}}$ is the renormalized effective coupling from Eq. 5.7 at $T = T_K^{1CK}$. It is of course the formation of Kondo singlets at these temperatures (in which terminal dots and the ‘0’-orbitals of their attached leads become strong-coupled under renormalization), that generates the effective model Eq. 5.8. 2CK physics is thus expected below T_K^{2CK} , given [40] from perturbative scaling (to third order) as

$$T_K^{2CK}/D \sim \rho \tilde{J}_{K,\text{eff}} \exp(-1/\rho \tilde{J}_{K,\text{eff}}), \quad (5.9)$$

The important question now is: how does this residual effective coupling, $\tilde{J}_{K,\text{eff}}$, flow under renormalization?

To answer this, we recall first that the effective temperature in the NRG is related to the iteration number via $T \sim \Lambda^{-N/2}$ (see Eq. 3.53 and Refs. [12, 13]). We also note that the operators for the Wilson chain orbitals also scale with iteration number. In particular, operators for the ‘0’-orbital of the Wilson chain can be shown [12, 13] to scale as $f_{\alpha 0\sigma} \sim \Lambda^{-N/4}$. Thus $\mathcal{J}_K \sim \Lambda^{-N/2}$, since the dot-lead exchange coupling is associated with a *pair* of ‘0’-orbital fermion operators. The key result is that the renormalized dot-lead coupling $\tilde{\mathcal{J}}_K \sim T_K^{1CK}$ for $T \sim T_K^{1CK}$. By contrast, the

interdot coupling $\mathcal{J}$ is not associated with any Wilson chain operators, and hence does *not* get renormalized with N .

As was pointed out in Ref. [34] in the context of the gapped Anderson model, once the ‘0’-orbital of a Wilson chain has been frozen out (*eg.* by formation of a Kondo singlet with an attached dot), the ‘1’-orbital operators scale as $f_{\alpha 1\sigma} \sim \Lambda^{-N/4}$. Thus the renormalized tunnel-coupling $\tilde{t}_0 \sim \Lambda^{-N/4}$, so that for $T \sim T_K^{1CK}$, the quantity $\tilde{t}_0^2/\tilde{\mathcal{J}}_K$ is $\mathcal{O}(1)$.

Overall then, from Eq. 5.7, the renormalized coupling $\rho\tilde{\mathcal{J}}_{K,\text{eff}}$ at $T \sim T_K^{1CK}$ can be estimated to have the functional dependence

$$\rho\tilde{\mathcal{J}}_{K,\text{eff}} \sim \frac{J}{T_K^{1CK}}. \quad (5.10)$$

In the next section, we confirm the above physical picture using NRG for the full model Eq. 4.1 for $N_c = 3$ in the regime $J < T_K^{1CK}$. In particular we show that 2CK physics *does* result at low temperatures in mirror-symmetric systems, as reflected in both thermodynamics and dynamics. We also examine the variation of the 2CK scale, comparing it to the perturbative prediction using Eq. 5.10 in Eq. 5.9, above. Finally, we consider larger odd chains, demonstrating that similar behaviour results in all cases.

5.1.2 NRG results for other odd chains

In this section, we consider odd chains, symmetrically coupled to two leads, with “small” interdot exchange couplings $J \ll J_K$. The physical picture discussed above for the trimer case ($N_c = 3$) indicates that for $J \lesssim T_K^{1CK}$, two-channel behaviour should again be accessible. Here we examine the full model Eq. 4.1 using NRG, considering the $N_c = 3$ case as well as larger chains with $N_c = 5$ and 7. We show that all such systems are described by the 2CK FP on the lowest energy/temperature scales.

We consider first the crossover case, where neither the large- J analysis of the previous chapter, nor the effective model Eq. 5.8 are valid. Of course, the NRG is a non-perturbative approach, and so accurate results may still be obtained in this regime. In Fig. 5.2 we plot the entropy $S_{\text{imp}}(T)$ *vs.* T/D for $N_c = 3, 5, 7$ (shown in the left, middle and right panels, respectively). In each case we use a common fixed $\rho J_K = 0.1$ (and consider explicitly mirror-symmetric systems: $\rho\delta = 0$), varying the interdot coupling via $\rho J = \lambda T_K^{1CK}$, with $\lambda = 10^n$ and $n = 4, 3, 2, 1$ (solid, dotted, dashed and dot-dashed lines). $T_K^{1CK}/D = 10^{-5}$ is the single-channel Kondo scale obtained when $J = 0$, as indicated with the vertical arrow above each panel. At ‘high’ (non-universal) temperature scales $T > J$, each system is described essentially in terms of N_c free, decoupled spins- $\frac{1}{2}$, and hence $S_{\text{imp}} = N_c \ln(2)$ results (this is

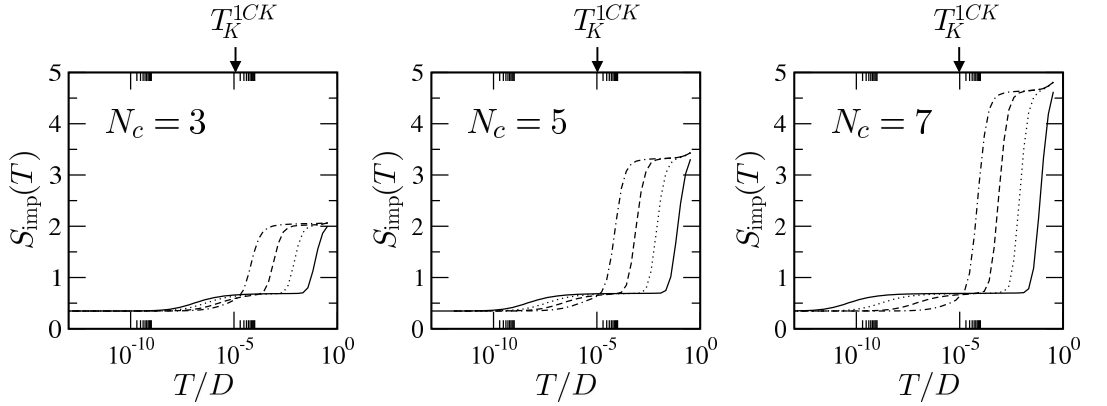


Figure 5.2: Entropy $S_{\text{imp}}(T)$ vs. T/D for $N_c = 3$ (left panel), 5 (middle panel) and 7 (right panel). Shown for common $\rho J_K = 0.1$ and (mirror-symmetric) $\rho\delta = 0$, varying $\rho J = \lambda T_K^{1CK}$ with $\lambda = 10^n$ and $n = 4, 3, 2, 1$ (solid, dotted, dashed and dot-dashed lines). T_K^{1CK} is the single-channel Kondo scale obtained when $J = 0$ (indicated with the vertical arrow).

the FO FP [13], as discussed in Chapter 4). On the scale of J for chains of any length, the entropy drops to $S_{\text{imp}} = \ln(2)$, characteristic of the LM FP (the magnetic susceptibility (not shown) follows the Curie law, confirming this [8]), which is reached when all but the lowest chain doublet is projected out.

Finally, on a scale T_K^{2CK} , the residual antiferromagnetic coupling between this chain doublet state and the leads drives each system to the 2CK FP, with its characteristic [43–45] entropy $S_{\text{imp}} = \frac{1}{2} \ln(2)$. This is the expected behaviour for chains with *large* interdot couplings, as discussed in Chapter 4. Indeed, considering first the solid lines in each panel (corresponding to $\rho J = 10^4 \times T_K^{1CK}$), the 2CK scale T_K^{2CK} is seen to decrease exponentially going from $N_c = 3 \rightarrow 5 \rightarrow 7$. This is explicable since the effective coupling of the lowest chain doublet state decreases with N_c (see Eq. 4.10), indicating therefore that such systems can indeed be thought of as being in the “large” J regime.

However, as the interdot couplings are reduced further (considering the progression $n = 4, 3, 2$), the scale for the ultimate flow to the 2CK FP (embodied in T_K^{2CK}) is seen to *increase*, so that in particular for $\rho J = 10 \times T_K^{1CK}$ (dot-dashed lines), RG flow in the vicinity of the LM FP is only barely observed in the entropy. Only a slight shoulder at $S_{\text{imp}} = \ln(2)$ is evident, with the 2CK FP being reached almost directly from the FO FP for each of $N_c = 3, 5, 7$.

The question of interest in this chapter is: what happens as the interdot couplings are reduced still further? The discussion of Sec. 5.1.1 above indicates that for $N_c = 3$, 2CK physics should again be observed for $J \lesssim T_K^{1CK}$. We consider this case explicitly in Fig. 5.3, where we again show the entropy $S_{\text{imp}}(T)$, but now vs. T/T_K^{1CK} , to demonstrate the universal behaviour in this regime. We plot chains of size $N_c = 3, 5, 7$ (solid, dotted and dashed lines) with common $\rho J_K = 0.1$, varying

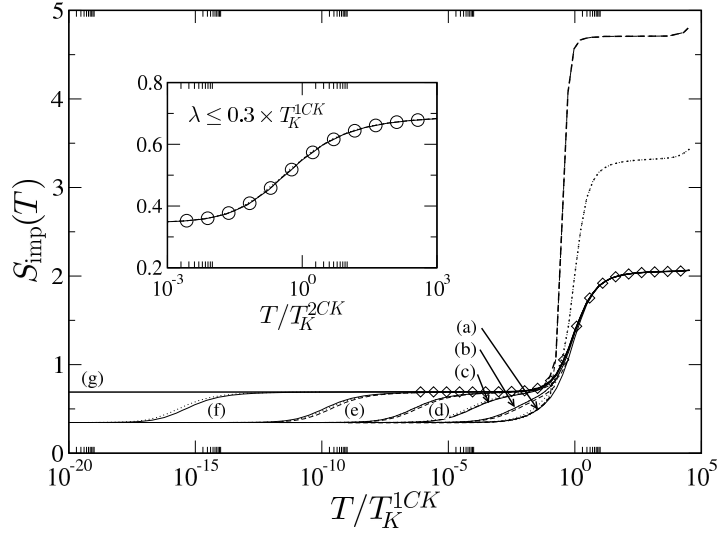


Figure 5.3: Entropy $S_{\text{imp}}(T)$ vs. T/T_K^{1CK} for $N_c = 3, 5, 7$ (solid, dotted and dashed lines) with common $\rho J_K = 0.1$ and (mirror-symmetric) $\rho\delta = 0$ (as in Fig. 5.2), but now varying $\rho J = \lambda T_K^{1CK}$ with $\lambda = 10^{-n/5}$ and $n = 0, 1, 2, 3, 4, 5$ [lines (a–f)], progressively approaching the $\rho J = 0$ limit [line (g)]. The diamond points are for $S_{\text{imp}}^{J=0}(T) = 2 \times S_{\text{imp}}^{1CK}(T) + \ln(2)$, corresponding to the expected behaviour for $J = 0$ in the $N_c = 3$ case. The inset shows the low-temperature behaviour rescaled in terms of T/T_K^{2CK} for $\lambda \leq 0.3 \times T_K^{1CK}$, showing the universal collapse onto the standard single-spin 2CK scaling curve (circles).

the interdot couplings via $\rho J = \lambda T_K^{1CK}$ as before, but now with $\lambda = 10^{-n/5}$ and $n = 0, 1, 2, 3, 4, 5, 6$ [lines (a–g)], progressively approaching the $\rho J = 0$ limit. Thus, the interdot couplings may be considered “small”, with $J \leq T_K^{1CK}$.

From Fig. 5.3, it is clearly seen that for $T \gg T_K^{1CK}$ (corresponding thereby to non-universal energy scales), all systems are described by the FO FP [13]. For $N_c = 3$ (solid lines) the limiting high-temperature entropy is thus $S_{\text{imp}} = 3\ln(2)$, while it is $S_{\text{imp}} = 5\ln(2)$ for $N_c = 5$ (dotted lines) and $S_{\text{imp}} = 7\ln(2)$ for $N_c = 7$ (dashed lines). For each N_c however, the entropy drops directly to the 2CK FP value [43–45] of $S_{\text{imp}} = \frac{1}{2}\ln(2)$ for lines (a), which correspond to $J = T_K^c$. No sign of the LM FP is seen for any chain size.

Considering now lines (b,c), the shape of the curves is seen to change, with a shoulder at $S_{\text{imp}} = \ln(2)$ now developing on the non-universal scale of J . As the interdot couplings are reduced still further [see lines (d–f)], a pronounced plateau at $S_{\text{imp}} = \ln(2)$ is observed. Again the magnetic susceptibility follows the Curie law (not shown), confirming that this behaviour is characteristic [13] of the LM FP, with RG flow persisting in the vicinity of the LM FP over a wider temperature range as J is decreased. Indeed, for lines (g), the systems are described by the LM FP over the entire temperature range shown.

However, for all lines (a–g), below T_K^{2CK} , the entropy drops to its ultimate $T = 0$ 2CK FP value of $S_{\text{imp}} = \frac{1}{2}\ln(2)$. The scale T_K^{2CK} itself is seen to rapidly diminish

with J ; we study its evolution in Fig. 5.4 below.

First, we comment that the above results are perfectly consistent with the perturbative analysis in Sec. 5.1.1. Initially, we consider the $N_c = 3$ case (solid lines). For $J < T_K^{1CK}$, the terminal dots undergo a *single*-channel Kondo effect [12,13] with their attached leads for $T \sim T_K^{1CK}$. The entropy thus drops from $3 \ln(2)$ to $\ln(2)$ on this scale; the residual $\ln(2)$ reflecting the free spin on dot 2. The FP Hamiltonian here is simply Eq. 4.1 for $N_c = 3$ with $J_K = \infty$ and $J = 0$ (see Sec. 3.4.1), and we denote it SC: $L \times LM \times SC$: R (with SC: α indicating the usual single-channel strong coupling Kondo singlet state formed with lead $\alpha = L, R$, and LM representing the free spin on dot 2).

In the $J = 0$ case, this is then the behaviour down to $T = 0$, and thus the entire temperature-dependence of the entropy is given by $S_{\text{imp}}^{J=0}(T) = 2 \times S_{\text{imp}}^{1CK}(T) + \ln(2)$, where $S_{\text{imp}}^{1CK}(T)$ is the entropy for a standard single-channel Kondo model [12,13] (the doubling reflecting the fact that both dot 1 and dot 3 are separately and simultaneously quenched in the mirror-symmetric systems considered) and the explicit $\ln(2)$ corresponds to the free spin- $\frac{1}{2}$ on dot 2. We plot $S_{\text{imp}}^{J=0}(T)$ as the diamond points in Fig. 5.3, which is seen to follow exactly line (g) for $N_c = 3$.

For non-zero J ($< T_K^{1CK}$), the SC: $L \times LM \times SC$: R FP is unstable, and so RG flow near it occurs only for $T_K^{2CK} > T > T_K^{1CK}$. Thus, lines (c–f) initially follow $S_{\text{imp}}^{J=0}(T)$, then depart from it, the residual coupling between dot 2 and the rest of the lead states driving the system to the 2CK FP below T_K^{2CK} . As expected from Eq. 5.9, this scale decreases rapidly with decreasing J , since the effective coupling itself has the form $\rho \tilde{J}_{K,\text{eff}} \sim J$ for fixed J_K (see Eq. 5.10).

Finally, we consider $N_c = 5$ (dotted lines) and $N_c = 7$ (dashed lines) in Fig. 5.3. The behaviour on the highest temperature scales is simply the FO FP, as previously discussed, and as is physically natural. Below T_K^{1CK} , the entropy is in fact expected to drop to $S_{\text{imp}} = (N_c - 2) \ln(2)$, since the spins on the terminal dots are quenched by the two separate single-channel Kondo effects. A residual entropy corresponding to the degrees of freedom of the remainder of the chain (which is again of odd length) is then expected². Indeed, in the $J = 0$ case for $N_c = 5, 7$, it is expected that $S_{\text{imp}} = (N_c - 2) \ln(2)$ describes the $T = 0$ entropy of the system.

In practice, evidence of this FP is not observed in Fig. 5.3, since on the scale of $T \sim J$ (which is comparable to T_K^{1CK} for the systems considered), the higher lying states of the residual $(N_c - 2)$ -length chain are projected out, leaving just the lowest doublet state. Thus in all cases for $T \lesssim T_K^{1CK}$, the LM FP is reached.

Details of the ‘bare’ Hamiltonian (for which Eq. 5.8 is a low-energy effective model), are then lost on renormalization under reduction of the temperature/energy scale, and all systems (scaled in terms of T_K^{1CK}) behave in exactly the same way —

²Note that in the $N_c = 3$ case, the remainder of the chain is simply dot 2, and hence the LM FP is reached directly.

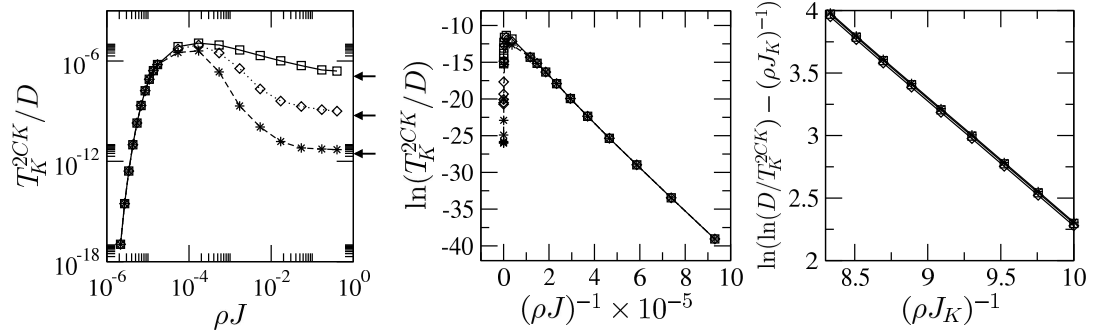


Figure 5.4: Variation of the Kondo scale T_K^{2CK} with the bare system parameters ρJ and ρJ_K for mirror-symmetric chains of length $N_c = 3, 5, 7$ (squares, diamonds and stars). *Left:* T_K^{2CK}/D vs. ρJ for fixed $\rho J_K = 0.1$. In the large J limit, the poor man's scaling result for the Kondo scale (Eq. 4.11) is recovered (indicated with arrows). *Middle:* $\ln(T_K^{2CK}/D)$ vs. $(\rho J)^{-1} \times 10^{-5}$, again for fixed $\rho J_K = 0.1$. *Right:* $\ln(\ln(D/T_K^{2CK}) - (\rho J_K)^{-1})$ vs. $(\rho J_K)^{-1}$ for fixed $\rho J = 3.4 \times 10^{-6}$. The linear form apparent in the middle and right panels for $J \ll T_K^{2CK}$ shows that $T_K^{2CK}/D \sim \exp(-1/\rho J_{K,\text{eff}})$, with $\rho J_{K,\text{eff}} \sim J/T_K^{1CK}$. Thus, the same effective single-spin 2CK model is indeed recovered at small J for all odd chains.

as indeed seen from the excellent agreement for all lines (a–g) and $N_c = 3, 5, 7$ in Fig. 5.3.

In the inset to the figure, we plot the lowest-temperature behaviour for lines (d–f) for $N_c = 3, 5, 7$, with the temperature axis rescaled in terms of T/T_K^{2CK} (and T_K^{2CK} determined in practice as usual through $S_{\text{imp}}(T_K^{2CK}) = 0.55$). The mapping of all such systems onto an effective single-spin 2CK model Eq. 5.8 is confirmed by the universal collapse to the 2CK scaling curve (circles).

We now examine the variation of the 2CK scale with the bare system parameters. In Sec. 5.1.1 we derived an effective low-energy 2CK model for the $N_c = 3$ case in the $J < T_K^{1CK}$ regime, valid for $T \sim T_K^{1CK}$, and with the effective coupling itself given by Eq. 5.10. In the left panel of Fig. 5.4, we plot T_K^{2CK}/D vs. ρJ for systems with common fixed $\rho J_K = 0.1$ and $N_c = 3, 5, 7$ (shown with squares, diamonds and stars, respectively). A clear non-monotonic variation is apparent. In the large- ρJ limit, the 2CK scale is expected to be described by Eq. 4.11, as derived in Sec. 4.1.2 of Chapter 4. For the parameters used in the left panel of Fig. 5.4, T_K^{2CK} calculated via Eq. 4.11 is indicated with the horizontal arrows in each case. That these are exponentially different for $N_c = 3, 5, 7$ reflects the different effective coupling of the ground chain doublet in each case, and hence the different configuration of the terminal spins in these states (see Sec. 4.1.1).

However (as shown in Fig. 5.2), as J decreases, the 2CK scale initially *increases*, with $T_K^{2CK} \approx T_K^{1CK}$ for $J \sim T_K^{1CK}$, which constitutes its maximum value — and since $T_K^{1CK}/D \sim \exp(-1/\rho J_K)$ is independent of ρJ and N_c , all systems have essentially the same T_K^{2CK} at this point.

As J is reduced further, T_K^{2CK} for all systems rapidly diminishes. This is expected from perturbative scaling on the effective 2CK model Eq. 5.8 (valid in the $J < T_K^{1CK}$ regime). Combining Eqs. 5.10 and 5.9, we obtain

$$\begin{aligned} T_K^{2CK}/D &\sim \left(\frac{J}{T_K^{1CK}} \right) \times \exp(-T_K^{1CK}/aJ) \\ &\sim \rho J \exp \left[\frac{1}{\rho J_K} - \frac{\exp(-1/\rho J_K)}{a\rho J} \right] \end{aligned} \quad (5.11)$$

where the last line follows using $T_K^{1CK}/D = \exp(-1/\rho J_K)$, and a is a constant $\mathcal{O}(1)$.

The functional form of Eq. 5.11 is tested in the middle and right panels of Fig. 5.4. In the middle panel we plot $\ln(T_K^{2CK}/D)$ (as determined directly from the NRG as before) *vs.* $(\rho J)^{-1} \times 10^{-5}$ for fixed $\rho J_K = 0.1$. For small J , the resulting straight line confirms the prediction that $T_K^{2CK}/D \sim \exp(A/\rho J)$ for constant ρJ_K . In the right panel, we now keep $\rho J = 3.4 \times 10^{-6}$ fixed, and vary ρJ_K . Specifically we plot $\ln(\ln(D/T_K^{2CK}) - (\rho J_K)^{-1})$ *vs.* $(\rho J_K)^{-1}$. The resulting straight line here establishes the functional dependence $T_K^{2CK}/D \sim (T_K^{1CK}/D)^{-1} \times \exp(B \times T_K^{1CK}/D)$.

Thus the variation of the 2CK scale in the $J < T_K^{1CK}$ regime given by Eq. 5.11 is confirmed for $N_c = 3, 5, 7$ by NRG. In particular, we find that the constant $a \approx 1.5$ from the above analysis.

Finally, we consider dynamical properties of systems in the $J < T_K^{1CK}$ regime. As in Sec. 4.2.2, we concentrate on the $T = 0$ spectral density $\rho^{N_c}(\omega)$, comparing results for chains of different length, as J is reduced. Specifically, in Fig. 5.5 we plot $D \rho^{N_c}(\omega)$ *vs.* ω/T_K^{1CK} for $N_c = 3, 5, 7$ (shown with solid, dotted and dashed lines, respectively) using a common fixed $\rho J_K = 0.1$, but varying the interdot couplings via $\rho J = \lambda T_K^{1CK}$ with $\lambda = 10^{-n/5}$ and $n = 0, 1, 2, 3, 4, 5, 6$ [lines (a–g)], progressively approaching the $\rho J = 0$ limit. Thus, the same systems are plotted as for the thermodynamics in Fig. 5.3.

For comparison, we have also plotted on the same graph a system with $\rho J = 10^{+4} \times T_K^{1CK}$, for each of $N_c = 3, 5, 7$ (see Fig. 5.5). The latter constitute the familiar “large” J limit, and the resulting behaviour is completely analogous to that presented in Fig. 4.2.2. On the scale of T_K^{2CK} (itself given from perturbative scaling via Eq. 4.11 in this regime), the 2CK resonance is observed, and $D \rho^{N_c}(\omega = 0) = \frac{1}{2}$ obtained as expected in each case (see Sec. 4.2.2 and Ref. [108]). That the 2CK scale is markedly different for different chain lengths is of course expected from the variation of the effective coupling between the ground chain doublet and the leads, as discussed previously, and as given in Eq. 4.10.

By contrast, for $J \lesssim T_K^{1CK}$, RG flow in the vicinity of the SC: $L \times$ LM $\times$ SC: R FP is observed. Here, the terminal dots undergo a *single*-channel Kondo effect [8] with their attached leads. For $N_c = 3$, the spin on dot 2 remains free, while for $N_c > 3$,

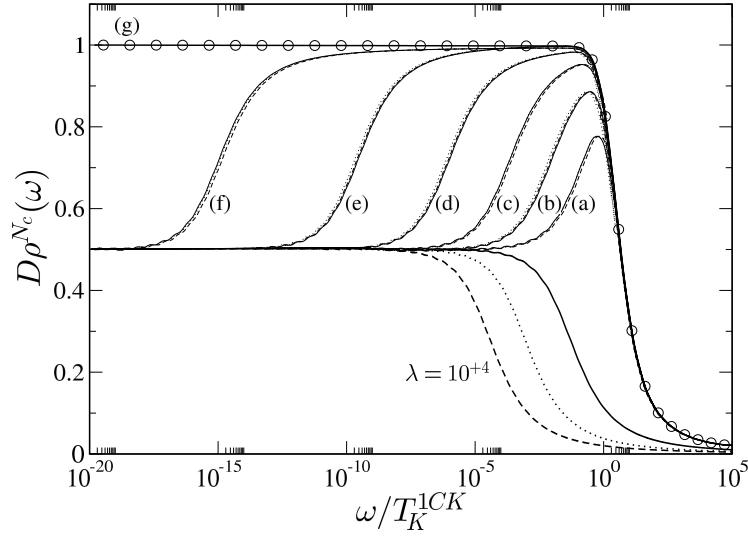


Figure 5.5: $T = 0$ spectrum $D\rho^{N_c}(\omega)$ vs. ω/T_K^{1CK} for $N_c = 3, 5, 7$ (solid, dotted and dashed lines, respectively), shown for the same systems as in Fig. 5.3 for the thermodynamics: $\rho J_K = 0.1$ and $\rho J = \lambda T_K^{1CK}$ with $\lambda = 10^{-n/5}$ and $n = 0, 1, 2, 3, 4, 5, 6$ [lines (a–g)], progressively approaching the $\rho J = 0$ limit. Also shown are systems away from this universal scaling regime, with $\rho J = 10^{+4} \times T_K^{1CK}$, which are close to the large J limit.

only the lowest doublet state of the remaining $(N_c - 2)$ -length chain is accessible at low-energies.

Flow near this effective single-channel strong-coupling FP (with each lead) must result in spectral behaviour typical [8] of the standard single-channel Kondo model. This is clearly seen in Fig. 5.5, with $D\rho^{N_c}(\omega)$ folding progressively onto $D\rho^{1CK}(\omega)$ (shown with circles) down to lower and lower frequencies as J is reduced [*ie.* going from (a→f)]. Indeed, case (g) is essentially indistinguishable from $D\rho^{1CK}(\omega)$ over the entire range of ω shown.

The behaviour of $D\rho^{1CK}(\omega)$ itself can of course be understood in terms of the standard single-channel Anderson model in the singly-occupied Kondo regime (where $D\rho^{1CK}(\omega) \equiv \pi\Gamma D(\omega)$ at low frequencies, as discussed in Sec. 3.6.2). At the Fermi level $\omega = 0$, the Friedel sum rule [8] gives $\pi\Gamma D(0) = 1$, and hence in the intermediate frequency range $T_K^{2CK} \ll |\omega| \ll T_K^{1CK}$, we expect $D\rho^{N_c}(\omega) \approx 1$, as clearly observed for lines (e–g) in Fig. 5.5.

Only on the scale of $\omega \sim T_K^{2CK}$ (itself described by Eq. 5.11 above) is the effective 1CK state destroyed, and the systems are then seen to flow to the half-unitarity limit value of $D\rho^{N_c}(\omega) = \frac{1}{2}$ typical [108] of the 2CK FP, which then describes the behaviour of the system down to $\omega = 0$.

We briefly comment that the physical behaviour discussed above is common to all odd chains: the lowest temperature/energy behaviour of Eq. 4.1 is *always* that of the 2CK FP for any finite positive interdot coupling J . However, the scale on

which systems flow to the stable 2CK FP diminishes rapidly for $J < T_K^{1CK}$, so that systems may be essentially described by a Fermi-liquid state (in which the terminal dots are exactly screened by conduction electrons in their attached leads) over a wide (but intermediate) range of temperatures/energies.

In the next section, we go on to consider *even* chains, focusing initially on the $N_c = 2$ case (which is of course the standard 2IK model) for systems where the mirror symmetry of the model is broken. We then turn to longer even chains, demonstrating that the resulting behaviour can again be understood in terms of the 2IK model.

5.2 Even chains

In the previous section, we considered the behaviour of odd chains in the small J regime. Below an effective single-channel Kondo scale T_K^{1CK} , the terminal dots undergo the Kondo effect with their attached leads. However, an effective antiferromagnetic coupling is generated for $T < T_K^{1CK}$ between the lowest doublet formed from the remaining $(N_c - 2)$ dots and the leads, which always drives the system to the 2CK FP on the lowest temperature/energy scales. The behaviour is expected to be somewhat different in the case of even chains however, and that is the focus of the present section.

First, we consider the $N_c = 2$ case, as this represents the simplest system in terms of which the essential physics of other even chains can be understood. By examining the case where the mirror symmetry of the model is broken, we show below that a simple physical picture of the low-temperature behaviour of all even chains can be obtained.

5.2.1 Two-impurity model revisited

In this section, we consider the $N_c = 2$ case of Eq. 4.1 in the “small” interdot coupling regime. This model is the famous ‘two-impurity’ Kondo model (2IK), which has been much studied previously *eg.* in Refs. [36, 37, 78, 109, 112, 113]. It represents the simplest case in which the tendency of the dots to form a local singlet state driven by the antiferromagnetic interdot exchange J competes with the formation of two separated single-channel Kondo states. A quantum phase transition between them is known to exist [37] at *finite* $J \sim T_K^{1CK}$, with the critical point of the model being the 2CK FP [37, 113].

That the critical point of the 2IK model in the mirror-symmetric case is the 2CK FP has been demonstrated with NRG [37], and confirmed using a conformal field theoretic analysis [112, 113], but its physical origin is somewhat obscure. Below, we revisit the 2IK model, considering explicitly the case where the mirror-

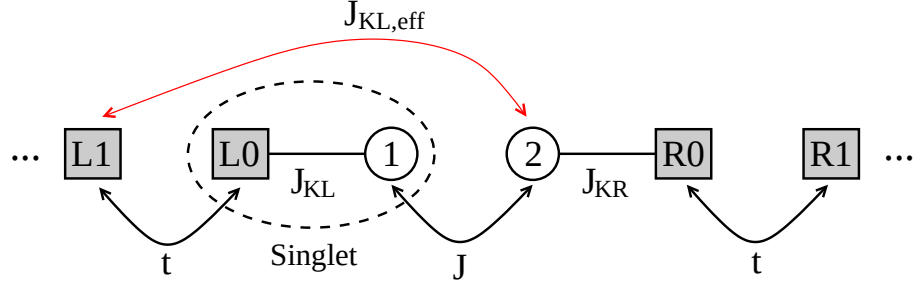


Figure 5.6: Illustration of the asymmetric ‘two-impurity’ model (Eq. 4.1 with $N_c = 2$). For $J \ll \min(J_{KL}, J_{KR})$ and $J_{KL} > J_{KR}$, dot 1 and the ‘L0’-orbital of the left Wilson chain form a singlet. However, there is a residual antiferromagnetic effective coupling, $J_{KL,\text{eff}}$, between dot 2 and the ‘L1’-orbital mediated by the singlet, and which depends on J . Tuning J so that $J_{KL,\text{eff}} \approx J_{KR}$ allows to access the 2CK FP.

symmetry of the setup is broken by distinct couplings to left and right leads. It is known [78, 112, 113] that the transition is robust to this symmetry breaking; here we employ physically motivated arguments similar to those in Ref. [78] to show that 2CK physics must be accessible in this system, and that the 2CK FP must describe the behaviour of the asymmetric 2IK system at the critical point. Indeed, we also show that the nature of the transition itself is fundamentally related to that in the standard channel-anisotropic single-spin 2CK model, and we derive an expression for the critical coupling strength J_c . For the first time, both thermodynamic and dynamical results calculated via NRG are presented for the asymmetric model near the transition. The behaviour of the model is examined in detail; the physical picture is confirmed and the analytic prediction for J_c is tested over a wide range of parameters. Finally, we go on to consider other asymmetrically-coupled even chains in the next section.

In Fig. 5.6, we present a schematic illustration of Eq. 4.1 for $N_c = 2$, where the exchange coupling between dot 1 and the left lead is stronger than the coupling between the dot 2 and the right lead: $J_{KL} > J_{KR}$. We also consider explicitly the case where the interdot coupling is *small*.

We discuss first the $J = 0$ limit, where the system is exactly equivalent to two separated single-channel Kondo models. However, since $J_{KL} \neq J_{KR}$, *two* universal low-energy scales result. These are given from perturbative scaling (see Sec. 2.3 and Ref. [19]) as

$$T_{K,\alpha}^{1CK}/D \sim \exp(-1/\rho J_{K\alpha}) \quad (5.12)$$

where for $\alpha = L$, the left lead screens the spin- $\frac{1}{2}$ on dot 1, while for $\alpha = R$, the right lead screens the spin- $\frac{1}{2}$ on dot 2. On the lowest possible temperature/energy scales, *both* dots are fully screened; we will refer to this stable FP as the SC: $L \times$ SC: R FP, the Hamiltonian for which being Eq. 4.1 for $N_c = 2$ with $J_{KL} = J_{KR} = \infty$ but

$J = 0$.

Due to the asymmetry of the setup, there is an exponential separation of the 1CK scales ($T_{K,L}^{1CK} \gg T_{K,R}^{1CK}$ follows from Eq. 5.12, since $J_{KL} > J_{KR}$). Thus, for $T \sim T_{K,L}^{1CK}$, dot 1 flows to strong-coupling (SC) with the left lead, forming thereby the familiar Kondo singlet with the ‘L0’-orbital, but dot 2 does not form a Kondo singlet with the ‘R0’-orbital of the right lead until the much lower temperature $T \sim T_{K,R}^{1CK}$.

On successive reduction of the temperature/energy scale, both J_{KL} and J_{KR} get renormalized, flowing toward their respective strong-coupling FP values, as discussed in Sec. 2.3. We can estimate the effective renormalized coupling between dot 2 and the right lead, $\tilde{J}_{KR}$, at $T = T_{K,L}^{1CK}$ by noting that $T_{K,R}^{1CK}$ is itself a *scaling invariant* [19]:

$$T_{K,R}^{1CK} \equiv D \exp(-1/\rho J_{KR}) = \tilde{D} \exp(-1/\rho \tilde{J}_{KR}) \quad (5.13)$$

where $\tilde{D}$ is the renormalized bandwidth. At $T = T_{K,L}^{1CK}$, the effective bandwidth³ is naturally reduced to $\tilde{D} \sim T_{K,L}^{1CK}$. Thus, rearranging Eq. 5.13 we obtain $T_{K,R}^{1CK}/T_{K,L}^{1CK} = \exp(-1/\rho \tilde{J}_{KR})$. Using Eq. 5.12 it then immediately follows that

$$\rho \tilde{J}_{KR} = \left[\frac{1}{\rho J_{KR}} - \frac{1}{\rho J_{KL}} \right]^{-1} \quad (5.14)$$

This will prove important shortly, when we consider the conditions necessary to observe 2CK physics in this system.

First, we consider the case of finite antiferromagnetic J . For “large” $J > T_{K,L}^{1CK}$ ($\gg T_{K,R}^{1CK}$), dots 1 and 2 lock up into a local singlet state on the temperature scale $T \sim J$, which cuts off RG flow to the strong-coupling (SC) FP for both left and right leads. We will refer to this stable FP as the ‘local singlet’ (LS) FP. The LS FP Hamiltonian is then simply Eq. 4.1 for $N_c = 2$ with $J_{KL} = J_{KR} = 0$ but $J = \infty$.

By contrast, for very small $J < T_{K,R}^{1CK}$ ($\ll T_{K,L}^{1CK}$), the system is naturally expected to be described by the SC:L $\times$ SC:R FP discussed above. The tendency to form a local singlet occurs only on the scale $T \sim J$, by which stage, the spin on each dot has already been quenched by a single-channel Kondo effect.

Although the ground state of both phases is a singlet state, they are not continuously connected, and so a transition must occur at a critical value of the interdot coupling, J_c . From the above arguments it follows that,

$$T_{K,R}^{1CK} < J_c < T_{K,L}^{1CK}. \quad (5.15)$$

³This can be understood physically in terms of the inaccessibility of higher lying conduction band states at low temperatures.

To understand the behaviour near the transition, we now consider interdot couplings in this intermediate range.

As discussed earlier, below $T \sim T_{K,L}^{1CK}$, dot 1 and the ‘L0’-orbital of the left Wilson chain flow to strong coupling and form a Kondo singlet state. The remaining states of the left lead still act as a bath of non-interacting conduction electrons however, which can compete to screen the spin on dot 2.

In an exactly analogous fashion to that described in Sec. 5.1.1, for couplings $J \lesssim T_{K,L}^{1CK}$, an *effective* coupling $J_{KL,\text{eff}}$ is generated between dot 2 and the ‘L1’-orbital, mediated by the Kondo singlet (see Fig. 5.6). For $T \sim T_{K,L}^{1CK}$, an effective model then arises of the form

$$H_{\text{trans}}^{\text{eff}} = \tilde{J}_{KL,\text{eff}} \hat{\mathbf{S}}_2 \cdot \hat{\mathbf{s}}_{L1} + \tilde{J}_{KR} \hat{\mathbf{S}}_2 \cdot \hat{\mathbf{s}}_{R0}. \quad (5.16)$$

$\tilde{J}_{KR}$ is the renormalized coupling between dot 2 and the ‘R0’-orbital of the right lead for $T \sim T_{K,L}^{1CK}$, as given in Eq. 5.14. $\tilde{J}_{KL,\text{eff}}$ is the effective coupling between dot 2 and the ‘L1’-orbital of the left lead (which is the $N_c = 2$ equivalent of Eq. 5.10), which can similarly be shown to be

$$\rho \tilde{J}_{KL,\text{eff}} \sim \frac{J}{T_{K,L}^{1CK}}. \quad (5.17)$$

Thus, in the region of the transition, $J \lesssim T_{K,L}^{1CK}$, the effective low-energy model $H_{\text{trans}}^{\text{eff}}$ is a 2CK model with *channel anisotropy*. However, J can be tuned so that $\tilde{J}_{KL,\text{eff}} = \tilde{J}_{KR}$, and hence the effective model is mirror-symmetric (even though the bare model is inherently asymmetric). Thus at this critical value of the interdot coupling, J_c , 2CK physics should be observed, with the 2CK FP stable at this single point. Setting Eqs. 5.14 and 5.17 equal and using the definition of $T_{K,L}^{1CK}$ in Eq. 5.12, gives

$$\begin{aligned} \rho J_c &\sim \rho \tilde{J}_{KR} \times T_{K,L}^{1CK} / D \\ &= b \left[\frac{1}{\rho J_{KR}} - \frac{1}{\rho J_{KL}} \right]^{-1} \times \exp(-1/\rho J_{KL}) \end{aligned} \quad (5.18)$$

where b is a constant $\mathcal{O}(1)$, which we shall determine directly with NRG below⁴.

First we comment that the 2CK FP is only stable at the point $J = J_c$ itself, and as it is distinct from the SC:L $\times$ SC:R FP and the LS FP, the 2CK FP is a genuine critical point of the model. Indeed, as the degree of channel anisotropy varies as J is varied (through Eq. 5.17), the transition itself is expected to be characteristic of the transition in the standard channel-anisotropic 2CK model, and we study this below.

⁴This result is in fact analogous to that quoted in Ref. [78] for a related model of two tunnel-coupled Andersonian sites

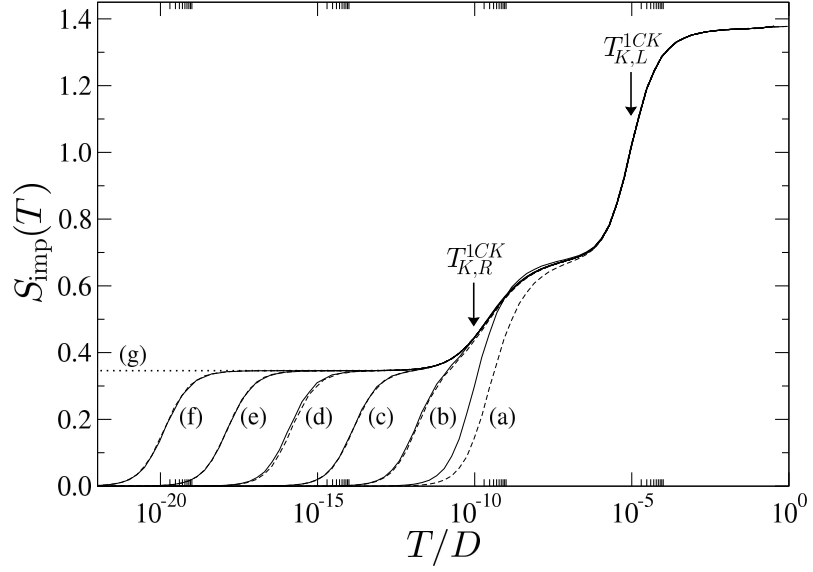


Figure 5.7: Entropy $S_{\text{imp}}(T)$ vs. T/D for the $N_c = 2$ case. Shown for fixed $\rho J_{KL} = 0.1$ and $\rho J_{KR} = 0.05$, varying the interdot exchange coupling via $\rho J = \rho J_c(1 + \lambda)$, where ρJ_c is the coupling at the quantum critical point [$\lambda = 0$; dotted line (g)]. Lines (a–f) progressively approach the transition, with $\lambda = \pm 10^{-n}$ and $n = 1, 2, 3, 4, 5, 6$. Solid lines show $\lambda < 0$ (corresponding to systems in the SC: $L \times$ SC: R Kondo phase) while dashed lines are for $\lambda > 0$ (which correspond to systems in the ‘local singlet’ phase). The single-channel Kondo scales $T_{K,L}^{1CK}$ and $T_{K,R}^{1CK}$ in the $J = 0$ limit are indicated with arrows.

In Fig. 5.7 we plot the entropy $S_{\text{imp}}(T)$ vs. T/D , obtained via NRG, for the 2IK model (Eq. 4.1 for $N_c = 2$) with $\rho J_{KL} = 0.1$ and $\rho J_{KR} = 0.05$. We vary the interdot couplings through $\rho J = \rho J_c(1 + \lambda)$, where $\rho J_c \approx 3.2278 \times 10^{-6}$ is the coupling at the quantum critical point [$\lambda = 0$; dotted line (g)].

Lines (a–f) progressively approach the transition, with $\lambda = \pm 10^{-n}$ and $n = 1, 2, 3, 4, 5, 6$. Solid lines show $\lambda < 0$ (corresponding to systems in the SC: $L \times$ SC: R Kondo phase) while dashed lines are for $\lambda > 0$ (which correspond to systems in the LS phase). For the dot-lead couplings given above, two single-channel Kondo scales are readily defined (in the $J = 0$ case, through Eq. 5.12), they are found to be $T_{K,L}/D = 10^{-5}$ and $T_{K,R}/D = 3 \times 10^{-10}$, as indicated with the vertical arrows in Fig. 5.7, and are thereby exponentially well-separated as desired.

Fig. 5.7 clearly shows the presence of a quantum phase transition: as ρJ is tuned through its critical value ρJ_c , the Kondo scale is seen to vanish. This Kondo scale of course corresponds to RG flow to the ultimate stable FP — which may be either SC: $L \times$ SC: R in the $\lambda < 0$ phase, or FS in the $\lambda > 0$ phase. We shall denote it simply T_K , and define T_K through the entropy such that $S_{\text{imp}}(T_K) = 0.2$, suitably between $S_{\text{imp}} = \frac{1}{2} \ln(2)$ and 0. We study the variation of T_K with ρJ in Fig. 5.8, but first examine the thermodynamics in Fig. 5.7.

We consider initially the solid line (a), which corresponds to $\rho J = 0.9 \times \rho J_c$,

and is as such deep in the $\text{SC}:L \times \text{SC}:R$ Kondo phase, well away from the transition. Thus, this system follows the $J = 0$ case very closely, and can essentially be described by two separated 1CK models. On the scale of $T_{K,L}^{1CK}$, dot 1 is quenched by coupling to the left lead, but dot 2 remains free. The entropy correspondingly drops from its limiting ‘high’-temperature free orbital (FO) FP value of $S_{\text{imp}}(T) = 2 \ln(2)$ to the LM FP value of $S_{\text{imp}}(T) = \ln(2)$. On the lower scale of $T_{K,R}^{1CK}$, dot 2 is quenched by the right lead, and the entropy drops to its final $\text{SC}:L \times \text{SC}:R$ FP value $S_{\text{imp}}(T) = 0$, which then remains the entropy down to $T = 0$. Thus deep in this phase, $T_K \simeq T_{K,R}^{1CK}$.

By contrast, the dashed line (a) is for $\rho J = 1.1 \times \rho J_c$, and is thus deep in the LS phase, again well away from the transition. On the scale of $T_{K,L}^{1CK}$, the spin on dot 1 is again screened by strong coupling to the left lead, and so the entropy drops from $2 \ln(2)$ to $\ln(2)$ as before. However, on the non-universal scale $T \sim J$, the Kondo singlet is destroyed, and a *local* singlet forms instead between dots 1 and 2. The entropy thus drops to its ultimate $T = 0$ value $S_{\text{imp}} = 0$. Deep in this phase therefore, $T_K \simeq J$.

Most interestingly however, is the situation as ρJ is tuned closer to the transition [lines (b–f)]. Lines (b) correspond to $\lambda = \pm 10^{-2}$; despite the fact that these systems are in different phases — and so the low- T FP describing the ground state behaviour of the system is naturally different — the thermodynamics of the two are nearly indistinguishable. As such the entropy is ‘blind’ to the ultimate low- T behaviour⁵. Lines (b) show a shoulder at $S_{\text{imp}}(T) = \frac{1}{2} \ln(2)$, emerging for $T \lesssim T_{K,R}^{1CK}$. This is of course characteristic [43–45] of the 2CK FP. The logarithmic divergence of the magnetic susceptibility and the NRG energy level structure (not shown) readily confirm the nature of the FP (see Secs. 3.4.3 and 3.5).

Indeed, a distinct plateau at $S_{\text{imp}}(T) = \frac{1}{2} \ln(2)$ is clearly observed in lines (c–f), with the length of the plateau being extended as the transition is approached more closely — and hence T_K is seen to diminish. RG flow thus persists in the vicinity of the unstable 2CK FP over a wider temperature/energy range. On the scale of $T \sim T_K$ however, the 2CK state is destroyed, and the system flows away to the stable FP for the phase; itself determined by the bare system parameters.

By contrast, for line (g) — corresponding to $\lambda = 0$, precisely *at* the transition — the 2CK FP is the stable FP of the model, and is the *critical* FP (CFP). A residual entropy $S_{\text{imp}}(T = 0) = \frac{1}{2} \ln(2)$ is thus observed at this point.

In all such cases however, systems flow to the 2CK FP on the same scale, which we will denote T_K^{2CK} . cursory inspection of Fig. 5.7 shows that this scale is essentially the smaller of the single-channel scales, $T_{K,R}^{1CK}$ (indicated on the figure), as now explained. The T_K^{2CK} scale characterizes the flow from the LM FP to the 2CK

⁵We will see however in Fig. 5.9 below, that such systems may still be distinguished from their dynamical properties.

FP, and is thus common to all systems near the transition (see Fig. 5.7). Using the usual definition $S_{\text{imp}}(T_K^{2CK}) = 0.55$ (chosen to be suitably between $\ln(2)$ and $\frac{1}{2}\ln(2)$), we find that $T_K^{2CK}/D = 7 \times 10^{-10}$ from Fig. 5.7. This can be understood by considering the case for $\lambda = 0$ [line (g)], precisely at the transition, where the 2CK FP is the stable FP of the model. Perturbative scaling for the low-energy effective 2CK model, Eq. 5.16, in the mirror-symmetric limit $\tilde{J}_{KL,\text{eff}} = \tilde{J}_{KR}$ that describes the critical point of the full asymmetric model, gives

$$T_K^{2CK}/\tilde{D} \sim \exp(-1/\rho\tilde{J}_{KR}) \quad (5.19)$$

where $\tilde{J}_{KR}$ is the renormalized coupling of dot 2 to the right lead, and $\tilde{D} \sim T_{K,L}^{1CK}$ is the renormalized bandwidth at the temperature $T \sim T_{K,L}^{1CK}$, for which the effective model Eq. 5.16 is valid. Using the definition of $\tilde{J}_{KR}$ from Eq. 5.14 together with the definition of $T_{K,L}^{1CK}$ from Eq. 5.12 in Eq. 5.19, it readily follows that

$$T_K^{2CK} \sim T_{K,R}^{1CK} \quad (5.20)$$

which is in accord with the value of T_K^{2CK} determined directly from NRG, and as seen clearly from visual inspection of Fig. 5.7.

In Fig. 5.8, we examine the variation of the lowest-energy scale, T_K/D *vs.* interdot coupling ρJ . We have shown the data on a log-log plot, and thus consider essentially all energy scales of J . As explained earlier, we define this T_K through the entropy via $S_{\text{imp}}(T_K) = 0.2$, and as such three distinct regimes arise in Fig. 5.8.

Firstly (and trivially), for “large” $J \gg T_{K,L}^{1CK}$, the dots lock up into a local singlet on the scale $T \sim J$, and so the dot contribution to the entropy is quenched. Thus one naturally expects “ $T_K \sim J$ ”, as found in Fig. 5.8, and demonstrated by comparison to the grey dot-dashed line in the $J \gg T_{K,L}^{1CK}$ regime.

For “small” $J \ll T_{K,R}^{1CK}$, one naturally expects that the dots are essentially decoupled and each undergoes its separate single-channel Kondo effect. Thus $T_K \sim T_{K,R}^{1CK}$, as the latter is the smaller of the two 1CK scales in the $J_{KL} > J_{KR}$ regime considered here. In fact, from Fig. 5.8, we see that this behaviour is seen to apply on much higher scales, so that in practice for $\rho J < 10^{-6}$, we find that $T_K \approx T_{K,R}^{1CK}$, as again shown by comparison to the grey dot-dashed line.

Finally and most importantly, is the region in the vicinity of the transition, which occurs at $\rho J_c \simeq 3.2278 \times 10^{-6}$. In the critical region $|\lambda| \equiv |J - J_c|/J_c \lesssim 0.01$, RG flow via the 2CK FP is observed: see lines (b–g) for the variation of the entropy near the transition in Fig. 5.7 (specifically, lines (b) corresponds to $|\lambda| \equiv |J - J_c|/J_c = 0.01$). As the transition is approached from either side, T_K is shown to vanish (see also, inset).

To understand how the scale vanishes, we first note that for the standard channel-

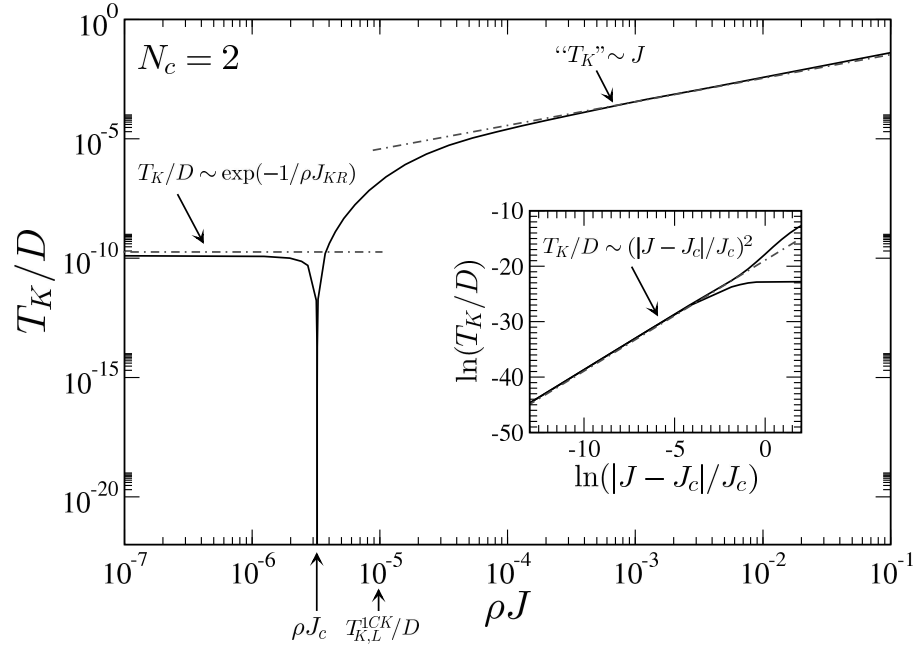


Figure 5.8: Variation of the low-energy scale T_K/D as a function of interdot coupling ρJ . Shown using fixed $\rho J_{KL} = 0.1$ and $\rho J_{KR} = 0.05$, for the $N_c = 2$ model. T_K is defined from the thermodynamics as the point at which $S_{\text{imp}}(T_K) = 0.2$, thereby describing the scale below which the internal degrees of freedom of the dots are quenched (see Fig. 5.7). For large J (*ie.* $J \gg T_{K,L}^{1CK}$), T_K corresponds to the scale where the dots form a local singlet, and hence “ $T_K \sim J$ ”. By contrast, for very small J (*ie.* $J \ll T_{K,L}^{1CK}$), the dots are essentially decoupled and separately undergo a single-channel Kondo effect with their attached lead. Since $J_{KL} > J_{KR}$, the lowest energy scale of the problem is the second-stage Kondo quenching of dot 2 by the right lead, and so $T_K \sim T_{K,R}^{1CK}$. In the critical region $|J - J_c|/J_c \lesssim 0.01$, the scale vanishes as $T_K/D \sim (|J - J_c|/J_c)^2$, as in the symmetric model.

anisotropic 2CK model, Eq. 2.20, the critical fixed point (which occurs when $J_{KL} = J_{KR}$) is the 2CK FP. For any asymmetry in the couplings to the left and right leads however, the system always flows to a strong-coupling FP, with the dot spin fully screened by the lead to which it was initially more strongly coupled, while the other lead decouples completely. The Kondo scale, T_K , which describes the flow to this FP, vanishes as the transition is approached according to $T_K \sim |J_{KL} - J_{KR}|^\nu$, with $\nu = 2$ characteristic of the transition.

The low-energy effective model, Eq. 5.16, which describes the transition in the asymmetric 2IK model shown in Figs. 5.7 and 5.8, is an effective anisotropic 2CK model. But $\tilde{J}_{KR}$ is fixed for constant J_{KL} and J_{KR} (according to Eq. 5.14), while $\tilde{J}_{KL,\text{eff}} \sim J$ (from Eq. 5.17), so it follows that the degree of channel-anisotropy is given by $(\tilde{J}_{KL,\text{eff}} - \tilde{J}_{KR}) \sim (J - J_c)$. As a consequence, the transition is expected to be characterized by the same power law decay,

$$T_K \stackrel{J \rightarrow J_c^\pm}{\sim} \mathcal{A} |J - J_c|^\nu \quad : \nu = 2 \quad (5.21)$$

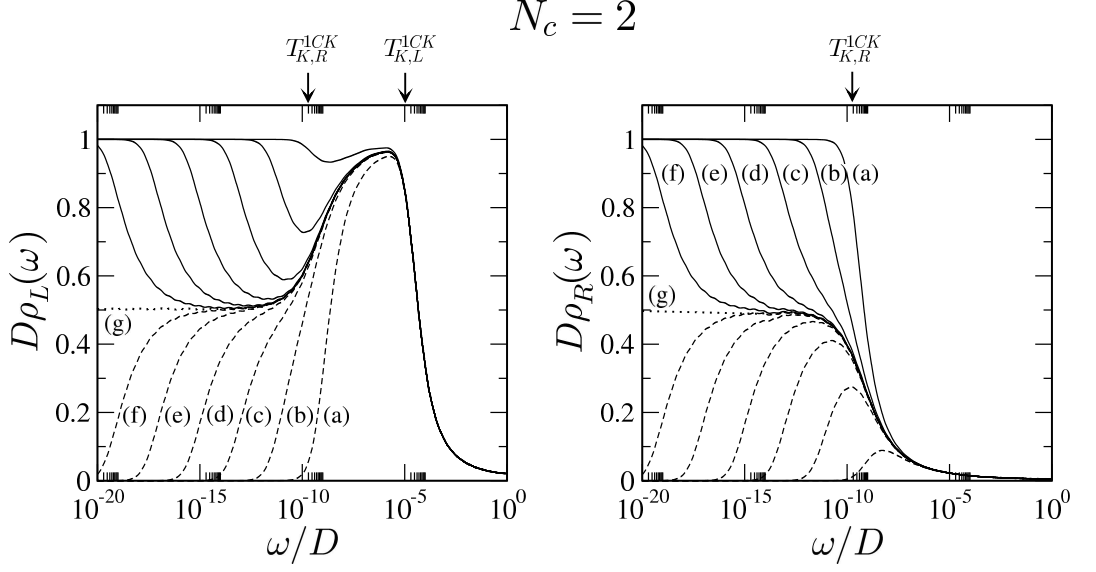


Figure 5.9: $T = 0$ spectra $D\rho_L(\omega)$ (left panel) and $D\rho_R(\omega)$ (right panel), both *vs.* ω/D for the $N_c = 2$ model. Shown for the same systems as plotted for the thermodynamics in Fig. 5.7: $\rho J_{KL} = 0.1$, $J_{KR} = 0.05$ and $\rho J = \rho J_c(1 + \lambda)$, where ρJ_c is the coupling at the quantum critical point [$\lambda = 0$; dotted line (g)]. Lines (a–f) progressively approach the transition, with $\lambda = \pm 10^{-n}$ and $n = 1, 2, 3, 4, 5, 6$. Solid lines show $\lambda < 0$ (corresponding to systems in the SC: $L \times$ SC: R Kondo phase) while dashed lines are for $\lambda > 0$ (which correspond to systems in the ‘local singlet’ phase). The vertical arrows show the Kondo scales, $T_{K,R}^{1CK}$ and $T_{K,L}^{1CK}$, in the $J = 0$ case.

with common amplitudes $\mathcal{A}$ approaching the transition from either side. Eq. 5.21 is confirmed in the inset to Fig. 5.8, where we plot $\ln(T_K/D)$ *vs.* $\ln(|J - J_c|/J_c)$, finding that the data collapse to a straight line of slope $\nu = 2$, corresponding to the critical exponent.

We now turn to dynamical properties of the 2IK model. As discussed in Sec. 4.2.2, in general *two* spectra can be defined for two-channel models, since one can consider spin-scattering in either the left or right leads. $D\rho_\alpha(\omega)$ is defined in terms of the t-matrix for lead $\alpha = L, R$ via $D\rho_\alpha(\omega) = -\pi\rho_T \text{Im}\{t_\alpha(\omega)\}$ (see Secs. 3.6.2, 3.6.3 and 4.2.2). Equations of motion methods [8, 139] then give $D\rho_\alpha(\omega)$ through Eqs. 4.16, 4.15, which can in turn be calculated directly with NRG.

Of course, in mirror-symmetric systems, $D\rho_L(\omega) = D\rho_R(\omega) \equiv D\rho(\omega)$ (as considered in Sec. 5.1.2 for example); but here the inherent asymmetry of the model (embodied in the distinct exchange couplings to left and right leads) means that two different spectra arise.

In Fig. 5.9, we study the $T = 0$ spectra $D\rho_\alpha(\omega)$ *vs.* ω/D , with $\alpha = L$ shown in the left panel, while $\alpha = R$ is shown in the right panel. We consider the same systems as presented for the thermodynamics in Fig. 5.7 for comparison: $\rho J_{KL} = 0.1$, $J_{KR} = 0.05$ and $\rho J = \rho J_c(1 + \lambda)$, where $\lambda = \pm 10^{-n}$, and lines (a→f) for integral

$n = 1 \rightarrow 6$ progressively approach the transition [$\lambda = 0$; line (g)].

We plot $\lambda < 0$ as the solid lines, which correspond to systems in the SC: $L \times$ SC: R Kondo phase, while dashed lines are used for $\lambda > 0$, which correspond to systems in the ‘local singlet’ (LS) phase, as before. From cursory inspection of Fig. 5.9, it is obvious that the left and right spectra are very different, as are the spectra belonging to systems in the different phases.

We will discuss first the solid lines in the left panel, which describe the behaviour of $D\rho_L(\omega)$ for systems in the SC: $L \times$ SC: R Kondo phase ($\lambda < 0$). For line (a), which may be considered well away from the transition, a resonance characteristic of the single-spin, single-channel Kondo model (see Sec. 3.6.2) is observed on the scale $|\omega| \sim T_{K,L}^{1CK}$. This is of course expected from the above discussion: since the interdot coupling $J < T_{K,L}^{1CK}$, dot 1 undergoes a single-channel Kondo effect with the left lead. The spectrum $D\rho_L(\omega)$ is then expected to be equivalent to $\pi\Gamma D(\omega)$ for the standard single-impurity Anderson model in the singly-occupied Kondo regime (see Sec. 3.6.2), and hence from the Friedel sum rule [8], $D\rho_L(\omega = 0) \equiv \pi\Gamma D(\omega = 0) = 1$, as seen in Fig. 5.9. Departure from this behaviour occurs on the non-universal scale of J , and is manifest in the solid line (a) as a small trough.

All systems are seen to undergo this effective single-channel resonance at $|\omega| \sim T_{K,L}^{1CK}$, but as J is tuned closer to the transition [considering now solid lines (b–f)], RG flow is now observed in the vicinity of the critical FP — which for the 2IK model is of course the 2CK FP, as discussed above. For line (d), the spectral density decays from the unitarity limit $D\rho_L(\omega) = 1$ for $|\omega| \lesssim T_{K,L}^{1CK}$ to the *half* unitarity value of $D\rho_L(\omega) = \frac{1}{2}$ which is characteristic [108] of the 2CK FP, as confirmed in Secs. 3.6.3 and 4.2.2. This occurs on the 2CK scale $|\omega| \sim T_K^{2CK} \approx T_{K,R}^{1CK}$, as given above in Eqs. 5.19 and 5.20.

On the lowest energy scale $|\omega| \sim T_K$, the system then flows away from the unstable 2CK FP and toward the ultimate stable SC: $L \times$ SC: R FP. Since the latter corresponds to two separated 1CK models, the unitarity limit $D\rho_L(\omega) = 1$ is recovered once more, and this describes the behaviour of the spectrum down to the Fermi level $\omega = 0$. The scale T_K , however, vanishes as the transition is approached, so that the systems are described by the 2CK FP down to lower and lower frequencies. Indeed, precisely at the transition itself [line (g)], $D\rho_L(\omega = 0) = \frac{1}{2}$, and so the 2CK FP describes the system at the Fermi level.

The dashed lines in the left panel of Fig. 5.9 (corresponding to systems in the LS phase; $\lambda > 0$) show similar behaviour for high- ω . Away from the transition, *eg.* line (a), the dots form a local singlet state on the scale of $|\omega| \sim J$. However, since $J < T_{K,L}^{1CK}$ (even for line (a)), a resonance is still observed for $|\omega| \sim T_{K,L}^{1CK}$, corresponding to the formation of a Kondo singlet between dot 1 and the left lead conduction band states, and is characteristic of the standard Kondo resonance of the 1CK model (or equivalently the Anderson model in the singly-occupied Kondo

regime, as argued above). Thus $D\rho_L(\omega) \approx 1$ results. However, this state is rapidly destroyed for $|\omega| \ll J$, and the LS FP value $D\rho_L(\omega) = 0$ is reached (which describes the system down to $\omega = 0$).

As the transition is approached, the 2CK FP controls the behaviour of the spectrum in the frequency window $T_K < |\omega| < T_K^{2CK}$, and so a plateau at $D\rho_L(\omega) = \frac{1}{2}$, characterizing incipient RG flow in the vicinity of the 2CK FP, is clearly observed in Fig. 5.9 for the dashed lines (d–f). Since the T_K scale vanishes as the transition is approached (see Fig. 5.8 and Eq. 5.21), the length of this plateau naturally increases, so that $D\rho_L(\omega = 0) = \frac{1}{2}$ of course results for $\lambda = 0$ where $T_K = 0$.

We now consider the analogous behaviour evident in the right panel of Fig. 5.9, where $D\rho_R(\omega)$ *vs.* ω/D is plotted for the same systems. Strikingly, *no* spectral features are observed on the scale of $|\omega| \sim T_{K,L}^{1CK}$. This is physically natural however: for small J , dot 2 flows to the strong coupling FP with the right lead only on the much lower scale of $|\omega| \sim T_{K,R}^{1CK}$ [see for example, solid line (a)], while for large J both dots lock up into a singlet on the non-universal scale of J [see dashed line (a)]. Near the transition [lines (b–g)], RG flow in the vicinity of the 2CK FP is only observed for $|\omega| < T_K^{2CK}$ ($\ll T_{K,L}^{1CK}$).

Of course, it is the flow to the strong coupling FP for dot 1 and the left lead that generates the effective coupling between dot 2 and the left lead (see Fig. 5.6 and Eq. 5.16). Thus, all systems near the transition naturally show a single-channel Kondo resonance $D\rho_L(\omega) \approx 1$, but no such spectral feature is observed in $D\rho_R(\omega)$ at $|\omega| \sim T_{K,L}^{1CK}$. However, evidence of the 2CK FP is observed *symmetrically* in $D\rho_L(\omega)$ and $D\rho_R(\omega)$ for $T_K < |\omega| < T_K^{2CK}$, both spectra showing a half-height plateau in this frequency window.

Ultimately, on the scale of $|\omega| \sim T_K$, both $D\rho_L(\omega)$ and $D\rho_R(\omega)$ reach their unitarity limit typical of the SC:L $\times$ SC:R FP for $\lambda < 0$. By contrast, in the LS phase ($\lambda > 0$), both $D\rho_L(\omega)$ and $D\rho_R(\omega)$ decay to zero below $|\omega| \sim T_K$.

To conclude our survey of the $N_c = 2$ asymmetric 2IK model, we finally examine the evolution of the critical coupling strength J_c itself with the bare dot-lead couplings J_{KL} and J_{KR} . We derived an expression for ρJ_c in Eq. 5.18 employing physically motivated perturbative scaling arguments. In Fig. 5.10 we test this expression using ρJ_c as obtained via NRG, for a wide range of couplings J_{KL} and J_{KR} .

In the left panel of Fig. 5.10, we plot $\rho J_c \times 10^6$ *vs.* $\rho \tilde{J}_{KR}$, as calculated from Eq. 5.14. We keep $\rho J_{KL} = 0.1$ fixed, and vary ρJ_{KR} . The resulting straight line demonstrates that $\rho J_c \sim \tilde{J}_{KR}$, as expected. In the middle panel, we now keep $\rho J_{KR} = 0.05$ fixed, and vary ρJ_{KL} . We plot $\ln(\rho J_c)$ *vs.* $(\rho J_{KL})^{-1}$, and a straight line (of slope -1) results, establishing the dependence $\rho J_c \sim \exp(-1/\rho J_{KL}) \sim T_{K,L}^{1CK}$ through Eq. 5.12.

In the right panel, we vary both J_{KL} and J_{KR} , plotting ρJ_c *vs.* $\rho \tilde{J}_{KR} T_{K,L}^{1CK}/D$

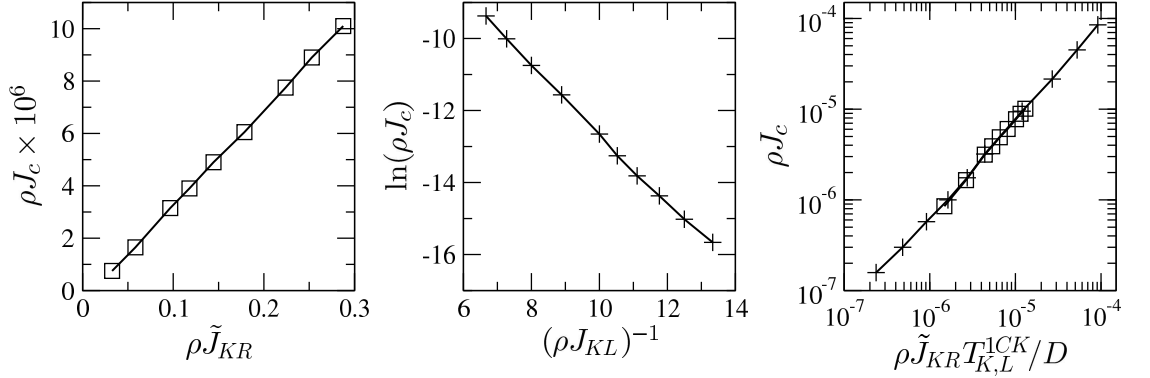


Figure 5.10: Dependence of the critical interdot coupling ρJ_c on the dot-lead couplings ρJ_{KL} and ρJ_{KR} . *Left:* $\rho J_c \times 10^6$ vs. $\rho \tilde{J}_{KR} = [1/\rho J_{KR} - 1/\rho J_{KL}]^{-1}$ for fixed $\rho J_{KL} = 0.1$. *Middle:* $\ln(\rho J_c)$ vs. $(\rho J_{KL})^{-1}$ for fixed $\rho J_{KR} = 0.05$. The linear relationship in the left and middle panels implies that $\rho J_c = b \times \rho \tilde{J}_{KR} T_{K,L}^{1CK}/D$ (since $T_{K,L}^{1CK}/D \sim \exp(-1/\rho J_{KL})$), which is plotted explicitly in the right panel. The right panel thus confirms Eq. 5.18, the gradient yielding $b = 0.72$.

for the systems shown in both the left and middle panels. The collapse to a common straight line confirms the functional dependence of Eq. 5.18, the slope yielding the constant $b \simeq 0.72$, which is $\mathcal{O}(1)$ as expected.

In this section, we have studied in detail the $N_c = 2$ case of Eq. 4.1 in the asymmetric limit $J_{KL} \neq J_{KR}$. We argued that the transition known to occur in such systems is described by an effective channel-anisotropic 2CK model, and hence the transition in the 2IK model must be fundamentally related to the transition in the 2CK model. As a consequence, the critical point must be the 2CK FP; we examined both thermodynamics and dynamics of the transition to confirm this physical picture. We also derived an expression for the critical coupling strength J_c ; agreement with NRG results again demonstrating the mapping of the full 2IK model onto the low-energy effective 2CK model near the transition.

In the next section, we show briefly that the physical behaviour of other even chains is fundamentally similar to that elucidated above.

5.2.2 Universal behaviour of other even chains

Having considered in detail the canonical $N_c = 2$ case of Eq. 4.1 in the previous section, we now go on to study briefly the generic behaviour of other even chains. A variant of Eq. 4.1 was considered in Ref. [78], in which chains of $N_c = 2$ and 4 *tunnel*-coupled dots were studied. For the $N_c = 4$ case, the limit considered in that work is one in which the two interior dots are much more strongly-coupled than the others, and so trivially form a singlet state. Their role then is simply to mediate an effective coupling between dots 1 and 4. Here we study chains with $N_c = 2, 4, 6$ with NRG, where the interdot couplings are all small (see Eq. 4.1), and demonstrate that

the same underlying physics as that elucidated in the previous section ubiquitously arises.

Before diving into the NRG results however, we give first a heuristic account of the expected behaviour of the larger even chains.

Away from the transition, the physical behaviour of all even chains is rather straightforward, and is completely analogous to the $N_c = 2$ case studied in the previous section. For large interdot coupling J , the stable FP is clearly the LS FP, since for $T \ll J$, high lying states of the even-length chain are projected out, leaving only the lowest state — which is always a spin *singlet* (see Sec. 4.1.1). As in the $N_c = 2$ case, this singlet decouples from the leads, as expected.

For very small J , the situation must also be similar to the $N_c = 2$ case. The terminal dots 1 and N_c each undergo separate *single*-channel Kondo effects with their attached leads on a scale determined by the bare dot-lead couplings (with $T_{K,L}^{1CK}$ and $T_{K,R}^{1CK}$ independent of J and given by Eq. 5.12). On the lower scale of $T \sim J$, the remaining $(N_c - 2)$ dots of the chain (which is of course again an *even* length chain) form a singlet state, and as such decouple from the rest of the system. This is essentially the SC: $L \times$ SC: R FP of the $N_c = 2$ case.

From consideration of the above limits, it is clear that for any even chain, a quantum phase transition *must* occur on tuning the interdot coupling J through its critical value J_c .

Let us now consider the intermediate coupling case, with J tuned close to the transition. We argued in the previous section for the $N_c = 2$ case that the transition is driven by an effective coupling mediated through the Kondo singlet formed between dot 1 and the left lead. For any even N_c , all systems close to the transition must therefore initially flow to an effective strong-coupling FP, where the spin on dot 1 is screened. Near this FP, dot 1 is thus essentially decoupled from the other $(N_c - 1)$ dots of the chain. The antiferromagnetic interdot coupling J between the remaining dots (which now constitute an *odd*-length chain) naturally favours the formation of a *doublet* ground state for $T \sim J$. As the temperature is lowered, the higher lying states of this residual chain are projected out, and the system flows toward the LM FP, for all even $N_c \geq 2$.

For $T \lesssim T_{K,L}^{1CK}$, dot 1 and the ‘L0’-orbital of the left Wilson chain are locked in a Kondo singlet, but a local Fermi-liquid description still applies. The remaining states of the left lead may act as a bath of non-interacting conduction electrons which can screen the spin- $\frac{1}{2}$ doublet of the residual $(N_c - 1)$ -length chain. An effective coupling is thus generated between this state and the ‘L1’-orbital (as in Sec. 5.2.1), which leads to an effective channel-anisotropic 2CK model.

Just as in the $N_c = 2$ case, the 2CK FP can then be accessed by tuning J to its critical value J_c , and so we do indeed expect to observe the same transition for all even-length chains.

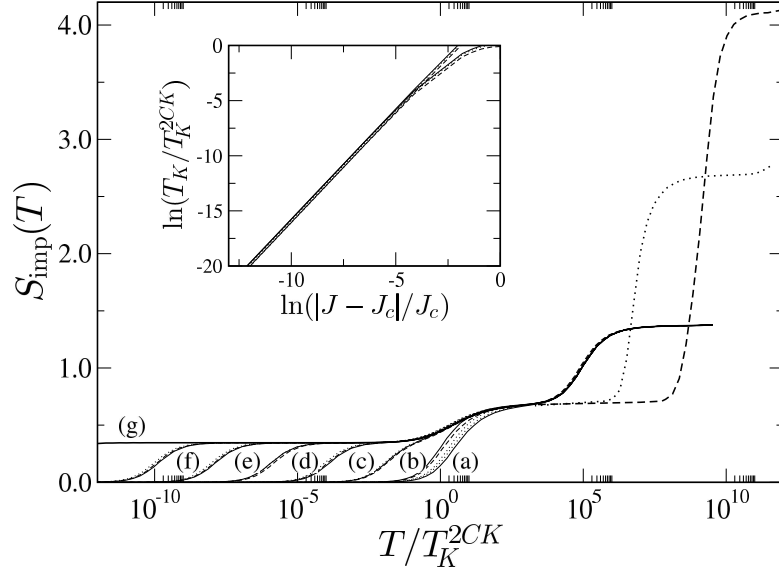


Figure 5.11: Entropy $S_{\text{imp}}(T)$ vs. T/T_K^{2CK} , comparing $N_c = 2, 4, 6$ (solid, dotted and dashed lines, respectively). Shown for systems with the same parameters as in Fig. 5.7: $\rho J_{KL} = 0.1$, $\rho J_{KR} = 0.05$, and $\rho J = \rho J_c(1 + \lambda)$, where ρJ_c is the coupling at the quantum critical point [$\lambda = 0$; line (g)]. Lines (a–f) progressively approach the transition, with $\lambda = \pm 10^{-n}$ and $n = 1, 2, 3, 4, 5, 6$. As shown, universality arises close to the transition on rescaling in terms of T_K^{2CK} , which is the 2CK scale at the critical point itself. The inset shows the power-law decay of T_K^{2CK} approaching the transition: $T_K/T_K^{2CK} \sim (|J - J_c|/J_c)^2$ in all cases.

Importantly, the residual effective coupling between the $(N_c - 1)$ -length chain and the leads is renormalized by a factor characteristic of the chain length. Indeed, since T_K^{2CK} is much smaller than $T_{K,L}^{1CK}$ — and hence is much smaller than J_c — the analysis for odd chains in the “large” J regime presented in Sec. 4.1.2 is now approximately valid. We would thus expect the effective residual coupling for $N_c = 4$ to be $\approx \frac{2}{3}$ that of the $N_c = 2$ case; while for $N_c = 6$, we expect it to be $\approx \frac{1}{2}$ that of the $N_c = 2$ case (see Eq. 4.10a of Sec. 4.1.2). This would result in exponentially separated 2CK scales, T_K^{2CK} , for chains with different N_c (see Eq. 5.19), although the transition itself is expected to be of exactly the same type in each case.

We now turn to the NRG results for even chains of different lengths near the transition, and confirm the above physical picture. The evolution of the entropy provides the clearest and most direct means of comparing the physical behaviour, and understanding the underlying FPs reached on renormalization under progressive reduction of the temperature. Thus, in Fig. 5.11, we plot $S_{\text{imp}}(T)$ vs. T/T_K^{2CK} for $N_c = 2, 4, 6$ (shown as the solid, dotted and dashed lines, respectively). We keep $\rho J_{KL} = 0.1$ and $\rho J_{KR} = 0.05$ fixed, varying the interdot coupling ρJ .

As for the results presented in the previous section, we define the interdot coupling J through the dimensionless quantity $\lambda = (J - J_c)/J_c$, which is consequently a measure of the proximity to the transition (which occurs at $\lambda = 0$, shown as the

lines (g) in Fig. 5.11). Specifically, we plot lines (a–f) so as to progressively approach the transition, with $\lambda = \pm 10^{-n}$ and $n = 1, 2, 3, 4, 5, 6$. Thus, the solid lines of Fig. 5.11 corresponding to the $N_c = 2$ case are precisely those shown in Fig. 5.7. The actual value of the critical coupling J_c is found from NRG to vary slightly with N_c . However, J_c is always $\mathcal{O}(T_{K,L}^{1CK})$ (as expected for the $N_c = 2$ case from Eq. 5.18, and for $N_c > 2$ from the above arguments). For the parameters used in Fig. 5.11, we find that $\rho J_c \simeq 3.2278 \times 10^{-6}$ for $N_c = 2$ (as in Sec. 5.2.1), $\rho J_c \simeq 4.8891 \times 10^{-6}$ for $N_c = 4$ and $\rho J_c \simeq 6.3290 \times 10^{-6}$ for $N_c = 6$.

We have also rescaled the temperature axis in terms of T_K^{2CK} so as to make comparison between the chains of different length in the critical region. As T_K^{2CK} is the scale characterizing flow from the LM FP to the 2CK FP, we will define it in practice through $S_{\text{imp}}(T_K^{2CK}) = 0.55$ at the critical point for each N_c . Indeed, it is found from NRG that $T_K^{2CK}/D = 10^{-5}$ for $N_c = 2$, $T_K^{2CK}/D = 3 \times 10^{-8}$ for $N_c = 4$, and $T_K^{2CK}/D = 6 \times 10^{-10}$ for $N_c = 6$, which is rough accord with the above heuristic arguments.

On the highest temperature scales, the dots are essentially decoupled from each other and the leads. This is the FO FP ($J_{KL} = J_{KR} = J = 0$ in Eq. 4.1); chains of different length are expected to behave very differently since the underlying number of degrees of freedom of a chain depends on N_c . An entropy of $S_{\text{imp}}(T) = N_c \ln(2)$ is expected, and as is indeed observed in Fig. 5.11 for $T \gg T_{K,L}^{1CK}$.

On the scale of $T \sim T_{K,L}^{1CK}$, the spin on dot 1 is quenched by coupling to the left lead, and so the entropy is expected to drop to $S_{\text{imp}}(T) = (N_c - 1) \ln(2)$. For $N_c > 2$ however, in practice the entropy drops straight to $S_{\text{imp}}(T) = \ln(2)$, since $J \approx T_{K,L}^{1CK}$ for the systems close to the transition considered here. Thus, the higher lying states of the residual $(N_c - 1)$ -length chain are projected out on roughly the same temperature scale. The lowest doublet state of this residual chain gives the $\ln(2)$ entropy.

As discussed above, an effective coupling is then generated between this spin- $\frac{1}{2}$ object and the leads, and RG flow in the vicinity of the 2CK FP is observed for all systems close to the transition. This is manifest in the entropy by flow on the scale of T_K^{2CK} to the characteristic [43–45] 2CK FP value of $S_{\text{imp}}(T) = \frac{1}{2} \ln(2)$.

Lines (b–f) show the behaviour as the transition is approached more closely (from either side). The $\frac{1}{2} \ln(2)$ plateau is clearly extended progressively in the sequence (b→f), indicating that the system is described by the 2CK FP down to lower and lower temperatures/energies. At the critical point itself (line (g); $\lambda = 0$), the 2CK FP is stable and so a residual entropy $S_{\text{imp}}(T = 0) = \frac{1}{2} \ln(2)$ results in each case.

We stress that universality arises on rescaling in terms of T/T_K^{2CK} , with the behaviour for all even chains being common at low-temperature near the transition, as seen from Fig. 5.11.

The inset shows the vanishing scale in the vicinity of the transition for the three

cases considered: $N_c = 2, 4, 6$ (again, shown with solid, dotted and dashed lines). Specifically, we plot $\ln(T_K/T_K^{2CK})$ vs. $\ln(|J - J_c|/J_c)$. The collapse to a common straight line of slope $\nu = 2$ confirms the power-law decay of T_K near the transition as given in Eq. 5.21 for all even chains considered.

We finally comment that, while the discussion in this section and in Sec. 5.2.1 has focused specifically on the case where there is an exponential separation of the 1CK scales $T_{K,L}^{1CK} \gg T_{K,R}^{1CK}$, a transition of exactly the same type is known [36, 37, 78, 109, 112, 113] to arise in the standard mirror-symmetric 2IK model, with the critical coupling in that case $J_c \sim T_K^{1CK}$. This is in fact consistent with Eq. 5.15; the channel-anisotropic model considered here is smoothly connected to the mirror-symmetric case, and so the transition and the nature of the critical point itself is expected to be the same in both cases. Indeed, we have also confirmed with NRG that the same underlying physical behaviour results for $N_c = 4$ and $N_c = 6$ chains in the mirror-symmetric $J_{KL} = J_{KR}$ limit.

5.3 Summary

In this chapter, we studied chains of dots coupled to two leads in the regime where the interdot coupling is small (see Eq. 4.1 and Fig. 4.1). We considered both odd chains (Sec. 5.1) and even chains (Sec. 5.2), demonstrating that very different behaviour results, but that in each case, the low-temperature/energy physics can be understood in terms of simpler effective models.

In Sec. 5.1, we showed that for odd chains, any finite antiferromagnetic interdot coupling, J , in mirror-symmetric systems results in behaviour controlled by the 2CK FP on the lowest temperature/energy scales. Indeed, in Sec. 5.1.1 we developed an effective model to describe the $N_c = 3$ trimer model at low temperatures.

For very small interdot coupling, the dots essentially remain free and uncoupled down to temperatures of order T_K^{1CK} , which corresponds to an effective *single-channel* scale, below which each of the terminal dots of the chain undergo a Kondo effect with their attached lead. The spins of the terminal dots are thus exactly screened by the conduction electrons in the leads, but a local Fermi-liquid description still applies, and so the remaining lead states constitute a bath of non-interacting electrons which can compete to screen the residual spins of the remaining dots. For temperatures $T < J$, the remaining $(N_c - 2)$ dots of the chain form a doublet state (the higher lying states being projected out at low temperatures). An effective coupling between this doublet and the leads, mediated through the Kondo singlets, is then generated (see Eq. 5.10), and so an effective 2CK model (Eq. 5.8) results.

This physical picture was tested directly with NRG in Sec. 5.1.2, where we confirmed the mapping of the full model for $N_c = 3, 5$ and 7 onto the effective 2CK

model at low temperatures by examining both thermodynamics and dynamics in detail. Indeed, the variation of the 2CK scale T_K^{2CK} with J as derived from scaling arguments in Eq. 5.11 was tested and confirmed in Fig. 5.4.

The common behaviour of the thermodynamics at low-temperatures was established in Fig. 5.3, where we demonstrate the universal crossover from the LM FP to the 2CK FP in all systems. The $T = 0$ spectrum $D\rho^{N_c}(\omega)$ presented in Fig. 5.5 shows more subtle behaviour. A resonance for $\omega \sim T_K^{1CK}$, in which the unitarity limit $D\rho^{N_c}(\omega) = 1$ is approximately reached, is indicative of RG flow in the vicinity of the SC FP. This is expected from the discussion presented in Sec. 5.1.1, since the terminal dots form a Kondo singlet state with their attached lead on this scale. At lower frequencies, however, the system is seen to flow to the 2CK FP, driven by the residual coupling between the lowest doublet of the remaining dots and the leads. On the scale of $\omega \sim T_K^{2CK}$ (itself given by Eq. 5.11), the characteristic 2CK FP *half*-unitarity limit value $D\rho^{N_c}(\omega) = \frac{1}{2}$ is reached, which then remains the behaviour of the spectrum down to the Fermi level $\omega = 0$.

In Sec. 5.2, we considered even chains with small interdot couplings. We focused initially on the 2IK model in the case where the mirror symmetry of the model was broken. The large and small J limits of the model clearly indicate the presence of a quantum phase transition in the model (and indeed for any even chain system). Applying similar arguments to those presented in Sec. 5.1, we derived an effective model (Eq. 5.16) to describe the transition in Sec. 5.2.1, and argued that the same effective model describes the transition of all even chains.

In the situation considered, the single-channel Kondo scales are well-separated ($T_{K,L}^{1CK} \gg T_{K,R}^{1CK}$ arising if $J_{KL} > J_{KR}$ from Eq. 5.12), and so dot 1 forms its Kondo singlet with the left lead on the scale $T \sim T_{K,L}^{1CK}$, but the remaining $(N_c - 1)$ dots of the chain still remain essentially free. As the temperature is lowered, all but the the lowest doublet state of this residual odd-length chain is projected out. An effective antiferromagnetic coupling to the left lead, mediated by the Kondo singlet, then results. The bare coupling to the right lead gives rise to an effective *channel-anisotropic* 2CK model, Eq. 5.16.

Varying the interdot coupling J allows to change the degree of channel-anisotropy in the low-energy effective model. Indeed, the effective 2CK model can be tuned to mirror symmetry by varying J , and hence the critical FP of the model must correspond to the 2CK FP. An expression for the critical coupling strength J_c was derived (Eq. 5.18) on the basis of this effective model.

This physical picture was confirmed using NRG for the full 2IK model, where we examined both thermodynamics (Fig. 5.7) and dynamics (Fig. 5.9) in detail. Specifically, we studied the variation of the Kondo scale in the vicinity of the transition (Fig. 5.8), and confirm the analytic prediction of the critical coupling strength (Fig. 5.10).

Finally, we showed with NRG that other even chains exhibit the same underlying physical behaviour. In particular, the transition and the nature of the critical point is found to be the same in all cases.

In Chapters 4 and 5, we have thus studied comprehensively the behaviour of chains of dots coupled to two leads, in all parameter regimes of interest. We used perturbative techniques and scaling arguments to derive low-energy effective models for such systems, which provided a clear physical picture of the expected low-temperature and low-energy behaviour. In all cases, the fundamental physics can be related to the single-spin 2CK model for odd chains, or the 2IK model for even chains. In the latter case, we also showed that the transition which occurs on tuning the interdot coupling can also be thought of in terms of an effective channel-anisotropic 2CK model.

In the following chapters, we turn to ring systems, and show that the possibility of magnetic frustration in such systems gives rise to subtle behaviour *not* accessible in the simpler 2CK or 2IK models.

CHAPTER 6

Frustration and phase transitions in triple quantum dots

In Chapters 4 and 5, we considered chains of quantum dots coupled to two leads, and showed that the resulting low-temperature and low-energy behaviour can be understood in terms of simpler paradigmatic quantum impurity models. Specifically, we demonstrated that all odd chains can be described by an effective single-spin two-channel Kondo (2CK) model, while even chains can be described by an effective two-impurity Kondo (2IK) model. We focused on universality in these systems, highlighting the common fixed-point (FP) structure.

Aspects of triple quantum dot (TQD) models, where three dots are coupled to two leads in a mirror-symmetric fashion, have been previously studied [68, 85, 111, 114], and are consistent with the general description of odd chains presented in Chapter 4. Numata *et al* study a TQD comprising tunnel-coupled Andersonian sites as a function of gate voltage in Ref. [65]. While inherently a Fermi liquid system, various interesting variants on the standard spin- $\frac{1}{2}$ Kondo effect are observed, including $SU(4)$ Kondo behaviour, and an exactly-screened spin-1 two-channel Kondo effect [65]. Other recent work by Žitko and Bonča in Ref. [85] showed that FPs from both the 2CK and the 2IK models are in fact accessible in a spin ring TQD model. The crossover between 2IK and 2CK behaviour on tuning the interdot couplings is studied as a third dot is coupled into a two-impurity two-channel system [85].

However, TQDs arranged in such a ring geometry also provide the simplest and most direct means of studying the effect of local frustration, arising from the internal degrees of freedom of a nanodevice, on Kondo physics [64, 85, 92]. In mirror-symmetric systems, all dot states can be classified by their parity under left $\leftrightarrow$ right interchange [62, 64]. This symmetry permits a level-crossing of states in the isolated trimer on varying the interdot couplings, with a pair of degenerate doublets comprising the ground state when all dots are equivalent. It was recently shown in

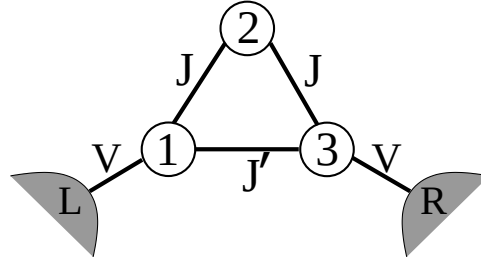


Figure 6.1: Schematic illustration of the two-channel quantum dot trimer.

Ref. [64] that this level-crossing is preserved in the full many-body system when a single lead is attached. The situation is however more subtle on coupling the trimer to two leads, which is the focus of the work presented in this chapter.

We study a ring of three quantum dots, mutually coupled by antiferromagnetic exchange interactions, and tunnel-coupled to two metallic leads (shown schematically in Fig. 6.1), as a function of the interdot exchange couplings. 2CK physics is found to predominate at low-energies in the mirror-symmetric systems considered [85], with a residual spin- $\frac{1}{2}$ overscreened by coupling to both leads. We show however that two *distinct* 2CK phases, with different ground state parities, arise on tuning the interdot exchange couplings. In consequence a frustration-induced quantum phase transition occurs, with the 2CK phases being separated by a novel quantum critical point, the nature of which is uncovered explicitly and analysed in detail. We derive an effective low-energy model to describe the transition, and employ the density matrix extension [20, 21] of Wilson’s numerical renormalization group (NRG) technique [12, 13, 27] to study both thermodynamic and dynamical properties of the system in detail.

6.1 2CK trimer model

We consider a system of three (single-level) quantum dots, arranged in a triangular geometry, as illustrated in Fig. 6.1. Dot ‘2’ is coupled to dots ‘1’ and ‘3’, which are coupled to each other and to their own metallic lead. As discussed in Chapter 2, the key ingredient for 2CK physics is the suppression of charge transfer between the two symmetrically coupled leads [40, 47, 49] — the necessity in essence of a central *spin*. To allow the possibility of accessing non-Fermi liquid 2CK behaviour on the lowest energy/temperature scales, we therefore consider a pure antiferromagnetic exchange interaction between the dots, forming thereby a Heisenberg ring, and model dot 2 strictly as a spin- $\frac{1}{2}$ object.

However, dots 1 and 3 are Anderson-like sites, permitting variable occupation by tunneling between these terminal dots and their connected leads. We focus explicitly

on a system tuned to left/right mirror symmetry (see Fig. 6.1), with Hamiltonian $H = H_L + H_{\text{hyb}} + H_{\text{tri}}$. Here $H_L = \sum_{\alpha, \mathbf{k}, \sigma} \epsilon_{\mathbf{k}} a_{\alpha \mathbf{k} \sigma}^\dagger a_{\alpha \mathbf{k} \sigma}$ refers to the two equivalent non-interacting leads ($\alpha = L, R$), which are tunnel-coupled to dots 1 and 3 via $H_{\text{hyb}} = \sum_{\mathbf{k}, \sigma} V(a_{L \mathbf{k} \sigma}^\dagger c_{1\sigma} + a_{R \mathbf{k} \sigma}^\dagger c_{3\sigma} + \text{H.c.})$. H_{tri} describes the trimer itself, with exchange couplings J and J' ,

$$H_{\text{tri}} = J \hat{\mathbf{S}}_2 \cdot (\hat{\mathbf{S}}_1 + \hat{\mathbf{S}}_3) + J' \hat{\mathbf{S}}_1 \cdot \hat{\mathbf{S}}_3 + \epsilon(\hat{n}_1 + \hat{n}_3) + U(\hat{n}_{1\uparrow} \hat{n}_{1\downarrow} + \hat{n}_{3\uparrow} \hat{n}_{3\downarrow}) \quad (6.1)$$

where $\hat{\mathbf{S}}_i$ is a spin- $\frac{1}{2}$ operator for dot i . For dots $i = 1, 3$, $\hat{n}_i = \sum_{\sigma} \hat{n}_{i\sigma} = \sum_{\sigma} c_{i\sigma}^\dagger c_{i\sigma}$ is the number operator, ϵ is the level energy and U is the intradot Coulomb repulsion. The full Hamiltonian H is thus invariant under simultaneous $1 \leftrightarrow 3$ and $L \leftrightarrow R$ permutation.

6.1.1 The isolated trimer

We are interested in the TQD deep in the $\mathcal{N} = 3$ Coulomb blockade valley, where each dot is in practice singly occupied. To this end we consider explicitly $\epsilon = -\frac{1}{2}U$, the $\mathcal{N} = 2$ or 4 states being much higher ($\sim \frac{1}{2}U$) in energy. H_{tri} (and the full H) is then particle-hole symmetric, although this is incidental: we require only that the singly-occupied manifold of TQD states lies lowest¹. This manifold comprises two doublets and a spin quartet, which is always $\max(J, J')$ higher than the doublets for antiferromagnetic exchange couplings.

To understand the nature of these states, we note that in the singly-occupied regime ($\hat{n}_1 = \hat{n}_3 = 1$), the TQD part of the Hamiltonian, Eq. 6.1, can be equivalently written as $H_{\text{tri}} = J \hat{\mathbf{S}}_2 \cdot \hat{\mathbf{S}}_{13} + \frac{1}{2} J' \hat{\mathbf{S}}_{13}^2$ (omitting irrelevant constants), and $\hat{\mathbf{S}}_{13} = (\hat{\mathbf{S}}_1 + \hat{\mathbf{S}}_3)$ is thus a conserved quantity: $[\hat{\mathbf{S}}_{13}, H_{\text{tri}}] = 0$. As we discussed in Sec. 4.1.1 of Chapter 4, this permits a specification of the eigenstates of H_{tri} in terms of the combined spin of dots 1 and 3, S_{13} , as well as the total TQD spin, S . This in turn allows a particularly simple description of the states from the vector coupling of S and S_{13} (see Eq. 4.2), which is importantly *independent* of J, J' .

The lowest doublet states of the TQD are thus

$$\begin{aligned} |+\rangle; S^z\rangle &= \hat{S}_2^\sigma \frac{1}{\sqrt{2}} \left(c_{1\uparrow}^\dagger c_{3\downarrow}^\dagger + c_{3\uparrow}^\dagger c_{1\downarrow}^\dagger \right) |\text{vac}\rangle \\ |-\rangle; S^z\rangle &= \frac{\sigma}{\sqrt{6}} \left[\hat{S}_2^\sigma (c_{1\uparrow}^\dagger c_{3\downarrow}^\dagger - c_{3\uparrow}^\dagger c_{1\downarrow}^\dagger) - 2\hat{S}_2^{-\sigma} c_{1\sigma}^\dagger c_{3\sigma}^\dagger \right] |\text{vac}\rangle \end{aligned} \quad (6.2)$$

with $S^z = \frac{\sigma}{2}$ and $\sigma = \pm$ for spins $\uparrow/\downarrow$, and $\hat{S}_2^\sigma \equiv \hat{S}_2^\pm$ the raising/lowering operator for the spin on dot 2. $|\text{vac}\rangle = \sum_{\sigma_2} |-\rangle; \sigma_2; -\rangle$ defines the ‘vacuum’ state of the local (dot) Hilbert space, in which dots 1 and 3 are unoccupied, and dot 2 carries a spin- $\frac{1}{2}$.

¹We have also considered the case where $\epsilon \neq -\frac{1}{2}U$, but the physical behaviour discussed here is remarkably robust to this asymmetry.

In particular, we note that $|-, S^z\rangle$ is simply the ground doublet state of a chain of 3 quantum dots (*ie.* in the limit $J' = 0$), given in Eq. 4.3.

The energy separation of the two doublets is $E_\Delta = E_+ - E_- = J - J'$, with $|+, S^z\rangle$ the ground state of the isolated TQD for $J' > J$ and $|-, S^z\rangle$ lowest for $J' < J$. When J' is dominant, dots 1 and 3 naturally lock up into a singlet (see $|+, S^z\rangle$, Eq. 6.2), leaving a free spin on dot 2; with $\langle \hat{\mathbf{S}}_1 \cdot \hat{\mathbf{S}}_3 \rangle = -\frac{3}{4}$ and $\langle \hat{\mathbf{S}}_1 \cdot \hat{\mathbf{S}}_2 \rangle = \langle \hat{\mathbf{S}}_3 \cdot \hat{\mathbf{S}}_2 \rangle = 0$. For $J' < J$ by contrast, dots 1 and 3 are now in a *triplet* configuration ($|-, S^z\rangle$ in Eq. 6.2), with $\langle \hat{\mathbf{S}}_1 \cdot \hat{\mathbf{S}}_3 \rangle = +\frac{1}{4}$ and $\langle \hat{\mathbf{S}}_1 \cdot \hat{\mathbf{S}}_2 \rangle = \langle \hat{\mathbf{S}}_3 \cdot \hat{\mathbf{S}}_2 \rangle = -\frac{1}{2}$.

The states are degenerate precisely at $J' = J$, reflecting the inherent magnetic frustration at that point. A level crossing of the doublets at $J' = J$ is permitted because each has different symmetry under $1 \leftrightarrow 3$ permutation. In Appendix A, we derive an expression for a parity operator, $\hat{P}_{i,j}$, which exchanges orbital labels i and j . It is given by

$$\begin{aligned} \hat{P}_{i,j} = & 2(\hat{\mathbf{I}}_i \cdot \hat{\mathbf{I}}_j - \hat{\mathbf{S}}_i \cdot \hat{\mathbf{S}}_j) + \sum_{k=\{i,j\},\sigma} \frac{1}{2} \hat{n}_{k\sigma} (\hat{n}_{k\sigma} - 1) \\ & + \sum_{\sigma} (c_{i\sigma}^\dagger c_{j\sigma} + \text{H.c.}) (2 - \hat{n}_i - \hat{n}_j) + \frac{1}{2} \end{aligned} \quad (6.3)$$

where $\hat{\mathbf{S}}_i$ is a spin- $\frac{1}{2}$ operator for site i , and $\hat{\mathbf{I}}_i$ is an isospin operator (with components $\hat{I}_i^z = \frac{1}{2}(\hat{n}_i - 1)$ and $\hat{I}_i^+ = c_{i\uparrow}^\dagger c_{i\downarrow}^\dagger$ and $\hat{I}_i^- = (\hat{I}_i^+)^\dagger$).

From Eq. 6.1 it is clear that exchanging dot labels 1 and 3 leaves H_{tri} unchanged. Indeed, it is straightforward to show that $\hat{P}_{1,3}$ commutes with the isolated TQD Hamiltonian, $[\hat{P}_{1,3}, H_{\text{tri}}] = 0$, and so all states of H_{tri} can be classified according to $1 \leftrightarrow 3$ parity. Since such a permutation operation is self-adjoint and self-inverse (involutory), it follows that $\hat{P}_{1,3}^2 = 1$, and so the eigenvalues of $\hat{P}_{1,3}$ are ± 1 only.

In the spin-only ('singly-occupied') regime, the parity operator may be expressed concisely as [150] $\hat{P}_{1,3} = (1 - \hat{\mathbf{S}}_{13}^2)$. Thus $\hat{P}_{1,3}|\pm; S^z\rangle = \pm|\pm; S^z\rangle$ describes the parity of the doublet states of H_{tri} , which is wholly equivalent to a specification of the states by S_{13} . We note that the full lead-coupled Hamiltonian H is not of course invariant to $1 \leftrightarrow 3$ interchange alone, but rather to simultaneous exchange of the 1,3 dot labels *and* the left/right leads (embodied in $\hat{P}_{L,R} = \hat{P}_{1,3} \prod_{\mathbf{k}} \hat{P}_{L\mathbf{k}, R\mathbf{k}}$, see Appendix A), which we will refer to as 'overall $L \leftrightarrow R$ ' symmetry in what follows.

6.1.2 Effective low-energy models

On tunnel-coupling to the leads, effective models describing the system on low-energy/temperature scales in the $\mathcal{N} = 3$ -electron valley of interest may be obtained by standard Schrieffer-Wolff transformations [8, 17], perturbatively eliminating virtual excitations into the $\mathcal{N} = 2$ - and 4-electron sectors of H to second order in H_{hyb} (and neglecting retardation effects [8] as usual). The calculations are lengthy, so

rather than giving full details we sketch below a somewhat simplified, but physically more transparent, account of the key results (Eqs. 6.7 and 6.13 below).

First we consider the effective low-energy model appropriate to the temperature range $(J, J') < T < U$, in which all dots become singly-occupied. Here the appropriate unity operator for the TQD Hilbert space is $\hat{1}_{\text{so}} = \sum_{\sigma_1, \sigma_2, \sigma_3} |\sigma_1; \sigma_2; \sigma_3\rangle \langle \sigma_1; \sigma_2; \sigma_3|$, with $\sigma_i = \uparrow/\downarrow$ the spin of dot i . To second order in the dot-lead tunneling V , a spin-model of form $H_s = H_L + H_{\text{eff}}^s + H_{\text{tri}}^s$ arises; where H_L describes the leads as above and:

$$\begin{aligned} H_{\text{tri}}^s &= J \hat{\mathbf{S}}_2 \cdot (\hat{\mathbf{S}}_1 + \hat{\mathbf{S}}_3) + J' \hat{\mathbf{S}}_1 \cdot \hat{\mathbf{S}}_3 \\ H_{\text{eff}}^s &= J_K (\hat{\mathbf{S}}_1 \cdot \hat{\mathbf{s}}_{L0} + \hat{\mathbf{S}}_3 \cdot \hat{\mathbf{s}}_{R0}) \end{aligned} \quad (6.4)$$

Here the effective exchange coupling is $\rho J_K = 8\Gamma/(\pi U)$, with ρ the lead density of states per orbital at the Fermi level as usual, and $\Gamma = \pi V^2 \rho_T$ is the hybridization, with total lead density of states $\rho_T = N\rho$, and N the number of orbitals/ $\mathbf{k}$ -states in the lead (such that NV^2 , and hence Γ , is finite in the continuum limit $N \rightarrow \infty$). In Eq. 6.4, $\hat{\mathbf{s}}_{\alpha 0}$ is the spin density of lead $\alpha = L(R)$ at dot 1(3), as given in Eq. 3.2.

The lowest states of H_{tri}^s are the doublets $|\pm; S^z\rangle$ given in Eq. 6.2. Provided they are not near-degenerate, only the lower doublet need be retained: $|+; S^z\rangle$ for $J' \gg J$ and $|-; S^z\rangle$ for $J' \ll J$. To first order in J_K , an effective low-energy model is then obtained simply by projecting into the reduced Hilbert space of the lowest doublet, using

$$\hat{1}_{\pm} = \sum_{S^z} |\pm; S^z\rangle \langle \pm; S^z| \quad (6.5)$$

for the appropriate $\gamma = +$ or $-$ doublet ground state. The resultant Hamiltonian $H_{\text{eff}, \gamma} = \hat{1}_{\gamma} H_{\text{eff}}^s \hat{1}_{\gamma}$ follows as

$$H_{\text{eff}, \gamma} = \frac{1}{2} J_K \hat{1}_{\gamma} (\hat{\mathbf{S}}_1 + \hat{\mathbf{S}}_3) \hat{1}_{\gamma} \cdot (\hat{\mathbf{s}}_{L0} + \hat{\mathbf{s}}_{R0}) \quad (6.6)$$

using the symmetry $\hat{1}_{\gamma} \hat{\mathbf{S}}_1 \hat{1}_{\gamma} = \hat{1}_{\gamma} \hat{\mathbf{S}}_3 \hat{1}_{\gamma}$ (which can also be shown explicitly using Eqs. 6.3 and 6.5).

Following the approach outlined in Sec. 4.1.2, it is readily shown that Eq. 6.6 is of two-channel Kondo form,

$$H_{\text{eff}, \gamma} = J_{K\gamma} \hat{\mathbf{S}}_{\gamma} \cdot (\hat{\mathbf{s}}_{L0} + \hat{\mathbf{s}}_{R0}), \quad (6.7)$$

where $\hat{\mathbf{S}}_{\gamma}$ is the spin- $\frac{1}{2}$ operator representing the appropriate doublet $\gamma = +$ or $-$, with components $\hat{S}_{\gamma}^z = \sum_{S^z} |\gamma; S^z\rangle S^z \langle \gamma; S^z|$ and $\hat{S}_{\gamma}^{\pm} = |\gamma; \pm \frac{1}{2}\rangle \langle \gamma; \mp \frac{1}{2}|$. At this level of calculation the effective exchange coupling (as in Sec. 4.1.2) is given by $J_{K\gamma} = \langle \gamma; +\frac{1}{2} | \hat{S}_1^z + \hat{S}_3^z | \gamma; +\frac{1}{2} \rangle J_K$. From Eq. 6.2, an antiferromagnetic effective Kondo coupling $J_{K-} = +\frac{2}{3} J_K$ then arises for the $|-; S^z\rangle$ ground state appropriate to $J' \ll J$

(which of course applies to the $J' = 0$ case studied explicitly in Sec. 4.1.2, and the same result is obtained for the effective coupling through Eq. 4.10). By contrast, for the $|+; S^z\rangle$ doublet (lowest for $J' \gg J$), $J_{K+} = 0$ results. In the latter case, there is in fact a weak residual antiferromagnetic coupling: a full $\mathcal{O}(V^2)$ Schrieffer-Wolff calculation gives precisely the two-channel Kondo model Eq. 6.7 as one would expect, but with $J_{K\pm}$ given by

$$\rho J_{K+} = \frac{4\Gamma}{\pi} \left\{ \frac{1}{3(J' - J) + 2U} - \frac{1}{3J' + J + 2U} \right\} \quad (6.8a)$$

$$\rho J_{K-} = \frac{4\Gamma}{3\pi} \left\{ \frac{9}{(J - J') + 2U} - \frac{1}{5J - J' + 2U} \right\}; \quad (6.8b)$$

yielding $\rho J_{K-} = \frac{2}{3}\rho J_K \propto \frac{\Gamma}{U}$ to leading order in $1/U$, and a much smaller but non-vanishing $\rho J_{K+} = \frac{4\Gamma J}{\pi U^2} + \mathcal{O}(\frac{1}{U^3})$ for the singlet-locked doublet $|+; S^z\rangle$, reflecting the residual antiferromagnetic coupling between the spin on dot 2 and the leads.

Hence, sufficiently deep in either regime $J' \ll J$ or $J' \gg J$, the low-energy behaviour of the system is that of a 2CK model. The lowest spin- $\frac{1}{2}$ state of the TQD is thus overscreened by conduction electrons, embodied in the infrared 2CK fixed point describing the non-Fermi liquid ground state [40, 47, 49], in which the partially quenched spin is characterised by a residual entropy of $S_{\text{imp}} = \frac{1}{2} \ln 2$ (setting $k_B = 1$ as usual). This overscreening sets in below the characteristic two-channel Kondo scale $T_{K,\gamma}^{2CK}$, which can be determined from perturbative scaling (see Sec. 2.4 and Ref. [40]), and is given by

$$T_{K,\gamma}^{2CK} \sim J_{K\gamma} \exp(-1/\rho J_{K\gamma}). \quad (6.9)$$

Since $\hat{P}_{1,3}$ commutes with all components of $\hat{\mathbf{S}}_\gamma$ in Eq. 6.7, $[\hat{H}_{\text{eff},\gamma}, \hat{P}_{1,3}] = 0$, whence $1 \leftrightarrow 3$ parity is conserved in the effective low-energy model. Since that parity is determined by $\gamma = +$ or $-$, there are two *distinct* 2CK phases, which one thus expects to be separated by a quantum phase transition (QPT).

In the vicinity of the transition, *ie.* close to $J' \simeq J$, neither of the two 2CK models in Eq. 6.7 is of course sufficient to describe the low-energy physics: the states $|+; S^z\rangle$ and $|-; S^z\rangle$ are now near-degenerate, so both must be retained in the low-energy trimer manifold. Hence, defining $\hat{1} = \hat{1}_+ + \hat{1}_-$ and proceeding in direct parallel to the discussion above, an effective low-energy model in the vicinity of the transition is obtained from $H_{\text{eff}}^{\text{trans}} = \hat{1}(H_{\text{eff}}^s + H_{\text{tri}}^s)\hat{1}$. From Eq. 6.4 for H_{eff}^s , using $\hat{\mathbf{S}}_1 = \hat{P}_{1,3}\hat{\mathbf{S}}_3\hat{P}_{1,3}$ such that $\langle \gamma; S^z | \hat{\mathbf{S}}_1 | \gamma'; S^{z'} \rangle = \gamma\gamma' \langle \gamma; S^z | \hat{\mathbf{S}}_3 | \gamma'; S^{z'} \rangle$ and hence

$\hat{1}_\gamma \hat{\mathbf{S}}_1 \hat{1}_{\gamma'} = \gamma \gamma' \hat{1}_\gamma \hat{\mathbf{S}}_3 \hat{1}_{\gamma'}$, one obtains

$$\begin{aligned} H_{\text{eff}}^{\text{trans}} = \sum_{\gamma=\pm} \frac{1}{2} J_K [\hat{1}_\gamma (\hat{\mathbf{S}}_1 + \hat{\mathbf{S}}_3) \hat{1}_\gamma \cdot (\hat{\mathbf{s}}_{L0} + \hat{\mathbf{s}}_{R0}) \\ + \hat{1}_\gamma (\hat{\mathbf{S}}_1 - \hat{\mathbf{S}}_3) \hat{1}_{-\gamma} \cdot (\hat{\mathbf{s}}_{L0} - \hat{\mathbf{s}}_{R0})] \\ + \frac{1}{2} E_\Delta (\hat{1}_+ - \hat{1}_-). \end{aligned} \quad (6.10)$$

The final term in Eq. 6.10 (arising from $\hat{1} H_{\text{tri}}^s \hat{1}$) is simply the energy difference between the $\gamma = +/ -$ doublets, and the first term is (see Eq. 6.6) the 2CK coupling of *each* doublet to the leads. It is helpful to recast Eq. 6.10 in terms of spin- $\frac{1}{2}$ operators for real spin $\hat{\mathbf{S}}$ ($= \sum_\gamma \hat{\mathbf{S}}_\gamma$) and pseudospin $\hat{\mathcal{T}}$ for the local Hilbert space, defined by

$$\hat{S}^z = \sum_{\gamma=\pm, S^z} |\gamma; S^z\rangle S^z \langle \gamma; S^z| \quad (6.11a)$$

$$\hat{\mathcal{T}}^z = \sum_{\gamma=\pm, S^z} |\gamma; S^z\rangle \frac{1}{2} \gamma \langle \gamma; S^z| \quad (6.11b)$$

and

$$\hat{S}^\pm = \sum_\gamma |\gamma; \pm \frac{1}{2}\rangle \langle \gamma; \mp \frac{1}{2}| \quad (6.12a)$$

$$\hat{\mathcal{T}}^\pm = \sum_{S^z} |\pm; S^z\rangle \langle \mp; S^z|. \quad (6.12b)$$

From Eq. 6.11, the TQD doublets $|\gamma; S^z\rangle$ are each eigenstates of $\hat{S}^z$ and $\hat{\mathcal{T}}^z$; in particular, the eigenvalues of $\hat{\mathcal{T}}^z \equiv \frac{1}{2}(\hat{1}_+ - \hat{1}_-)$ correspond simply to (half) the parity of the appropriate doublet. By contrast, the doublets are interconverted by $\hat{\mathcal{T}}^\pm$ (Eq. 6.12b), $\hat{\mathcal{T}}^+ | -; S^z \rangle = | +; S^z \rangle$ and $\hat{\mathcal{T}}^- | +; S^z \rangle = | -; S^z \rangle$, acting to switch parity.

After simple if laborious algebra, Eq. 6.10 reduces to

$$\begin{aligned} H_{\text{eff}}^{\text{trans}} = (\frac{1}{2} J_A + J_B \hat{\mathcal{T}}^z) \hat{\mathbf{S}} \cdot (\hat{\mathbf{s}}_{L0} + \hat{\mathbf{s}}_{R0}) \\ + J_{\text{mix}} (\hat{\mathcal{T}}^+ + \hat{\mathcal{T}}^-) \hat{\mathbf{S}} \cdot (\hat{\mathbf{s}}_{L0} - \hat{\mathbf{s}}_{R0}) \\ + E_\Delta \hat{\mathcal{T}}^z, \end{aligned} \quad (6.13)$$

in terms of spin/pseudospin operators, with

$$J_A = (J_{K+} + J_{K-}) \quad J_B = (J_{K+} - J_{K-}) \quad (6.14)$$

and $J_{\text{mix}} = \langle +; +\frac{1}{2} | \hat{S}_1^z - \hat{S}_3^z | -; +\frac{1}{2} \rangle J_K = \frac{1}{\sqrt{3}} J_K$ using Eq. 6.2. In fact, a full $\mathcal{O}(V^2)$ Schrieffer-Wolff calculation again gives precisely the effective Hamiltonian Eq. 6.13,

with

$$\rho J_{\text{mix}} = \frac{2\Gamma}{\sqrt{3}\pi} \left\{ \frac{1}{3J' + J + 2U} + \frac{1}{5J - J' + 2U} + \frac{3}{3(J' - J) + 2U} + \frac{3}{(J - J') + 2U} \right\} \quad (6.15)$$

recovering $J_{\text{mix}} = \frac{1}{\sqrt{3}}J_K$ to leading order in $1/U$, and $J_{K\pm}$ as given by Eq. 6.8.

Eq. 6.13 is the essential low-energy model applicable to the vicinity of the QPT; we study it directly via NRG in Sec. 6.4. The pseudospin operators can naturally be classified according to $1 \leftrightarrow 3$ parity, the components of $\hat{\mathcal{T}}$ having different parity under $\hat{P}_{1,3}$: using $\hat{P}_{1,3}|\gamma; S^z\rangle\langle\gamma'; S^z| = \gamma\gamma'\langle\gamma'; S^z|\langle\gamma; S^z|\hat{P}_{1,3}$, Eqs. 6.11b and 6.12b give $\hat{P}_{1,3}\hat{\mathcal{T}}^z = +\hat{\mathcal{T}}^z\hat{P}_{1,3}$, while $\hat{P}_{1,3}\hat{\mathcal{T}}^\pm = -\hat{\mathcal{T}}^\pm\hat{P}_{1,3}$ for the raising/lowering components. By contrast, all components of spin $\hat{\mathbf{S}}$ (Eqs. 6.11a, 6.12a) commute with $\hat{P}_{1,3}$. Hence, since the global (overall $L \leftrightarrow R$) parity must be conserved ($[H_{\text{eff}}^{\text{trans}}, \hat{P}_{L,R}] = 0$), interactions involving the $\hat{\mathcal{T}}^z$ component of pseudospin can only couple to *even* combinations $\hat{\mathbf{S}}_{L0} + \hat{\mathbf{S}}_{R0}$ of the lead spin densities (symmetric under interchange of the L/R lead labels), as in the first term of Eq. 6.13 (or 6.10); while by the same token interactions involving $\hat{\mathcal{T}}^\pm$ must be associated with the *odd* (antisymmetric) combination $\hat{\mathbf{S}}_{L0} - \hat{\mathbf{S}}_{R0}$, as in the second term of Eq. 6.13. In the vicinity of the QPT the latter is of course the key interaction in $H_{\text{eff}}^{\text{trans}}$, since in switching the parity of the TQD states it in essence drives the transition between the two 2CK phases.

Finally, note that the last term of Eq. 6.13, equivalent to a magnetic field acting on the pseudospin, energetically favours the $|-, S^z\rangle$ doublet ($\mathcal{T}^z = -\frac{1}{2}$) when their energy separation $E_\Delta > 0$, and $|+, S^z\rangle$ ($\mathcal{T}^z = +\frac{1}{2}$) for $E_\Delta < 0$. Hence, when $|E_\Delta|$ is sufficiently large that only one of the doublets need be retained in the low-energy TQD manifold, the $\hat{\mathcal{T}}^\pm$ terms are obviously suppressed; and Eq. 6.13 then reduces as it must to one or other of the 2CK models Eq. 6.7. In fact, as shown in Sec. 6.3, for any $|E_\Delta| \neq 0$, the $E_\Delta\hat{\mathcal{T}}^z$ term in Eq. 6.13 ensures that one or other of the 2CK fixed points ultimately remains the stable low-temperature FP.

By contrast, precisely at the point of frustration where $|E_\Delta| = 0$, the $\hat{\mathcal{T}}^\pm$ terms in Eq. 6.13 destabilize the 2CK FPs. The resultant $H_{\text{eff}}^{\text{trans}}$ then describes the *quantum critical point* which separates the two 2CK phases, and which we consider in detail in Sec. 6.3.

6.2 Properties of the 2CK Phases

The physical picture thus indicates that 2CK physics dominates the low-energy behaviour of the model, but that a QPT occurring as a function of J' exists between two 2CK phases of distinct parity.

We now analyse the properties of each 2CK phase of the full model, using Wil-

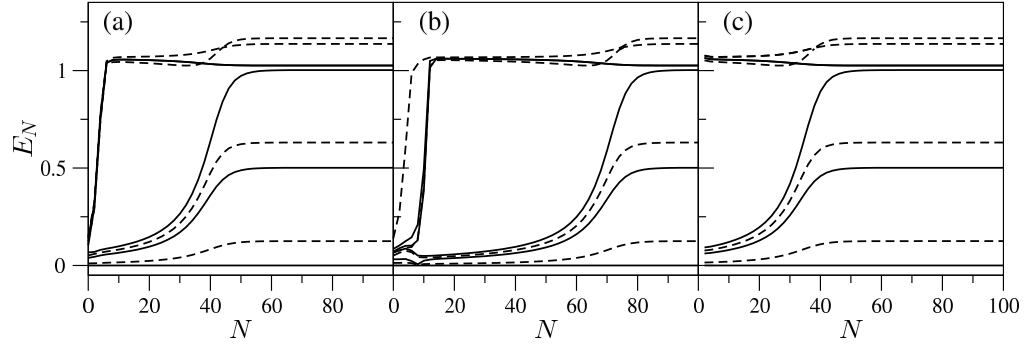


Figure 6.2: Lowest five NRG energy levels of the left-charge/right-charge/spin subspaces $(Q_L, Q_R, S^z) \equiv (0, 0, \frac{1}{2})$ [solid lines] and $(0, 1, 0)/(1, 0, 0)$ [dashed], versus (even) iteration number, N . Shown for $\rho J = 0.1$, $\tilde{U} = U/(\pi\Gamma) = 7$, with $\rho J' = 0$ [panel (a)] and $\rho J' = 0.105$ [panel (b)]. For comparison, panel (c) shows corresponding results for a pure (single-spin) 2CK model with $\rho J_K = 0.055$.

son's NRG technique [12, 13, 27], employing a complete basis set of the Wilson chain [20] to calculate the full density matrix [20, 21] as described in Chapter 3. Calculations are typically performed for an NRG discretization parameter $\Lambda = 3$, retaining the lowest $N_s = 4000$ states per iteration. As above, we choose for convenience $\epsilon = -\frac{1}{2}U$, and consider a symmetric constant density of states for each lead, with density of states per conduction orbital $\rho = 1/(2D)$, and bandwidth $D = 100\Gamma \gg 1$ (such that results shown are essentially independent of D). In all calculations shown, we use a fixed $\rho J = 0.1$ and $\tilde{U} \equiv U/(\pi\Gamma) = 7$, varying the exchange J' (see Fig. 6.1)².

Fig. 6.2 shows the evolution of the lowest energy levels of the system as a function of NRG iteration number N , exemplifying RG flow between different FPs of the model. Panel (a) is for a system deep in the $J' < J$ regime (specifically $\rho J' = 0$, as studied as the $N_c = 3$ case in Chapter 4), while panel (b) shows the energy levels for $\rho J' = 0.105$ ($> \rho J$). For comparison, panel (c) is for a pure (single spin- $\frac{1}{2}$) 2CK model of form Eq. 6.7, *ie.* $H = J_K \hat{\mathbf{S}} \cdot (\hat{\mathbf{s}}_{L0} + \hat{\mathbf{s}}_{R0})$, with a Kondo coupling $\rho J_K = 0.055$ chosen to be the same as the effective coupling ρJ_{K-} of the ground state TQD doublet in (a) (as obtained from Eq. 6.8(b)). In both cases (a) and (b), the levels are seen to converge quite rapidly to their $N \rightarrow \infty$ values, which are clearly those of the 2CK FP in Fig. 6.2(c). These levels are of course characteristic of the 2CK FP, and — after a trivial rescaling by a factor which depends on the NRG discretization parameter Λ — are described by the fractions $0, \frac{1}{8}, \frac{1}{2}, \frac{5}{8}, 1...$ as determined from a conformal field theory analysis of the FP [46, 48], and as

²The essential physics is of course the same whether $J \sim U$ or $\ll U$, since the dots remain singly-occupied. We consider here a relatively large $J/U \sim \mathcal{O}(1)$ largely for numerical convenience, and clarity of the resulting physical behaviour, albeit noting that quantum dots in graphene typically have [104] $J/U \sim \frac{1}{3}$.

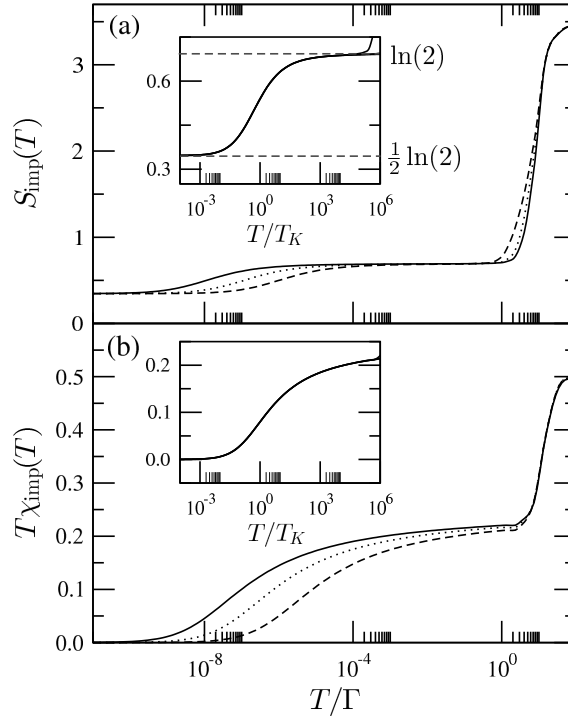


Figure 6.3: Thermodynamics of the $J' < J$ phase. Shown for fixed $\tilde{U} = 7$ and $\rho J = 0.1$, varying $\rho J' = 0$ (solid lines), 0.0375 (dotted) and 0.075 (dashed). Panel (a) shows $S_{\text{imp}}(T)$, (b) shows $T\chi_{\text{imp}}(T)$, both *vs.* T/Γ . Insets show the universality arising on rescaling in terms of the 2CK Kondo temperature, T_K , all curves collapsing to a common form.

exemplified in Fig. 3.6.

The iteration number by which the levels converge to the set of 2CK FP levels is however clearly different in (a) and (b), reflecting the different Kondo scales characteristic of the two cases. Case (b) ($J' > J$) flows close to the local moment (LM) FP between $N = 10$ to 60 (with levels naturally characteristic of the LM FP in that range), and approaches the stable 2CK FP by $N \simeq 80$. By contrast, convergence to the 2CK FP in (a) and (c) both occur at $N \approx 50$ (with a much shorter range of N close to the LM FP). Since the iteration number is related to an effective temperature through $T/\Gamma \sim \Lambda^{-N/2}$ (see Eq. 3.53 and Refs. [12,13]), the 2CK Kondo scales (which here we simply denote “ T_K ”) of the three examples in Fig. 6.2 are thus exponentially small (as expected from Eq. 6.9). However, T_K/Γ for (b) is some 8 orders of magnitude smaller than that of (a), reflecting the distinct nature of the coupling in the two cases, as discussed in Sec. 6.1.2.

6.2.1 Thermodynamics

NRG results for thermodynamics in each phase are now considered. We focus on the ‘impurity’ (TQD) contribution [13,27] to the entropy, $S_{\text{imp}}(T)$, and the uniform

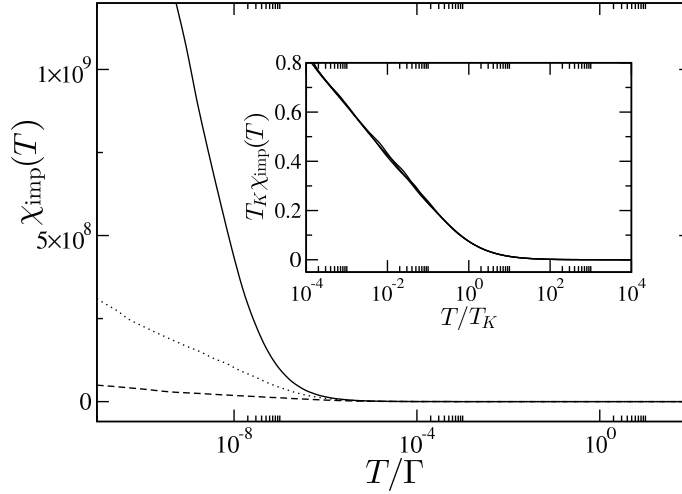


Figure 6.4: Spin susceptibility $\chi_{\text{imp}}(T)$ vs T/Γ in the $J' < J$ regime, for same parameters as Fig. 6.3. Inset: scaling collapse onto the universal form $T_K \chi_{\text{imp}}(T) = \alpha \ln(T_K/T)$.

spin susceptibility, $T\chi_{\text{imp}}(T)$, which provide clear signatures of the underlying FPs of the model, and the relevant energy scales associated with the crossovers between them, as discussed in Sec. 3.5.

$J' < J$

For the $J' \ll J$ regime the effective 2CK model Eq. 6.7 should describe the system for $T \ll |J - J'| = |E_\Delta|$, where the lowest TQD doublet (in this case the odd parity state $|-, S^z\rangle$) couples symmetrically to the leads. 2CK physics is thus expected below $T \sim T_K \equiv T_{K-}^{2CK}$.

For the full model, Fig. 6.3 shows both $S_{\text{imp}}(T)$ [panel (a)] and $T\chi_{\text{imp}}(T)$ [panel (b)] for fixed $\tilde{U} = 7$ and $\rho J = 0.1$, with $J'/J = 0, 0.375$ and 0.75 , all deep in the $J' < J$ regime. In each case, at high temperatures $T \gtrsim U$ the behaviour is governed by the free orbital [13] (FO) FP, with all possible states of the TQD thermally accessible, and hence $S_{\text{imp}} = \ln(32)$ results (corresponding to the entropy associated with two free sites and one free spin). For $T \lesssim U$ the dots become in essence singly occupied, and hence an entropy of $\ln(8)$ is expected³. Below $T \sim |E_\Delta|$ all but the lowest trimer doublet is projected out. Thus S_{imp} approaches $\ln(2)$, signifying the LM FP where the lowest doublet is essentially a free spin- $\frac{1}{2}$ disconnected from the leads (the LM FP Hamiltonian being Eq. 6.7 with $J_{K-} \equiv 0$).

The LM FP is however unstable, and the system always flows to the stable 2CK FP below $T \sim T_K$, recovering (Fig. 6.3(a)) the $\frac{1}{2} \ln 2$ residual entropy known to be characteristic of the 2CK FP [43–45]. As discussed in Sec. 3.5, in practice we

³In practice the systems in Fig. 6.3 flow directly to the LM FP from the FO FP, with no $\ln(8)$ entropy plateau since there is not a wide scale separation between U and J .

may define a Kondo temperature $T_K \equiv T_K^S$ through the entropy, via $S_{\text{imp}}(T_K^S) = 0.55$ (suitably between $\ln 2$ and $\frac{1}{2} \ln 2$); or alternatively $T_K \equiv T_K^\chi$ through the spin susceptibility via $T_K^\chi \chi_{\text{imp}}(T_K^\chi) = 0.07$ (as in Ref. [13]). Deep in the 2CK phases the two definitions are equivalent ($T_K^\chi \equiv T_K^S \equiv T_K$), probing as they do the common characteristic scale associated with flow to the 2CK FP. The inset to Fig. 6.3(a) shows the entropy of the three systems rescaled in terms of T/T_K ; showing scaling collapse to a common functional form, *ie.* the universality characteristic of the crossover from the LM FP to the stable 2CK FP [45], and as demonstrated explicitly in Fig. 3.10.

The underlying FPs of the model are likewise evident from $T\chi_{\text{imp}}(T)$, Fig. 6.3(b). The highest T behaviour corresponds to two uncorrelated sites (dots 1 and 3 of the TQD) and a free spin (dot 2). Hence $T\chi_{\text{imp}}(T) = 2 \times \frac{1}{8} + \frac{1}{4} = \frac{1}{2}$, readily understood as the mean $\langle (S^z)^2 \rangle$ of the quasidegenerate states. On decreasing T the LM FP is again rapidly reached, the lowest TQD doublet following the free spin- $\frac{1}{2}$ Curie law $T\chi_{\text{imp}}(T) = \frac{1}{4}$. Below T_K the spin susceptibility is quenched [43, 45, 46] in the sense that $T\chi_{\text{imp}}(T) \rightarrow 0$ as $T \rightarrow 0$. In the inset to Fig. 6.3(b) the data are rescaled in terms of T/T_K , again showing universality in the approach to the 2CK FP [45].

The characteristic low- T logarithmic divergence [43, 45, 46] of $\chi_{\text{imp}}(T)$ itself is evident in Fig. 6.4 for the same parameters as Fig. 6.3. The slopes of the divergence vary widely between the three cases, but all collapse to the universal form [45] $T_K \chi_{\text{imp}}(T) = \alpha \ln(T_K/T)$ (with α a constant), as seen in the inset of the figure.

$J' > J$

From the arguments of Sec. 6.1.2, 2CK physics is again expected at low-energies in the $J' \gg J$ regime, where the even-parity $|+; S^z\rangle$ doublet is now the lowest TQD state. This is confirmed in Fig. 6.5, where (in direct parallel to Fig. 6.3 for $J' \ll J$) thermodynamics are shown for fixed $\tilde{U} = 7$ and $\rho J = 0.1$, but now with $J'/J = 1.05$, 1.15 and 1.25 (solid, dotted and dashed lines, respectively). Of course, for non-universal temperature scales $T > U$, all states of the dots are thermally accessible, and so once again all systems are described by the FO FP (with its characteristic $S_{\text{imp}} = \ln(32)$ entropy and $T\chi_{\text{imp}} = \frac{1}{2}$ susceptibility). As the temperature is lowered, the entropy naturally drops, since higher lying states become depopulated. However, a short $\ln(4)$ plateau is also observed in the case of $J'/J = 1.05$ (solid line), as the quartet has been projected out but, over a small temperature range, the lowest doublets remain quasidegenerate. Such behaviour is only observed when $J \simeq J'$, and we return to this in Sec. 6.3.

In all cases, the unstable LM FP is rapidly reached on lowering the temperature still further, as in the case $J' < J$, considered in Fig. 6.3. Residual antiferromagnetic correlations between the $|+; S^z\rangle$ doublet and the leads, described by Eq. 6.7, drive

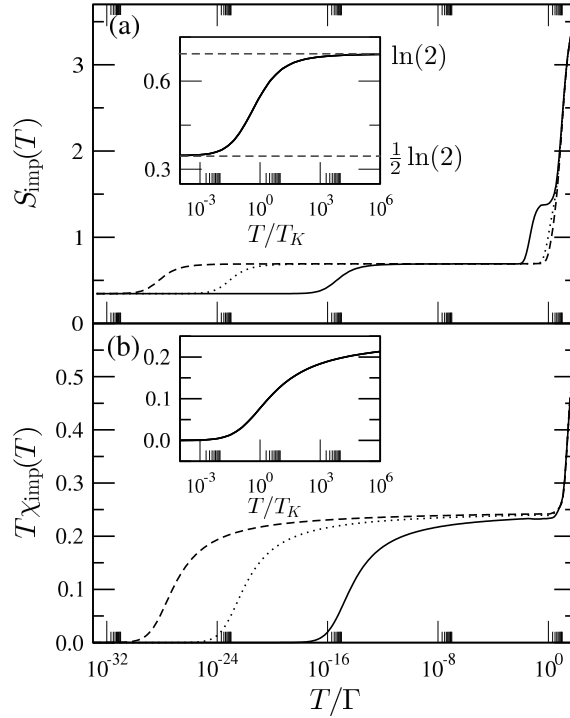


Figure 6.5: Thermodynamics of the $J' > J$ phase. Shown for fixed $\tilde{U} = 7$, $\rho J = 0.1$, varying $\rho J' = 0.105$ (solid lines), 0.115 (dotted) and 0.125 (dashed). Panel (a) again shows $S_{\text{imp}}(T)$, (b) shows $T\chi_{\text{imp}}(T)$, both *vs* T/Γ . Insets show rescaling in terms of the Kondo temperature, T_K , yielding the same universal 2CK scaling curves as in Fig. 6.3.

the system to the 2CK FP below $T \sim T_K$. The entropy thus drops to $S_{\text{imp}} = \frac{1}{2} \ln(32)$, while $T\chi_{\text{imp}} = 0$. As expected, $\chi_{\text{imp}}(T)$ itself (not shown) is again found to diverge logarithmically below T_K . Indeed, the scaling forms for $S_{\text{imp}}(T)$ and $T\chi_{\text{imp}}(T)$ *vs.* T/T_K shown in the insets of Fig. 6.5, are precisely those arising for $J' \ll J$ and shown in Fig. 6.3.

While the low-energy physics in the two regimes $J' \ll J$ and $J' \gg J$ have common 2CK scaling behaviour (which confirms the mapping in both phases onto the same effective single-spin 2CK model), we add that the Kondo scales T_K themselves evolve very differently with J' . We consider this explicitly in Sec. 6.2.3 (see Fig. 6.10), but it is also directly evident even from cursory comparison of Figs. 6.5 and 6.3.

6.2.2 Dynamics

We turn now to dynamics, focusing largely on the local single-particle spectrum of dot 1 (or, equivalently by symmetry, dot 3): $D_1(\omega) = -\frac{1}{\pi} \text{Im}\{G_1(\omega)\}$, with $G_1(\omega)$ the local retarded Green function (as for the conventional Anderson model discussed

in Sec. 3.6.1). We obtain it through the Dyson equation,

$$[G_1(\omega)]^{-1} = [G_1^0(\omega)]^{-1} - \Sigma_1(\omega), \quad (6.16)$$

where $G_1^0(\omega)$ is the non-interacting propagator (*ie.* for $U = 0 = J = J'$); and $\Sigma_1(\omega)$ is the proper electron self-energy, with $\Sigma_1(\omega) \equiv \Sigma_1^R(\omega) - i\Sigma_1^I(\omega)$ (such that $\Sigma_1^I(\omega) \geq 0$). The non-interacting $G_1^0(\omega)$ is given trivially by [8] $[G_1^0(\omega)]^{-1} = \omega^+ - \epsilon - \Gamma(\omega)$ (with $\omega^+ = \omega + i0^+$), where $\Gamma(\omega) = \sum_{\mathbf{k}} V^2 [\omega^+ - \epsilon_{\mathbf{k}}]^{-1}$ is the usual one-electron hybridization function for coupling of dot 1 to the left lead: $\Gamma(\omega) \equiv \Gamma^R(\omega) - i\Gamma^I(\omega)$, with $\Gamma^I(\omega) = \Gamma (= \pi V^2 \rho_T)$ for all $|\omega| < D$ inside the band, and $\Gamma^R(\omega = 0) \simeq 0$.

An expression for the electron self-energy $\Sigma_1(\omega)$ is also readily obtained using equation of motion methods [8, 139]. It is given by

$$\begin{aligned} \Sigma_1(\omega) = [G_1(\omega)]^{-1} & \left\{ U \langle \langle c_{1\uparrow} \hat{n}_{1\downarrow}; c_{1\uparrow}^\dagger \rangle \rangle_\omega \right. \\ & + \frac{1}{2} J \langle \langle c_{1\downarrow} \hat{S}_2^- + c_{1\uparrow} \hat{S}_2^z; c_{1\uparrow}^\dagger \rangle \rangle_\omega \\ & \left. + \frac{1}{2} J' \langle \langle c_{1\downarrow} \hat{S}_3^- + c_{1\uparrow} \hat{S}_3^z; c_{1\uparrow}^\dagger \rangle \rangle_\omega \right\} \end{aligned} \quad (6.17)$$

where as usual, $\langle \langle \hat{A}; \hat{B} \rangle \rangle_\omega$ is the Fourier transform of the retarded correlator $\langle \langle \hat{A}(t_1); \hat{B}(t_2) \rangle \rangle = -i\theta(t_1 - t_2) \langle \{ \hat{A}(t_1), \hat{B}(t_2) \} \rangle$, and where the local Green function itself is given by $G_1(\omega) = \langle \langle c_{1\sigma}; c_{1\sigma}^\dagger \rangle \rangle_\omega$ (independent of spin σ in the absence of a magnetic field). The self-energy can be calculated directly within the density matrix formulation of the NRG [20, 21, 27, 126] via Eq. 6.17, and $G_1(\omega)$ itself can then be obtained from Eq. 6.16. $D_1(\omega)$ calculated in this way is highly accurate [27, 126], with many of the artifacts known to arise from the discretization of the leads being removed [27, 126], and automatically guarantees correct normalization of the spectrum [20, 21].

To motivate study of the spectrum $D_1 (\equiv D_1(\omega; T))$, we note that it controls the zero-bias conductance through dot 1. The TQD does not of course mediate current from the L to R leads, since the internal couplings between constituent dots are pure exchange (Fig. 6.1 and Eq. 6.1). However the L and R leads in Fig. 6.1 can obviously each be ‘split’ in two (symmetrically, to preserve overall $L \leftrightarrow R$ symmetry), enabling a current to be driven through dot 1 or dot 3, with the same zero-bias conductance resulting in either case, by symmetry. Following Meir and Wingreen [56], the resultant conductance follows as

$$\frac{G_c(T)}{G_0} = \int_{-\infty}^{\infty} -\frac{\partial f(\omega)}{\partial \omega} \pi \Gamma D_1(\omega; T) d\omega \quad (6.18)$$

where $f(\omega) = [e^{\omega/T} + 1]^{-1}$ is the Fermi function (with $\omega = 0$ the Fermi level) and $G_0 = 2e^2/h$ the (spin-summed) conductance quantum. The (ω, T) -dependence of D_1

thus controls the conductance, and for $T = 0$ in particular $G_c(T = 0)/G_0 = \pi\Gamma D_1(\omega = 0; T = 0)$. From Eq. 6.16, the local propagator for $\omega = 0 = T$ may be expressed as $[G_1(\omega = 0)]^{-1} = -\epsilon^* + i\Gamma^*$ in terms of the renormalized single-particle level ϵ^* and renormalized hybridization Γ^* , given by

$$\epsilon^* = \epsilon + \Sigma_1^R(0) \quad (6.19a)$$

$$\Gamma^* = \Gamma + \Sigma_1^I(0) \quad (6.19b)$$

in terms of the $\omega = 0$ value of the self-energy at $T = 0$; and hence from Eq. 6.18:

$$\frac{G_c(T = 0)}{G_0} = \pi\Gamma D_1(0; 0) = \frac{\Gamma}{\Gamma^*} \left(\frac{1}{1 + \left(\frac{\epsilon^*}{\Gamma^*}\right)^2} \right). \quad (6.20)$$

This expression will be used shortly to determine the zero-bias conductance in the 2CK phase.

We have argued above that, sufficiently deep in either regime $J' < J$ or $J' > J$, the low-energy physics of the full TQD model must reduce to that of a single spin- $\frac{1}{2}$ 2CK model (with the form of Eq. 6.7).

While various dynamical properties associated with the 2CK FP have been studied previously, no local single-particle spectrum of the standard 2CK model can be defined *per se*, since the dot is of course strictly singly-occupied, being modelled as a *spin*. However, the local spectrum for systems comprising Andersonian dots tunnel-coupled to two leads has been studied in *eg.* Ref. [68], and the self-energy calculated for the same system in Ref. [141]. The conductance near the 2CK FP of coupled dot models has also been examined in *eq.* Refs. [67, 151] — although such tunnel-coupled systems that permit inter-lead charge transfer are ultimately Fermi-liquids at $\omega = 0$, and are not described by the 2CK FP as $T \rightarrow 0$.

The quadrupolar single-impurity Anderson model studied in Ref. [108] is however described by the 2CK FP on the lowest temperature/energy scales, as is the $O(3)$ symmetric Anderson model, which is exactly equivalent to the 2CK model in the large U limit [106, 107]. This model is examined in detail in Refs. [106, 107], and the spectral density is explicitly calculated. Indeed, the spectrum of the zero-orbital of the Wilson chain is studied in the 2CK model itself in Ref. [152].

NRG results for single-particle dynamics of the full TQD ring model are considered below, but first a question arises: can a direct comparison be made between the spectrum $\pi\Gamma D_1(\omega)$, and the dynamical quantities studied near the 2CK FP of the other models mentioned above? In particular, to which dynamical property of a pure 2CK model should the spectral density $\pi\Gamma D_1(\omega)$ be compared? To answer

these questions, note first that Eq. 6.18 may be written equivalently as

$$\frac{G_c(T)}{G_0} = \int_{-\infty}^{\infty} -\frac{\partial f(\omega)}{\partial \omega} \left[-\pi \rho_T \text{Im}\{t_L(\omega)\} \right] d\omega \quad (6.21)$$

in terms of the t-matrix, $t_L(\omega)$, for the L lead, with $t_\alpha(\omega)$ defined in the usual way in terms of scattering of electron states in the $\alpha = L, R$ lead (see Sec. 3.6.2), via

$$G_{\alpha\mathbf{k},\alpha\mathbf{k}'}(\omega) = \frac{\delta_{\mathbf{k}\mathbf{k}'}}{\omega^+ - \epsilon_{\mathbf{k}}} + \frac{1}{\omega^+ - \epsilon_{\mathbf{k}}} t_\alpha(\omega) \frac{1}{\omega^+ - \epsilon_{\mathbf{k}'}} \quad (6.22)$$

where $G_{\alpha\mathbf{k},\alpha\mathbf{k}'}(\omega) = \langle\langle a_{\alpha\mathbf{k}\sigma}; a_{\alpha\mathbf{k}'\sigma}^\dagger \rangle\rangle_\omega$ is the propagator for the lead states. Using equation of motion methods [8, 139] it is straightforward to show that $t_L(\omega) = V^2 G_1(\omega)$ (likewise $t_R(\omega) = V^2 G_3(\omega) \equiv t_L(\omega)$), and so

$$\pi\Gamma D_1(\omega; T) = -\pi\rho_T \text{Im}\{t_L(\omega)\} \quad (6.23)$$

where $\Gamma = \pi V^2 \rho_T$, hence the equivalence of Eqs. 6.18 and 6.21.

Proceeding analogously to the approach adopted in Ref. [127], in Sec. 3.6.3 we define the spectral density of the (mirror-symmetric) single-spin 2CK model as

$$D\rho^{2CK}(\omega) = -\pi\rho_T \text{Im}\{t_\alpha^{2CK}(\omega)\} \quad (6.24)$$

where $t_\alpha^{2CK}(\omega)$ is the scattering t-matrix for lead $\alpha = L, R$ (with $t_L^{2CK}(\omega) = t_R^{2CK}(\omega) \equiv t^{2CK}(\omega)$ by symmetry), given explicitly in Eqs. 3.79 and 3.80. Comparison between $\pi\Gamma D_1(\omega; T)$ for the full TQD model (Eq. 6.23), and $D\rho^{2CK}(\omega)$ for the standard 2CK model (Eq. 6.24) obviously yields the desired correspondence, since the t-matrices of both systems describe the same 2CK FP at low energies/temperatures.

Thus, the conductance through dot 1 (or equivalently by symmetry, dot 3) in the TQD model can be calculated through Eq. 6.21, and can then be compared with the results near the 2CK FP in *eg.* Refs. [67, 68, 151]. Indeed, by establishing the form of the t-matrix in the quadrupolar Anderson model [108] and the $O(3)$ symmetric Anderson model [106], one can directly compare the spectral densities to $\pi\Gamma D_1(\omega)$ through Eq. 6.23, which we consider below.

Dynamics: results

Fig. 6.6 shows the $T = 0$ spectrum $\pi\Gamma D_1(\omega)$ *vs.* ω/Γ , in the $J' < J$ regime (for the same bare parameters as Fig. 6.3 for thermodynamics). The main panel shows results on a log scale for $\omega > 0$; and particle-hole symmetry for $\epsilon = -\frac{1}{2}U$ means $D_1(\omega) = D_1(-\omega)$ (as seen in the inset). The figure also shows $D\rho^{2CK}(\omega)$ for the single-spin 2CK model (for $\rho J_K = 0.07$, ensuring an exponentially small Kondo scale but otherwise chosen arbitrarily).

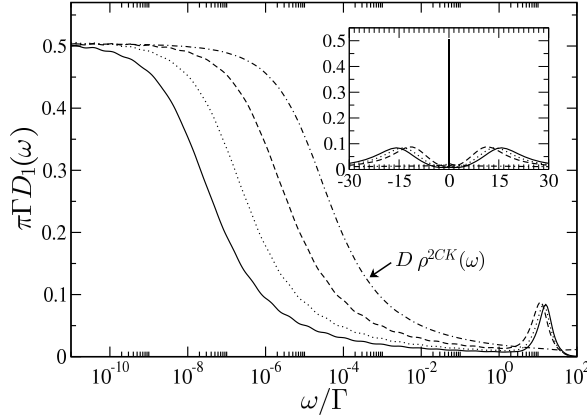


Figure 6.6: $T=0$ local spectrum $\pi\Gamma D_1(\omega)$ vs. ω/Γ in the $J' < J$ regime. Shown (as in Fig. 6.3) for fixed $\tilde{U} = 7$ and $\rho J = 0.1$, varying $J'/J = 0$ (solid line), 0.375 (dotted) and 0.75 (dashed). The dot-dashed line is the spectral density $D\rho^{2CK}(\omega)$ (Eq. 6.24) for a single-spin 2CK model (Eq. 2.24), with $\rho J_K = 0.07$. Inset: results shown on a linear frequency scale.

We first comment on the high-energy spectral features (‘Hubbard satellites’) in $D_1(\omega)$. As usual, these reflect simple one-electron addition to the isolated TQD ground state. The lowest such excitation from the $|-, S^z\rangle$ TQD ground state incurs an energy cost $\Delta E_- = \frac{1}{4}(J - J') - \epsilon$. On tunnel coupling to the leads these features are naturally broadened, but the satellites are centred on $\omega \simeq \Delta E_-$, indeed seen from Fig. 6.6 to shift slightly to lower ω on increasing J' . In the $J' > J$ regime (not shown), directly analogous behaviour arises. Here the $|+, S^z\rangle$ doublet is the TQD ground state, the Hubbard satellites in $D_1(\omega)$ are now centred around $\omega \simeq \Delta E_+ = \frac{3}{4}(J' - J) - \epsilon$, and hence shift to *higher* frequency as J' is increased. By contrast, see Fig. 6.6, Hubbard satellites are simply absent in $\rho^{2CK}(\omega)$ – addition/removal excitations are suppressed by construction in modelling a dot strictly as a spin, and as previously discussed in Secs. 3.6.3 and 4.2.2.

The most important characteristic of the spectra in Fig. 6.6 is of course the low-energy Kondo resonance, the form of which reflects RG flow in the vicinity of the stable 2CK fixed point. At the Fermi level $\omega = 0$ in particular, $\pi\Gamma D_1(\omega = 0) = \frac{1}{2}$ in all cases (likewise $D\rho^{2CK}(0) = \frac{1}{2}$), a hallmark of the 2CK FP. This result was established for $D\rho^{2CK}(0)$ in Sec. 3.6.3, and was again confirmed for odd chains of spins in Chapter 4. Indeed, that the spectral density at the 2CK FP reaches *half* the unitarity limit is consistent with results known from study of the two-channel (quadrupolar) single-impurity Anderson model [108, 141] and the $O(3)$ symmetric Anderson model [106].

Universal scaling of single-particle dynamics is considered in Fig. 6.7, where $\pi\Gamma D_1(\omega)$ vs. ω/T_K is shown (with T_K defined in practice from thermodynamics, as in Sec. 6.2.1). The figure includes the three examples shown in Fig. 6.6 for the

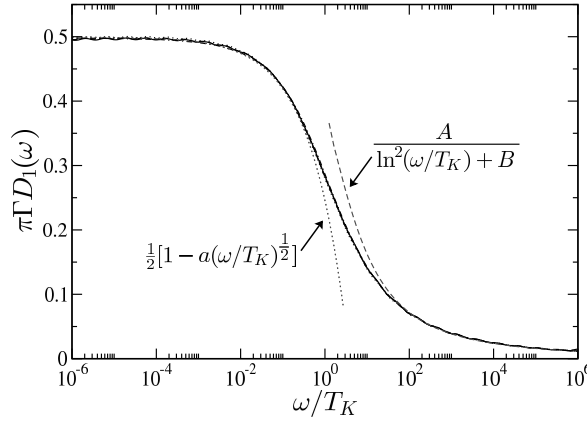


Figure 6.7: $T = 0$ scaling spectrum for the 2CK phases. $\pi\Gamma D_1(\omega)$ vs. ω/T_K is shown both in the $J' < J$ regime (for the bare parameter sets used in Fig. 6.3) and for the $J' > J$ regime (with the parameters used in Fig. 6.5). $D\rho^{2CK}(\omega)$ vs. ω/T_K for the single-spin 2CK model is also shown. All spectra collapse to the same universal form. The dotted line shows the low- $|\omega|/T_K$ asymptotic behaviour $\pi\Gamma D_1(\omega) = \frac{1}{2}[1 - a(|\omega|/T_K)^{\frac{1}{2}}]$, while the dashed line describes the high- $|\omega|/T_K$ scaling behaviour, $\pi\Gamma D_1(\omega) = A/[\ln^2(|\omega|/T_K) + B]$.

$J' < J$ (odd parity ground state) regime, as well as spectra for the $J' > J$ (even parity) regime for the same parameters as Fig. 6.5, together with $D\rho^{2CK}(\omega)$ vs. ω/T_K for the pure 2CK model. As seen from Fig. 6.7, all spectra collapse perfectly to a universal scaling form, confirming that the TQD model – be it in the $J' > J$ or $J' < J$ regime – is described by the effective 2CK model Eq. 6.7 at low-energies.

Since $\pi\Gamma D_1(\omega)$ for all systems deep in the 2CK phases of the TQD model collapse precisely to the universal scaling form for the single-spin 2CK model (presented previously in Fig. 4.6), the asymptotic behaviour of the spectrum must be the same as that discussed in Sec. 4.2.2. In particular, the leading low-frequency asymptotic behaviour of the scaling spectrum is

$$\pi\Gamma D_1(\omega) \underset{\frac{|\omega|}{T_K} \ll 1}{\sim} \frac{1}{2}[1 - a(|\omega|/T_K)^{\frac{1}{2}}] \quad (6.25)$$

with the constant $a \simeq 0.47$, while for $|\omega|/T_K \gg 1$ by contrast, the asymptotic behaviour is

$$\pi\Gamma D_1(\omega) \underset{\frac{|\omega|}{T_K} \gg 1}{\sim} A/[\ln^2(|\omega|/T_K) + B] \quad (6.26)$$

with A and B pure constants $\mathcal{O}(1)$. Eqs. 6.25 and 6.26 constitute the TQD analogue of Eqs. 4.17 and 4.18 which describe the asymptotics of $D\rho^{N_c}(\omega)$ for odd spin chains (including of course the $N_c = 1$ case, corresponding thereby to the standard single-spin 2CK model). Thus the behaviour is likewise consistent at low frequencies with that of the quadrupolar Anderson model studied in Ref. [108]. Indeed, at high frequencies, the behaviour is asymptotically common to that of single-channel

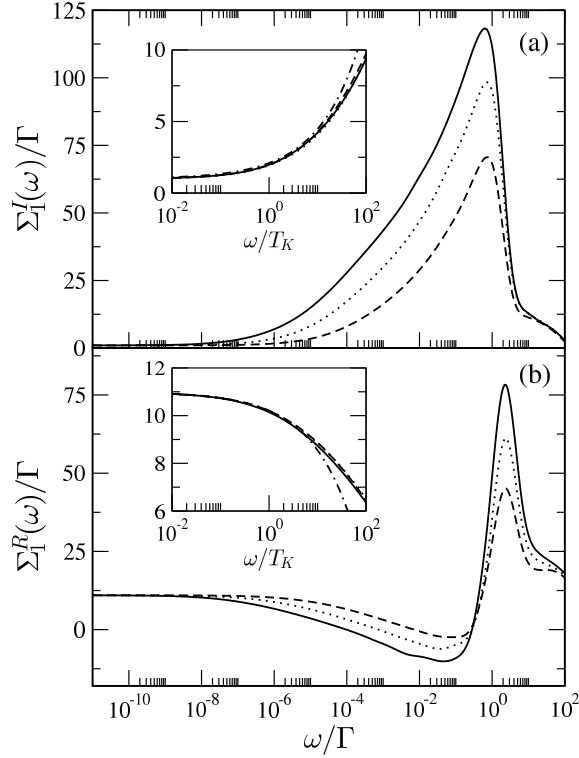


Figure 6.8: Electron self-energy $\Sigma_1(\omega)/\Gamma$ vs. ω/Γ for the same parameters as Fig. 6.6. Panel (a): imaginary part, $\Sigma_1^I(\omega)/\Gamma$; panel (b): real part, $\Sigma_1^R(\omega)/\Gamma$. Insets: universal scaling forms as a function of ω/T_K , with the dot-dashed lines showing the low-frequency asymptotic behaviour $\Sigma_1^I(\omega)/\Gamma = 1 + c|\omega/T_K|^{\frac{1}{2}}$, and $\Sigma_1^R(\omega)/\Gamma = -\epsilon/\Gamma - \text{sgn}(\omega)c'|\omega/T_K|^{\frac{1}{2}}$.

models studied in Refs. [31, 33], since the origin of these high energy leading $\sim 1/\ln^2(|\omega|/T_K)$ logarithms is spin-flip scattering processes [8], which naturally occur for both single-channel and two-channel models.

We consider now the electron self-energy of dot 1 in the full TQD model, the real and imaginary parts of which are shown in Fig. 6.8 and naturally exhibit scaling in terms of ω/T_K . For $\Sigma_1^I(\omega)$ we find the low- ω/T_K asymptotic behaviour to be $\Sigma_1^I(\omega)/\Gamma = 1 + c|\omega/T_K^{2CK}|^{\frac{1}{2}}$ as shown explicitly in the inset to panel (a). At the Fermi level in particular, $\Sigma_1^I(\omega = 0) = \Gamma$, in marked contrast to a Fermi liquid phase for which $\Sigma^I(\omega = 0) = 0$ generically; and leading to a renormalized hybridization (Eq. 6.19b) $\Gamma^* = \Gamma + \Sigma_1^I(\omega = 0) = 2\Gamma$. The real part of the self-energy is shown in panel (b), and at the Fermi level in particular is found to be $\Sigma_1^R(\omega = 0) = -\epsilon$, such that the renormalized level $\epsilon^* = 0$ (Eq. 6.19a).

Since $\Gamma^* = 2\Gamma$ and $\epsilon^* = 0$, it follows from Eq. 6.20 that the $T = 0$ zero-bias conductance for the TQD model reduces to one-half the unitarity limit, *ie.* $G_c(T = 0)/G_0 = \frac{1}{2}$, as known to be the case for a single-spin 2CK model [47, 67, 151, 152]. Moreover, although the explicit case for which we have shown results is $\epsilon = -U/2$

where the TQD model is particle-hole symmetric, we note that $\Gamma^* = 2\Gamma$ and $\epsilon_* = 0$ — and hence $\pi\Gamma D_1(\omega) = \frac{1}{2}$ and $G_c(0)/G_0 = \frac{1}{2}$ — is also found to hold exactly on moving away from particle-hole symmetry. Indeed, only when the TQD is far away from the $\mathcal{N} = 3$ regime does the physical picture discussed here change qualitatively.

The results above refer to dynamics for $T = 0$, and we now touch on $T > 0$. Universality implies $\pi\Gamma D_1(\omega; T)$ depends on ω/T_K and T/T_K . Without loss of generality it may be cast as

$$\pi\Gamma D_1(\omega; T) = \pi\Gamma D_1(0; T) - \frac{a}{2} \left(\frac{|\omega|}{T_K} \right)^{\frac{1}{2}} g \left(\frac{\omega}{T_K}; \frac{T}{T_K} \right) \quad (6.27)$$

where the scaling function g satisfies $g(0; 0) = 1$, so that at $T = 0$, Eq. 6.27 reduces asymptotically to Eq. 6.25 for $\pi\Gamma D_1(\omega; T = 0)$. For the Fermi level $\omega = 0$ in particular, the leading low- T/T_K dependence of $\pi\Gamma D_1(0; T)$ is found from NRG to be

$$\pi\Gamma D_1(0; T) \underset{\frac{T}{T_K} \ll 1}{\sim} \frac{1}{2} [1 - b (T/T_K)^{\frac{1}{2}}] \quad (6.28)$$

with $b \simeq a$ a constant. Employing Eq. 6.27 in Eq. 6.18 for $G_c(T)$, and rescaling the resultant non-trivial integral (arising from the second term of Eq. 6.27) by exploiting the fact that the Fermi function depends solely on ω/T , gives the leading low- T/T_K behaviour of the zero-bias conductance as

$$\frac{G_c(T)}{G_0} = \frac{1}{2} [1 - \gamma (T/T_K)^{\frac{1}{2}}] \quad (6.29)$$

where γ is a constant ($\gamma = b + a'$ with $a' = a\sqrt{\pi}\eta(\frac{1}{2}) \simeq 1.07a$ and $\eta(z)$ the Dirichlet η -function). And the behaviour Eq. 6.29 is precisely that known to arise for the single-spin 2CK model [47, 67, 151, 152].

Finally, we consider briefly the local dynamic spin susceptibility of dot 1 in the 2CK phases, given by $\chi_1(\omega) = -\frac{1}{\pi} \text{Im} \langle \langle \hat{S}_1^z; \hat{S}_1^z \rangle \rangle_\omega$. Fig. 6.9 shows $\chi_1(\omega)$ *vs.* ω/Γ (for $T = 0$) in the $J' < J$ regime, with the same bare parameter sets as Fig. 6.6 (the behaviour discussed below being applicable in both 2CK phases). In the standard single-channel Anderson model, $\chi_1(\omega)$ exhibits characteristic low- ω Fermi liquid behaviour [8, 140], $\chi_1(\omega) \propto \omega$. By contrast, it is known [106, 108] that at the 2CK FP, $\chi_1(0)$ plateaus at a finite constant; itself proportional to the slope of the log divergence of $\chi_{\text{imp}}(T)$ as $T \rightarrow 0$. In Fig. 6.4 (inset) for the full TQD model we showed the uniform static spin susceptibility to have a low- T log divergence of form $\chi_{\text{imp}}(T) = \frac{\alpha}{T_K} \ln(T_K/T)$, with slope α/T_K . Thus we also expect $T_K\chi_1(\omega)$ to exhibit universality as a function of ω/T_K ; as indeed confirmed in the inset of Fig. 6.9.

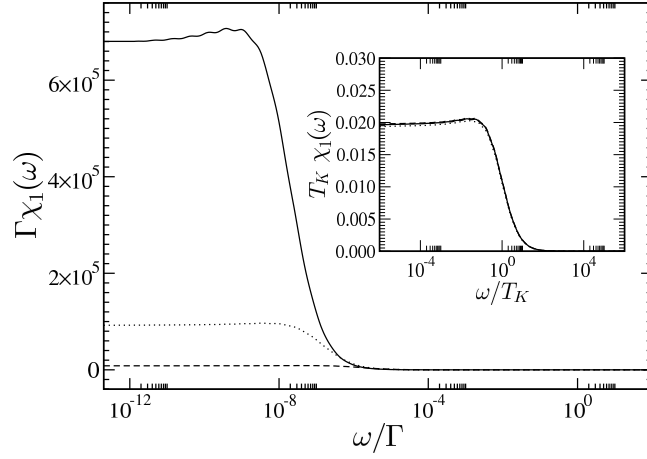


Figure 6.9: Local dynamic susceptibility $\Gamma\chi_1(\omega)$ vs. ω/Γ at $T = 0$ for the same bare parameters as Fig. 6.6. Inset: showing universal scaling of $T_K\chi_1(\omega)$ vs. ω/T_K .

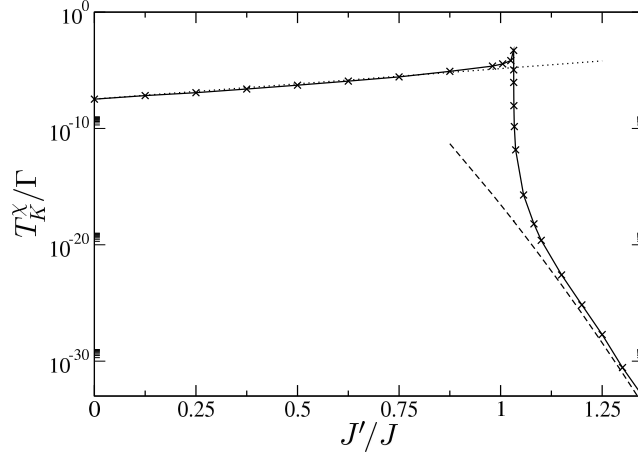


Figure 6.10: Kondo temperature T_K^X/Γ (points, with solid line as guide to eye) vs. J'/J for fixed $\tilde{U} = 7$ and $\rho J = 0.1$; as defined (Sec. 6.2.1) via $T_K^X\chi_{\text{imp}}(T_K^X) = 0.07$. Kondo scales obtained from perturbative scaling (Eq. 6.9) are also shown, with ρJ_{K+} (for $J'/J > 1$) from Eq. 6.8(a) (dashed line) and ρJ_{K-} (for $J'/J < 1$) from Eq. 6.8(b) (dotted); with a trivial constant prefactor adjusted to fit the data in each case.

6.2.3 Kondo Scales

The energy scale on which 2CK physics emerges in the full TQD model is of course the two-channel Kondo temperature. T_K itself varies markedly with the bare model parameters, with qualitatively different behaviour for $J'/J < 1$ and $J'/J > 1$ that reflects the distinct nature (Sec. 6.1.2) of the lowest-energy TQD doublets in the two regimes, $|-, S^z\rangle$ and $|+, S^z\rangle$ respectively. This is shown in Fig. 6.10, considering explicitly the Kondo scale $T_K \equiv T_K^X$ obtained (as in Sec. 6.2.1) from the uniform susceptibility, and showing T_K^X/Γ vs. J'/J . In the $J' < J$ regime a relatively

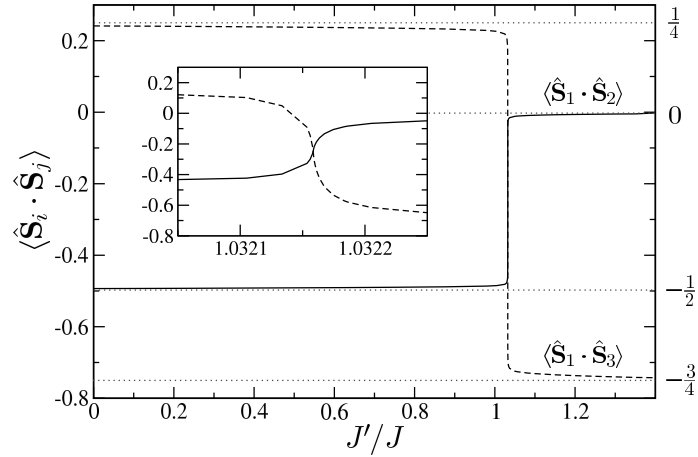


Figure 6.11: $T = 0$ spin-spin correlation functions $\langle \hat{\mathbf{S}}_1 \cdot \hat{\mathbf{S}}_2 \rangle$ (solid line) and $\langle \hat{\mathbf{S}}_1 \cdot \hat{\mathbf{S}}_3 \rangle$ (dashed) vs. J'/J , for fixed $\bar{U} = 7$ and $\rho J = 0.1$. Inset: magnification around the point of frustration, where $\langle \hat{\mathbf{S}}_1 \cdot \hat{\mathbf{S}}_2 \rangle = \langle \hat{\mathbf{S}}_1 \cdot \hat{\mathbf{S}}_3 \rangle$, occurring at $J'/J = 1.03216\dots$

modest increase in T_K occurs on increasing J'/J ; while for $J' > J$ by contrast T_K diminishes very rapidly, reflecting physically the weak residual antiferromagnetic coupling (Sec. 6.1.2) between the spin on dot 2 and the leads, when the singlet-locked $|+; S^z\rangle$ doublet is the TQD ground state.

In Sec. 6.1.2 we showed that the full TQD H maps onto an effective single-spin 2CK model (Eq. 6.7) in each of the $J' < J$ and $> J$ regimes, provided the separation between the TQD doublets $|E_\Delta| = |J - J'|$ is sufficiently large that one or other alone dominates the low-energy physics. The resultant Kondo temperatures for the two regimes are then given from perturbative scaling by Eqs. 6.9 and 6.8. These are compared directly to the NRG results for T_K^x in Fig. 6.10, and are seen to agree quantitatively for $|E_\Delta|/J \gtrsim 0.1$, *ie.* throughout the great majority of each of the two 2CK regimes.

6.3 Quantum phase transition

When $|E_\Delta| = |J - J'|$ is sufficiently small however, neither TQD doublet alone dominates the low-energy physics, both must then be included in the low-energy trimer manifold, and as shown in Sec. 6.1.2 the low-energy behaviour is no longer described by an effective single-spin 2CK model, but rather by Eq. 6.13, with coupling between doublets of distinct parity embodied in the pseudospin raising/lowering terms. We show in the following that these additional terms in the effective Hamiltonian drive a quantum phase transition between the two 2CK phases, occurring at the point of inherent magnetic frustration.

In the *isolated* TQD, frustration occurs at $J' = J$ where the TQD doublets

are degenerate, a trivial level-crossing ‘transition’ occurring in this case as $J'_c = J$ is crossed. As a result, ground state properties in general change discontinuously across J'_c , exemplified *eg.* by the spin correlation functions $\langle \hat{\mathbf{S}}_1 \cdot \hat{\mathbf{S}}_2 \rangle$ and $\langle \hat{\mathbf{S}}_1 \cdot \hat{\mathbf{S}}_3 \rangle$ which (as in Sec. 6.1.1) change abruptly at J'_c from $-\frac{1}{2}$ and $+\frac{1}{4}$ respectively in the $(-)$ -parity phase $J' < J'_c$ to 0 and $-\frac{3}{4}$ respectively in the $(+)$ -parity phase for $J' > J'_c$. That situation changes qualitatively on coupling to the leads, as illustrated in Fig. 6.11 where the $T = 0$ spin correlators $\langle \hat{\mathbf{S}}_1 \cdot \hat{\mathbf{S}}_2 \rangle$ and $\langle \hat{\mathbf{S}}_1 \cdot \hat{\mathbf{S}}_3 \rangle$ are shown as a function of J'/J for the full model [85]. While their behaviour sufficiently deep in either of the 2CK regimes naturally accords with expectations from the isolated TQD, they now vary continuously with J'/J , as seen clearly from the magnification of the crossover region in the inset. The value of J'/J for which $\langle \hat{\mathbf{S}}_1 \cdot \hat{\mathbf{S}}_3 \rangle = \langle \hat{\mathbf{S}}_1 \cdot \hat{\mathbf{S}}_2 \rangle$ ($\equiv \langle \hat{\mathbf{S}}_3 \cdot \hat{\mathbf{S}}_2 \rangle$) is the point of complete magnetic frustration, and as seen from the inset to Fig. 6.11 is naturally slightly renormalized from unity, to $J'_c/J = 1.03216\dots$ in the example shown.

We shall see in the following sections that the QPT occurs at $\tilde{E}_\Delta = J'_c - J' = 0$, with a quantum critical point separating the two 2CK phases of distinct parity.

6.3.1 Physical picture of the transition

Before showing NRG results, we give heuristic physical arguments for the behaviour of the system in the vicinity of the QPT, based on the effective low-energy Hamiltonian $H_{\text{eff}}^{\text{trans}}$ (Eq. 6.13) in which both TQD doublet states are retained in the low-energy trimer manifold. $H_{\text{eff}}^{\text{trans}}$ is cast in terms of spin- $\frac{1}{2}$ operators for both real spin ($\hat{\mathbf{S}}$) and pseudospin ($\hat{\mathbf{T}}$) for the local TQD Hilbert space, the distinct parity of the two doublets being reflected in the $\mathcal{T}^z = \pm\frac{1}{2}$ components of pseudospin.

In Eq. 6.13 the exchange couplings $\frac{1}{2}(J_A \pm J_B)$ ($\equiv J_{K\pm}$) are both > 0 (antiferromagnetic), in which case it is readily argued (and confirmed explicitly by NRG) that the low-energy FP structure of $H_{\text{eff}}^{\text{trans}}$ is independent of J_B (although of course the energy scales on which these FPs are reached under renormalization will inevitably be somewhat different). For simplicity in the following we thus consider $J_B = 0$ in Eq. 6.13, *ie.*

$$\begin{aligned} H_{\text{eff}}^{\text{trans}} = & \frac{1}{2}J_A \hat{\mathbf{S}} \cdot (\hat{\mathbf{s}}_{L0} + \hat{\mathbf{s}}_{R0}) \\ & + J_{\text{mix}}(\hat{\mathcal{T}}^+ + \hat{\mathcal{T}}^-)\hat{\mathbf{S}} \cdot (\hat{\mathbf{s}}_{L0} - \hat{\mathbf{s}}_{R0}) \\ & + \tilde{E}_\Delta \hat{\mathcal{T}}^z, \end{aligned} \quad (6.30)$$

with $\tilde{E}_\Delta = J'_c - J'$ (rather than the ‘bare’ $E_\Delta = J - J'$, allowing simply for the slight renormalization of J'_c away from the value $J'_c = J$ in the isolated TQD, as above).

For $\tilde{E}_\Delta \neq 0$, a ‘magnetic field’ acts on the z -component of pseudospin, and as mentioned in Sec. 6.1.2 the low-energy physics is ultimately that of a single-

spin 2CK FP (we return to it below). But now consider $\tilde{E}_\Delta = 0$ in Eq. 6.30; *ie.* $J' = J'_c$, corresponding to the transition itself. In this case no field acts on the pseudospin, its ‘ z -component’ as such being arbitrary. Recalling that $\hat{T}^+ + \hat{T}^- = 2\hat{T}^x$ in Eq. 6.30, and then performing a trivial rotation of the pseudospin axes from $(x, y, z) \rightarrow (z, x, y)$, Eq. 6.30 may be written as:

$$H_{\text{eff}}^{\text{trans}}(\tilde{E}_\Delta = 0) = \left(\frac{1}{2}J_A + 2J_{\text{mix}}\hat{T}^z\right)\hat{\mathbf{S}} \cdot \hat{\mathbf{s}}_{L0} + \left(\frac{1}{2}J_A - 2J_{\text{mix}}\hat{T}^z\right)\hat{\mathbf{S}} \cdot \hat{\mathbf{s}}_{R0} \quad (6.31)$$

This Hamiltonian commutes with $\hat{T}^z$, so is strictly separable into disjoint $\mathcal{T}^z = +\frac{1}{2}$ and $-\frac{1}{2}$ sectors. As a consequence, the pseudospin is free. But in either given $\mathcal{T}^z$ sector, the spin $\hat{\mathbf{S}}$ clearly couples asymmetrically to the L and R channels: one has *channel anisotropy*. In the single spin- $\frac{1}{2}$ 2CK model, channel anisotropy is of course well known [40,42,45,46,49,124] to destabilise the 2CK FP. As discussed in Secs. 2.4, 3.4.3 and 4.3.1, the spin- $\frac{1}{2}$ is instead now fully quenched by the channel to which it is most strongly antiferromagnetically exchange-coupled, and is decoupled from the second conduction channel/lead. The ultimate stable fixed point is then equivalent to the *single channel* strong coupling FP plus an extra free chain, which we denote SC: α as before, with $\alpha = L, R$ the more strongly coupled lead. We stress that the SC: α FP is inherently a single-channel object, with the second lead decoupled entirely; only the *corrections* to the FP involve the second lead. Indeed, for systems not close to mirror-symmetry, we showed in Figs. 4.7 and 4.10 of Chapter 4 that the approach to the SC: α FP from the LM FP evident in both thermodynamics and dynamics is effectively that of a single-channel Anderson model on low temperature/energy scales. The FP is itself reached below an effective single-channel Kondo temperature scale $T_K^{1CK} \equiv T_K^{SC} \propto \exp(-1/\rho J_>)$ (see Eq. 4.12) with $J_>$ the coupling to lead α (which is the larger of the L/R exchange couplings).

In the present context, Eq. 6.31, the situation is then clear: in the $\mathcal{T}^z = +\frac{1}{2}$ sector the spin is wholly quenched by coupling to the L lead/channel ($J_{\text{mix}} > 0$), while for $\mathcal{T}^z = -\frac{1}{2}$ it is quenched by coupling to the R lead; the temperature scale for quenching in either case being the aforementioned effective one-channel Kondo scale $T_K^{1CK} \propto \exp(-1/\rho J_>)$, and here $J_> \equiv \frac{1}{2}J_A + J_{\text{mix}}$.

The stable FP is clearly a doubled version of the SC: α FP, with the ‘doubling’ reflecting the free pseudospin. Thus an associated $T = 0$ residual entropy of $S_{\text{imp}} = \ln 2$, and a finite uniform spin susceptibility $\chi_{\text{imp}}(0) \propto 1/T_K^{1CK}$ symptomatic of the one-channel quenched spin- $\frac{1}{2}$ results. Since this FP is distinct from the stable 2CK FP arising for $\tilde{E}_\Delta \neq 0$ away from the QPT, it corresponds to a critical FP (CFP), with Eq. 6.31 the effective Hamiltonian for the quantum critical point (QCP) itself. Despite the inherent channel anisotropy in either pseudospin sector, the CFP itself comprises both SC: L and SC: R FPs, and so overall L/R symmetry is of course

respected at the transition (as discussed further below).

The ‘entire’ T -dependence of thermodynamics at the QCP is also readily inferred, since the pseudospin is ubiquitously free and spin-quenching is characterised by the single, finite scale T_K^{1CK} . For $T \gg T_K^{1CK}$ one expects $S_{\text{imp}}(T) = \ln 4$ (reflecting the free pseudospin *and* the free spin), with a free spin- $\frac{1}{2}$ Curie law $T\chi_{\text{imp}}(T) \sim \frac{1}{4}$; the ‘ $SU(2) \times SU(2)$ ’ FP Hamiltonian here being Eq. 6.31 with all exchange couplings set to zero. $T \sim T_K^{1CK}$ then sets the scale for spin quenching and the crossover to the CFP discussed above. Hence, at the QCP, the T -dependence of the entropy should be given by $S_{\text{imp}}(T) = \ln 2 + S_{\text{imp}}^{1CK}(T)$, with $S_{\text{imp}}^{1CK}(T)$ the entropy for a single-channel Kondo model with Kondo scale T_K^{1CK} . Likewise the uniform spin susceptibility should be $\chi_{\text{imp}}(T) = \chi_{\text{imp}}^{1CK}(T)$.

Having considered the QCP we return briefly to a non-vanishing $|\tilde{E}_\Delta| \ll T_K^{1CK}$, small compared to the 1CK scale. In this case we expect flow to the CFP to be cut off at a characteristic 2CK scale, $T \sim T_K$, below which the system flows to the stable 2CK FP; and with $T_K \equiv T_K(\tilde{E}_\Delta)$ vanishing as $|\tilde{E}_\Delta| \rightarrow 0$, indicative of the QPT. We examine this via NRG in the following section, but note here that the considerations above would lead us to expect a crossover in $S_{\text{imp}}(T)$ from $\ln 4$ to $\ln 2$ on the scale $T \sim T_K^{1CK}$, followed by a crossover for $T \sim T_K$ to the $\frac{1}{2} \ln 2$ characteristic of the stable 2CK FP. Likewise for $\chi_{\text{imp}}(T)$ we anticipate the Curie law $\chi_{\text{imp}}(T) \sim 1/4T$ for $T \gg T_K^{1CK}$, increasing to $\chi_{\text{imp}}(T) \propto 1/T_K^{1CK}$ for $T \sim T_K^{1CK}$, before crossing over to the divergent 2CK behaviour $\chi_{\text{imp}}(T) \propto \ln(T_K/T)$ for $T \lesssim T_K$.

Finally, for a larger non-zero $|\tilde{E}_\Delta| \gg T_K^{1CK}$, no RG flow in the vicinity of the CFP is expected, and the T_K^{1CK} scale is then irrelevant: below $T \sim |\tilde{E}_\Delta| \gg T_K^{1CK}$ one or other of the pseudospin z -components is simply frozen out, $S_{\text{imp}}(T)$ crossing over from $\ln 4$ to $\ln 2$ (here indicative of a frozen pseudospin but a free spin- $\frac{1}{2}$), and then to the stable 2CK FP value $\frac{1}{2} \ln 2$ on the 2CK scale $T \sim T_K$. The physics here is simply that of a single spin- $\frac{1}{2}$ 2CK model, as already considered in the preceding sections.

6.3.2 Critical fixed point: NRG

The physical arguments given above imply that the NRG energy levels associated with the critical FP itself, should consist of *both* a set of single-channel strong coupling FP levels, reflecting spin-quenching to one lead (as arises for an AF-coupled single-channel spin- $\frac{1}{2}$ Kondo model); *and* a set of levels for a free conduction band, reflecting decoupling of the spin from the other lead (as arises at the trivial weak coupling FP for a ferromagnetically coupled single-channel spin- $\frac{1}{2}$ Kondo model [8]).

Before proceeding we simply demonstrate that this is indeed the case. The left panel of Fig. 6.12 shows the lowest NRG energy levels of the full TQD model at the transition ($J' = J'_c$), as a function of iteration number, N . The CFP levels are well

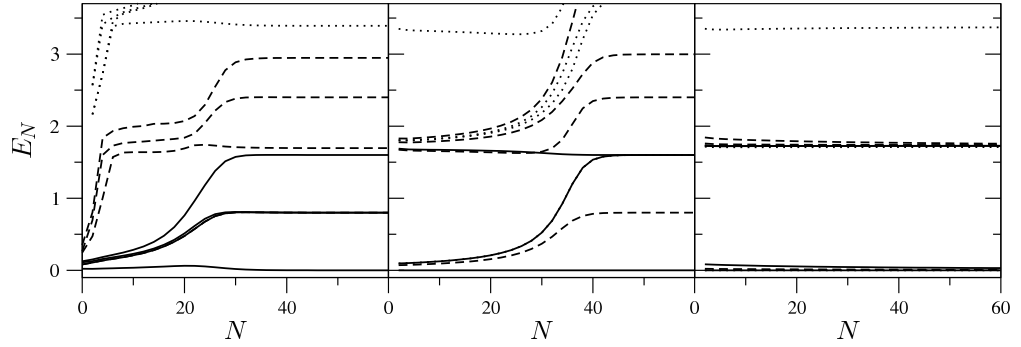


Figure 6.12: NRG energy levels for even iteration number, N . The lowest 4 levels are shown in each charge/spin subspace for: the full TQD model precisely at the transition [*left panel*], a 1CK model with $\rho J_K = +0.056$ [*middle*] and $\rho J_K = -0.056$ [*right*]. For the full model, subspaces shown are $(Q_L, Q_R, S^z) \equiv (0, 1, 0)/(1, 0, 0)$ [solid lines], $(0, 1, 1)/(1, 0, 1)$ [dashed], and $(0, 3, 0)/(3, 0, 0)$ [dotted]. For the 1CK models, the subspaces are $(Q, S^z) \equiv (0, 0)$ [solid lines], $(1, \frac{1}{2})$ [dashed], and $(0, 1)$ [dotted].

converged by $N = 40$ (flow to the CFP from the $SU(2) \times SU(2)$ FP beginning for $N \approx 26$). For comparison we also show the lowest NRG levels for a representative 1CK model with antiferromagnetic coupling (middle panel) and with ferromagnetic coupling (right panel). The CFP level structure can indeed be seen to comprise *both* sets of strong coupling (middle panel) and weak coupling (right panel) levels. The lowest levels of the system at the CFP thus appear to be the same as those of a standard single-spin 2CK model with channel anisotropy, as presented in the left panel of Fig. 3.6. However, there is a key difference: the CFP comprises *both* SC:L and SC:R FPs, and hence the L/R mirror symmetry of the problem is not of course broken. Unlike the levels of the channel-anisotropic single-spin 2CK model (see Fig. 3.6), the levels in the subspaces $(Q_L, Q_R, S^z) \equiv (x, y, S^z)$ and (y, x, S^z) are degenerate in Fig. 6.12 for the full TQD model. The strong coupling and weak coupling levels thus form *symmetrically* in each channel.

6.3.3 Thermodynamics of the transition

We turn now to thermodynamics in the vicinity of the transition, obtained via NRG for the full TQD model; considering temperatures $T \ll \Gamma$ (*ie.* without comment on non-universal high-temperatures, where the same behaviour as in Sec. 6.2.1 naturally occurs).

Fig. 6.13 shows the T/Γ -dependence of the entropy $S_{\text{imp}}(T)$. Results are given for fixed $\tilde{U} = 7$ and $\rho J = 0.1$, varying J' as the transition — occurring at $J' = J'_c$ determined as above from the spin correlators — is approached from either side, according to $\tilde{E}_\Delta = (J'_c - J') = \pm \lambda T_K^c$; with results shown for $\lambda = 10^n$ and $n = 0, -1, -2, -3, -4$ [lines (a-e) in Fig. 6.13], chosen to approach progressively the transition, itself oc-

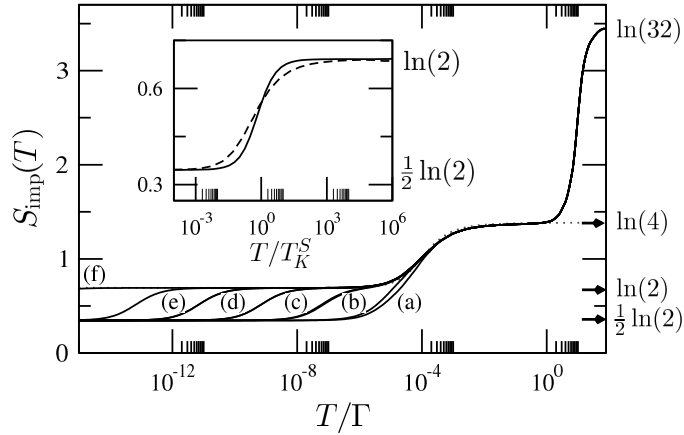


Figure 6.13: Entropy $S_{\text{imp}}(T)$ vs. T/Γ on progressively approaching the QPT as: $\tilde{E}_\Delta = (J'_c - J') = \pm \lambda T_K^c$, with $T_K^c/\Gamma = 10^{-4}$ (as discussed in text) and results shown for $\lambda = 10^n$ with $n = 0, -1, -2, -3, -4$ (lines (a)-(e) respectively). The QCP itself ($\lambda = 0$) is shown as line (f), while the dotted line shows $\ln 2 + S_{\text{imp}}^{1CK}(T)$ calculated for a single-channel Kondo model with $T_K^{1CK} = T_K^c$; the two coinciding for all $T/\Gamma \lesssim 1$. Inset: results in (b)-(e) rescaled (solid line) in terms of the vanishing Kondo scale $T_K \equiv T_K^S$, showing universal crossover from the CFP to the stable 2CK FP; and contrasted to that arising in the single-spin 2CK model (dashed line).

curing at $\lambda = 0$ [shown as line (f)]. Here, $T_K^c/\Gamma = 10^{-4}$ is the value, at $J' = J'_c$, of the Kondo scale T_K^χ obtained from $T\chi_{\text{imp}}(T)$ as in Sec. 6.2.1; and we will in fact shortly identify T_K^c as corresponding to the effective single-channel Kondo scale T_K^{1CK} discussed in Sec. 6.3.1 and associated with the QCP. Lines (a) in Fig. 6.13 are thus for J' being $\pm T_K^c$ away from the transition; while (b-e) show the behaviour for $|J'_c - J'| \ll T_K^c$ as the QPT is approached.

$S_{\text{imp}}(T)$ self-evidently shows a QPT: one sees clearly a low-energy scale $T_K \equiv T_K^S$ in the vicinity of the transition, reflected in the crossover to the stable 2CK FP value $S_{\text{imp}} = \frac{1}{2} \ln 2$ (and determined in practice via $S_{\text{imp}}(T_K^S) = 0.55$ as in Sec. 6.2.1); with T_K vanishing precisely at the transition itself (line (f)).

The obvious first question is how $T_K \equiv T_K(\tilde{E}_\Delta)$ vanishes as $\tilde{E}_\Delta = J'_c - J' \rightarrow 0$ on approaching the QPT. The answer is

$$T_K \stackrel{J' \rightarrow J'_c \pm}{\sim} \mathcal{A} |J'_c - J'|^\nu \quad : \nu = 2 \quad (6.32)$$

with exponent $\nu = 2$, and common amplitudes $\mathcal{A}$ on approaching J'_c from either side. This is shown in the inset panel (c) to Fig. 6.14 (itself discussed further below). The solid lines therein show T_K/Γ vs. $|J'_c - J'|/T_K^c$ on a log-log scale, as the transition $J' \rightarrow J'_c$ is approached from both sides. The dashed line has a slope $\nu = 2$, onto which the T_K fall cleanly for $|J'_c - J'| \lesssim T_K^c$; so that T_K^c is as such the ‘boundary’ scale below which Eq. 6.32 holds and the critical regime is entered. We add also

that an exponent $\nu = 2$ reflects the non-trivial nature of the transition: for a first order level-crossing transition, as arises [64] if the TQD is instead coupled to a single lead/channel at dot 2 (see Fig. 6.1), one instead finds [64] $\nu = 1$.

We also note that a critical exponent $\nu = 2$ arises [42, 45, 46, 49, 124] in the standard single-spin 2CK model as the degree of channel asymmetry vanishes, $\delta \rightarrow 0$ (see Eq. 4.9), which was also studied for odd chains in Sec. 4.3.1 (see in particular Eq. 4.19). This further suggests that the nature of the transition in the full TQD model is one driven by channel anisotropy. The behaviour of the L/R asymmetric 2CK model is generally characterized by single-channel Kondo quenching of the dot spin to yield a Fermi liquid, with the non-Fermi liquid 2CK FP only describing the ground state for strictly mirror-symmetric systems. Interestingly, the situation is essentially reversed in the TQD model: the behaviour of the system is in general described by the 2CK FP, with the effective single-channel Kondo quenching of the spin occurring only at the critical point, $\tilde{E}_\Delta = 0$.

Consider now the QCP itself, $J' = J'_c$ (line (f) in Fig. 6.13). From the arguments given in Sec. 6.3.1 we anticipate $S_{\text{imp}}^{QCP}(T) = \ln 2 + S_{\text{imp}}^{1CK}(T)$, where the explicit $\ln 2$ reflects the free pseudospin and $S_{\text{imp}}^{1CK}(T)$ is the entropy for a *single*-channel spin- $\frac{1}{2}$ Kondo model. This is indeed verified in Fig. 6.13, where $\ln 2 + S_{\text{imp}}^{1CK}(T)$ is calculated explicitly for a single-channel Kondo model with T_K^{1CK} chosen such that $T_K^{1CK} = T_K^c$. It is seen (dotted line) to coincide perfectly with $S_{\text{imp}}^{QCP}(T)$ for all $T \lesssim \Gamma$; including the $\ln 4$ entropy plateau reflecting the free pseudospin *and* spin (the ‘ $SU(2) \times SU(2)$ ’ FP of Sec. 6.3.1), and the crossover at $T \sim T_K^{1CK} = T_K^c$ to the CFP characterised by $S_{\text{imp}} = \ln 2$, where the pseudospin remains free but the spin is wholly quenched.

Moving away from the QCP, consider now the sequence (b $\rightarrow$ e) in Fig. 6.13, as the transition is progressively approached. In all cases $S_{\text{imp}}(T)$ follows the QCP $S_{\text{imp}}^{QCP}(T)$ all the way from the $\ln 4$ regime, through the crossover at the common temperature $T \sim T_K^c = T_K^{1CK}$ (which is of course finite at the transition), to the $\ln 2$ symptomatic of the CFP; before ultimately descending to the stable 2CK FP with $S_{\text{imp}} = \frac{1}{2} \ln 2$ on the scale $T \sim T_K \equiv T_K^S$. Since T_K vanishes as the transition is approached, $S_{\text{imp}}(T)$ should exhibit universality in terms of T/T_K . That it does is shown in the inset to Fig. 6.13, where all lines (b-e) collapse to a common scaling curve (solid line). This scaling is of course characteristic of flow from the vicinity of the *critical* FP to the stable 2CK FP. As such it is thus expected to be distinct from the universal crossover in the *single* spin 2CK model (Sec. 6.2.1), from the $\ln 2$ entropy plateau associated with the free spin- $\frac{1}{2}$ *local moment* FP to the stable 2CK FP; indeed confirmed in the inset to Fig. 6.13, where the latter is shown as a dashed line. Note also in this regard that lines (a) in Fig. 6.13, for $J'_c - J' = \pm T_K^c$, constitute in effect the boundary between effective single-spin 2CK behaviour (arising for $|\tilde{E}_\Delta| = |J'_c - J'| \gtrsim T_K^c \equiv T_K^{1CK}$) and the critical regime $|J'_c - J'| \lesssim T_K^c$;

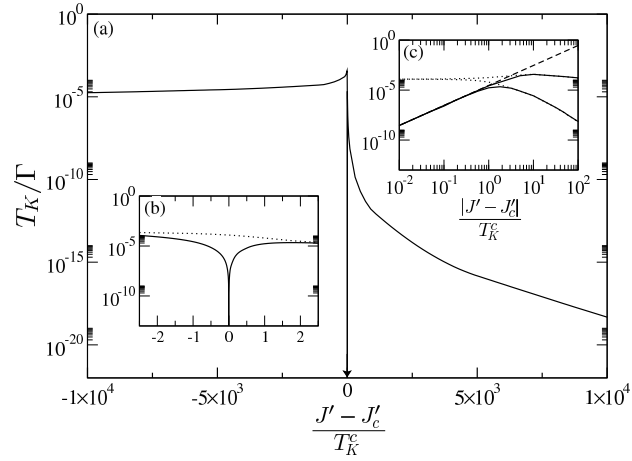


Figure 6.14: Variation of the Kondo scale $T_K \equiv T_K^S$: T_K/Γ vs. $(J' - J'_c)/T_K^c$ (with fixed $\tilde{U} = 7$ and $\rho J = 0.1$, for which $T_K^c/\Gamma = 10^{-4}$). Inset (b) shows an expanded view in the vicinity of the transition (solid line); inset (c) shows the same results (solid) on a log-log scale, together with the power-law decay $T_K \propto |J'_c - J'|^2$ (dashed line) as the transition is approached. In both insets, T_K^χ is also shown (dotted lines), and remains finite at the transition.

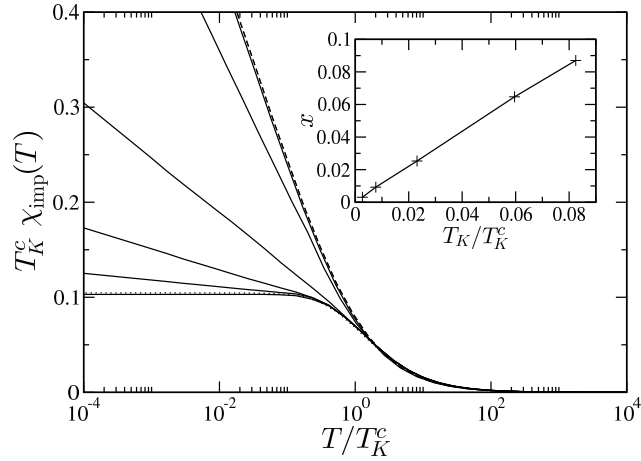


Figure 6.15: Uniform spin susceptibility $T_K^c \chi_{\text{imp}}(T)$ vs. T/T_K^c for fixed $\tilde{U} = 7$ and $\rho J = 0.1$, varying J' as: $\tilde{E}_\Delta = (J'_c - J') = \lambda T_K^c$ with $\lambda = 10^{n/4}$ and $n = 1, 0, -1, -2, -3$ (solid lines, in order of decreasing slope). The QCP itself ($\lambda = 0$) is the bottom solid line. Also shown (dotted) is a 1CK model chosen such that $T_K^{1CK} = T_K^c$, which describes the QCP; and a single-spin 2CK model with $T_K = T_K^c$ (dashed). Near the transition $\chi_{\text{imp}}(T)$ diverges as $T_K^c \chi_{\text{imp}}(T) \sim x \ln(T_K/T)$, with amplitude $x \sim T_K/T_K^c$ as shown in the inset (see also text).

as reflected in the direct flow of $S_{\text{imp}}(T)$ from $\ln 4$ to $\frac{1}{2} \ln 2$ occurring at that point.

Fig. 6.15 shows the T -dependence of the uniform spin susceptibility, $T_K^c \chi_{\text{imp}}(T)$ vs. T/T_K^c (with $T_K^c/\Gamma = 10^{-4}$ as above), on approaching the transition according to $\tilde{E}_\Delta = J'_c - J' = \lambda T_K^c$; but now with $\lambda = 10^{n/4}$ and $n = 1, 0, -1, -2, -3$ (solid lines, in order of decreasing slope), showing as such the region where RG flow near the

CFP is first observed (roughly between lines (a) and (b) in Fig. 6.13). The figure also shows the behaviour at the QCP itself ($\lambda = 0$, bottom solid line), as well as the spin susceptibility for a single-spin 2CK model (dashed line).

For the QCP itself, we expect $\chi_{\text{imp}}^{QCP}(T) = \chi_{\text{imp}}^{1CK}(T)$ from the arguments of Sec. 6.3.1; with $\chi_{\text{imp}}^{1CK}(T)$ the spin susceptibility for a single-channel spin- $\frac{1}{2}$ Kondo model with Kondo scale $T_K^{1CK} \equiv T_K^c$, such that at $T = 0$ in particular $\chi_{\text{imp}}^{1CK}(T = 0)$ is characteristically finite (as discussed in relation to Fig. 3.10). That is indeed verified in Fig. 6.15, where the result for the single-channel Kondo model is shown as a dotted line.

For $n = 1$ by contrast, *ie.* $J'_c - J' \approx 2T_K^c$, the susceptibility follows essentially perfectly the dashed line; thus being described by a single-spin 2CK model, precisely as arises deep in either 2CK phase of the full TQD model (see Fig. 6.4), and characterised by the low- T logarithmic divergence $T_K^c \chi_{\text{imp}}(T) \propto \ln(T_K/T)$. On moving closer to the transition (decreasing n), the susceptibilities progressively ‘fold on’ to the QCP result over an increasingly wider T/T_K^c -range; indeed even for $J'_c - J' = 0.1T_K^c$ ($n = -4$, not included in Fig. 6.15), the resultant susceptibility is barely distinguishable from the QCP line over most of the T/T_K^c range shown. As seen from the figure however, in all cases except the QCP itself, the ultimate low- T behaviour is the logarithmic divergence expected for the stable 2CK FP, $T_K^c \chi_{\text{imp}}(T) \sim x \ln(T_K/T)$; with an amplitude x visible from the gradients in Fig. 6.15 and seen to diminish steadily as the transition is approached. While numerical accuracy prevents a definitive determination of x much closer to the transition, extrapolation of the results in Fig. 6.15 (as shown in the inset) suggest x vanishes as $x \propto T_K/T_K^c \propto (1 - J'/J'_c)^2$ from Eq. 6.32).

Finally, as discussed only partially above (see Eq. 6.32), we return to the evolution of the Kondo scale shown in Fig. 6.14; the main panel of which shows $T_K \equiv T_K^S$ *vs.* $(J' - J'_c)/T_K^c$ as determined from the T -dependence of the entropy (Fig. 6.13). Inset (b) to Fig. 6.14 shows an expanded view of T_K in the vicinity of the transition ($|J' - J'_c|/T_K^c \lesssim 2$), together (dotted line) with the scale T_K^X determined in practice from the spin susceptibility via [13] $T_K^X \chi_{\text{imp}}(T_K^X) = 0.07$ (as employed in Sec. 6.2.1). While $T_K \equiv T_K^S$ in inset (b) naturally shows the vanishing of the Kondo scale as the QPT is approached, T_K^X is seen to remain finite at the transition, as seen also in Fig. 6.10 of Sec. 6.2.3. This is precisely as it should be. The ‘true’, ultimately vanishing Kondo scale T_K is of course evident in the evolution of both $S_{\text{imp}}(T)$ (Fig. 6.13) and $\chi_{\text{imp}}(T)$ itself (Fig. 6.15). But $T \times \chi_{\text{imp}}(T)$ — from which T_K^X has been defined — vanishes as $T \rightarrow 0$ (the explicit factor of T ‘killing’ the low- T logarithmic divergence in $\chi_{\text{imp}}(T)$ itself). Indeed, as readily inferred from Fig. 6.15 (and verified by explicit calculation), $T \chi_{\text{imp}}(T)$ close to the transition ($|J'_c - J'|/T_K^c \lesssim 0.1$ or so) is indistinguishable from the QCP behaviour $T \chi_{\text{imp}}^{1CK}(T)$; and as such is naturally characterised by the finite temperature scale $T_K^{1CK} \equiv T_K^X$. The above, important

distinction between T_K and T_K^χ is however applicable only close to the transition. As seen clearly from inset (b) to Fig. 6.14, the scales $T_K \equiv T_K^S$ and T_K^χ coincide away from the transition (in practice for $|J'_c - J'|/T_K^c \gtrsim 2$ or so); as noted and used in Sec. 6.2.1 when considering the model deep in either of the 2CK phases.

6.3.4 Dynamics of the transition

Here we focus again on the single-particle spectrum $D_1(\omega)$ of dot 1 (or equivalently, $D_3(\omega)$ for dot 3). The $T = 0$ spectrum $\pi\Gamma D_1(\omega)$ vs. ω/Γ is shown in Fig. 6.16 for $\tilde{U} = 7$ and $\rho J = 0.1$; varying $\tilde{E}_\Delta = J'_c - J'$ on approaching the transition from the (+) parity phase $J' > J'_c$, according to $\tilde{E}_\Delta = -\lambda T_K^c$ with $\lambda = 10^{n/2}$ and integral $n = +4 \rightarrow -4$ for lines a $\rightarrow$ i respectively. The spectrum at the transition itself ($\lambda = 0$) is indistinguishable from case (i).

Two particular spectral features should be noted. First, the spectrum at the Fermi level is pinned at $\pi\Gamma D_1(\omega = 0) = \frac{1}{2}$ in all cases, including the transition itself. Second, the width of the Kondo resonance clearly increases as the transition is approached, being of order $T_K^c \equiv T_K^{1CK}$ at the transition (with $T_K^c/\Gamma = 10^{-4}$ as usual); in which sense the vanishing T_K scale evident *eg.* in the evolution of the entropy (Fig. 6.13), does *not* show up in single-particle dynamics.

That $\pi\Gamma D_1(\omega = 0)$ should be $\frac{1}{2}$ away from the transition is (as in Sec. 6.2.2) a natural consequence of the stable 2CK FP that ultimately arises (Sec. 6.3.3). To understand why $\pi\Gamma D_1(\omega = 0) = \frac{1}{2}$ at the transition itself, first recall the general result from Sec. 6.2.2 that $\pi\Gamma D_1(\omega) = -\pi\rho_T \text{Im} t_L(\omega)$, with $t_\alpha(\omega)$ the t-matrix for scattering of electron states in the $\alpha = L, R$ lead. As discussed in Sec. 6.3.1, the effective Hamiltonian for the QCP (Eq. 6.31) is strictly separable into disjoint $\mathcal{T}^z = \pm\frac{1}{2}$ sectors, the two sectors possessing common eigenvalues. In this case it is straightforward to show that $t_\alpha(\omega) = \frac{1}{2}[t_\alpha(\mathcal{T}^z = +\frac{1}{2}; \omega) + t_\alpha(\mathcal{T}^z = -\frac{1}{2}; \omega)]$, where $t_\alpha(\mathcal{T}^z; \omega)$ is the t_α -matrix calculated for a *fixed* $\mathcal{T}^z$ in the QCP Hamiltonian Eq. 6.31 (with $t_L(\mathcal{T}^z = \pm\frac{1}{2}; \omega) = t_R(\mathcal{T}^z = \mp\frac{1}{2}; \omega)$ such that $t_L(\omega) = t_R(\omega)$ overall, as symmetry requires generally).

Consider then $t_L(\omega)$: as explained in Sec. 6.3.1, at the critical fixed point the spin- $\frac{1}{2}$ $\hat{\mathbf{S}}$ is quenched in a *one*-channel fashion, by antiferromagnetic coupling to the L -lead for $\mathcal{T}^z = +\frac{1}{2}$, but to the R -lead for $\mathcal{T}^z = -\frac{1}{2}$. In consequence, $t_L(\mathcal{T}^z = +\frac{1}{2}; \omega = 0)$ is equivalently the t-matrix, $t^{1CK}(\omega = 0)$, for a *one*-channel antiferromagnetic spin- $\frac{1}{2}$ Kondo model. But $t_L(\mathcal{T}^z = -\frac{1}{2}; \omega = 0) = 0$ by contrast, since for $\mathcal{T}^z = -\frac{1}{2}$ the spin is quenched by coupling to the R -lead, while the L -lead is entirely decoupled from it (so no spin-scattering of electrons due to dot 1 occurs in the L -lead). Hence, $t_L(\omega = 0) \equiv \frac{1}{2}t^{1CK}(\omega = 0)$. For a one-channel spin- $\frac{1}{2}$ Kondo model itself, $-\pi\rho_T \text{Im} t^{1CK}(\omega) \equiv \pi\Gamma D^{1CK}(\omega)$, with $D^{1CK}(\omega)$ the single-particle spectrum of a one-channel, single-level Anderson impurity model in the

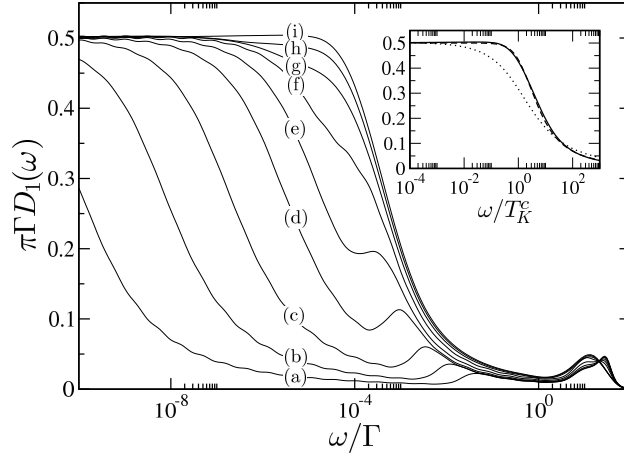


Figure 6.16: $\pi\Gamma D_1(\omega)$ vs. ω/Γ , varying $\tilde{E}_\Delta = J'_c - J'$ as the transition is approached from the (+) parity 2CK phase: $\tilde{E}_\Delta = -\lambda T_K^c$ with $\lambda = 10^{n/2}$ and $n = +4 \rightarrow -4$ (a→i respectively). The QCP spectrum ($\lambda = 0$) is indistinguishable from case (i). Inset: QCP scaling spectrum vs. ω/T_K^c (solid line, in practice coinciding with all spectra for $\lambda \lesssim 10^{-2}$). The QCP spectrum is seen to be the scaling spectrum $\frac{1}{2}\pi\Gamma D^{1CK}(\omega)$ (dashed line) for a single-channel Anderson impurity model. The dotted line shows the distinct scaling spectrum of a single-spin 2CK model (onto which cases (a)-(c) scale).

singly-occupied Kondo regime of the model (as is physically obvious, but follows more formally from the arguments presented in Sec. 3.6.2). Overall we thus infer that $\pi\Gamma D_1(0) = -\pi\rho_T \text{Im}t_L(0) \equiv \frac{1}{2}\pi\Gamma D^{1CK}(0)$. But $\pi\Gamma D^{1CK}(0) = 1$ by virtue of the Friedel sum rule [8]; whence $\pi\Gamma D_1(0) = \frac{1}{2}$ arises, as indeed found, see Fig. 6.16.

While the arguments above strictly apply only to $\omega = 0$ (and as such the CFP), one naturally expects the frequency dependence of the Kondo resonance in $\pi\Gamma D_1(\omega)$ at the QCP to be that of $\frac{1}{2}\pi\Gamma D^{1CK}(\omega)$. That this is so is demonstrated in the inset to Fig. 6.16. The scaling spectrum $\frac{1}{2}\pi\Gamma D^{1CK}(\omega)$ for the Anderson model (as a function of ω/T_K^{1CK}) is shown as a dashed line, and compared to $\pi\Gamma D_1(\omega)$ vs. ω/T_K^c for the full TQD model at the QCP (solid line); the two coincide perfectly. In particular, the low-frequency spectral behaviour ($|\omega|/T_K^c \ll 1$) at the transition is thus of quadratic Fermi liquid form [8],

$$\pi\Gamma D_1(\omega) \sim \frac{1}{2} [1 - a'(\omega/T_K^c)^2] \quad (6.33)$$

with a' a constant of order unity. This is of course in marked contrast to the behaviour arising deep in either of the 2CK phases (Sec. 6.2.2). The scaling spectrum in that case is also shown in Fig. 6.16 (inset, dotted line), and instead exhibits the characteristic square-root frequency dependence of Eq. 6.25.

Cases (a)-(c) in Fig. 6.16 are relatively deep in the (+)-parity 2CK phase ($|\tilde{E}_\Delta| \geq 10T_K^c$). Their dynamics are thus in essence those of the single-spin 2CK model discussed in Sec. 6.2.2: when scaled in terms of their Kondo scale T_K , the spectra

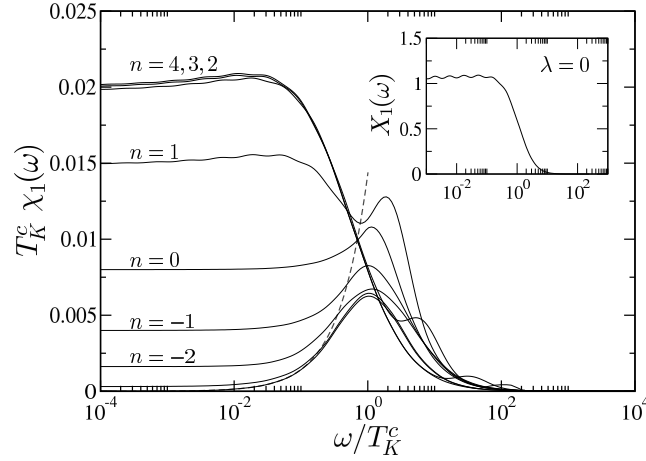


Figure 6.17: Local dynamic susceptibility $T_K^c \chi_1(\omega)$ vs. ω/T_K^c , varying $\tilde{E}_\Delta = J'_c - J'$ on approaching the transition from the (–)-parity 2CK phase: $\tilde{E}_\Delta = \lambda T_K^c$ with $\lambda = 10^{n/2}$ and $n = +4 \rightarrow -4$. $T_K^c \chi_1(0)$ vanishes as the transition is approached. The dashed line, $T_K^c \chi_1(\omega) \propto \omega$, shows the low- ω Fermi liquid behaviour of the single-channel Anderson model arising at the QCP ($\lambda = 0$). Inset: $X_1(\omega) = \chi_1(\omega)/(2\omega[\text{Re}\langle S_1^z; S_1^z \rangle]_{\omega=0})^2$ vs. ω/T_K^c at the transition ($\lambda = 0$), showing recovery of the Korrington-Shiba relation $X_1(\omega = 0) = 1$.

all collapse onto the 2CK scaling spectrum shown in the inset (dotted line), departure from such occurring only on non-universal scales $\omega \sim |\tilde{E}_\Delta|$ (where a subsidiary peak arises, see main figure). Close to the transition by contrast — exemplified by case (i) in Fig. 6.16 ($|\tilde{E}_\Delta| = 10^{-2}T_K^c$) — the single-particle dynamics are essentially indistinguishable from that of the QCP, as is physically natural. The crossover from the CFP to the 2CK FP (which occurs on the scale of T_K for any $|\tilde{E}_\Delta| \neq 0$), is only barely evident in the crossover of the low-frequency asymptotic form of $\pi\Gamma D_1(\omega)$, described by Eq. 6.33 near the CFP, to Eq. 6.25 when finally approaching the 2CK FP. But since both are close to their half-unitarity-limit value of $\pi\Gamma D_1(\omega) = \frac{1}{2}$ at low-frequencies, systems close to the transition (as in line (i) in Fig. 6.16) essentially represent the QCP spectrum itself.

As expected, spectra (d)-(h) do not conform to either limiting form (QCP or 2CK), but instead represent crossover behaviour between the two.

Finally, we consider the $T = 0$ local dynamic susceptibility for dot 1 in the vicinity of the transition. Fig. 6.17 shows $T_K^c \chi_1(\omega)$ vs. ω/T_K^c , varying $\tilde{E}_\Delta = J'_c - J'$ on approaching the transition from the (–)-parity 2CK phase $J' < J'_c$, according to $\tilde{E}_\Delta = \lambda T_K^c$ with $\lambda = 10^{n/2}$ and $n = +4 \rightarrow -4$. The cases $n = 2, 3, 4$ (with $\tilde{E}_\Delta \geq 10T_K^c$) are quite deep in the 2CK phase (where the T_K scale is roughly constant, see Fig. 6.14), so they are essentially equivalent to the 2CK scaling curves of Fig. 6.9 (inset).

As the transition is approached however, the height of the $\omega \rightarrow 0$ plateau in Fig. 6.17 is seen steadily to diminish; the behaviour found being of form $T_K^c \chi_1(\omega =$

0) $\sim T_K/T_K^c$, with the Kondo scale $T_K \rightarrow 0$. This is readily understood: as mentioned in Sec. 6.2.2 it is known [106, 108] that at the 2CK FP, $\chi_1(0)$ plateaus at a constant, itself proportional to the slope of the low-temperature log divergence of $\chi_{\text{imp}}(T)$; and in Fig. 6.15 we showed the latter to vanish $\propto T_K \rightarrow 0$. Hence $\chi_1(0) = 0$ at the transition itself. As expected from the nature of the QCP, the leading low- ω dependence of $\chi_1(\omega)$ is then the Fermi liquid behaviour characteristic of the single-channel Anderson model [8, 140], $\chi_1(\omega) \propto \omega$, which we showed explicitly in Fig. 3.13, and is seen in Fig. 6.17 (dashed line) to be present in the full TQD model at the critical point. Indeed for $\tilde{E}_\Delta \lesssim T_K^c$, the leading low- ω behaviour of $T_K^c \chi_1(\omega)$ is in fact well described by $T_K^c \chi_1(\omega) \sim T_K^c \chi_1(0) + \alpha \omega$ (with α a constant). Close to the QCP, $\chi_1(\omega)$ is also seen to contain an absorption centred on $\omega = T_K^c$ ($\equiv T_K^{1CK}$), likewise characteristic of the Anderson model [8, 140] (see Fig. 3.13).

The inset to Fig. 6.17 shows $X_1(\omega) = \chi_1(\omega)/(2\omega[\text{Re}\langle\langle S_1^z; S_1^z \rangle\rangle_{\omega=0}]^2)$ vs. ω/T_K^c at the transition itself. For the single-channel Anderson model, the $\omega \rightarrow 0$ behaviour of $X_1(\omega)$ is given exactly by the Korringa-Shiba relation [8, 140] $X_1(\omega = 0) = 1$, which is seen from the figure to be well satisfied in practice (to within a few %), again confirming the physical picture of the CFP discussed in Sec. 6.3.1.

6.4 Reduced model for the transition

In the preceding sections, the effective low-energy model Eq. 6.13 (or Eq. 6.30) has been important in understanding the behaviour of the full TQD system in the vicinity of the QPT. We have also performed direct NRG calculations on the effective low-energy model itself, varying independently the bare parameters J_A, J_B, J_{mix} and E_Δ (or $\tilde{E}_\Delta$); and now comment briefly on the results of such. Specifically, we here consider explicitly the effective model with $J_A = 0 = J_B$, which we have confirmed describes the same physics as arises with generically non-zero J_A or J_B (reflecting the fact that the key element in the effective Hamiltonian Eq. 6.13 is the pseudospin raising/lowering term, H_{mix} below, which in switching the parity of the TQD states effectively drives the QPT).

We thus consider the reduced model $H_{\text{red}} = H_L + H_{\text{mix}} + H_{\text{mag}}$, with H_L the Hamiltonian for the leads and

$$H_{\text{mix}} = J_{\text{mix}}(\hat{T}^+ + \hat{T}^-)\hat{\mathbf{S}} \cdot (\hat{\mathbf{s}}_{L0} - \hat{\mathbf{s}}_{R0}), \quad (6.34a)$$

$$H_{\text{mag}} = \tilde{E}_\Delta \hat{T}^z. \quad (6.34b)$$

The underlying FPs of H_{red} are readily inferred. The $SU(2) \times SU(2)$ FP corresponds to $J_{\text{mix}} = 0 = \tilde{E}_\Delta$ in Eq. 6.34, and as such to both a free spin and a free pseudospin; this of course is the high-temperature FP of H_{red} , generating *eg.* the associated $\ln 4$ entropy. Two LM FPs also arise, corresponding formally to $J_{\text{mix}} = 0$ in Eq. 6.34

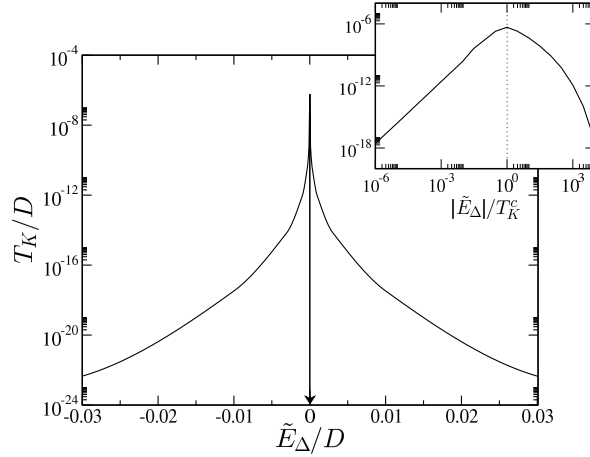


Figure 6.18: Evolution of the 2CK scale for the reduced model Eq. 6.34: T_K/D vs. $\tilde{E}_\Delta/D$ (with D the conduction bandwidth), for fixed $\rho J_{\text{mix}} = 0.075$. Inset: T_K/D vs. $|\tilde{E}_\Delta|/T_K^c$ on logarithmic axes, with $T_K \sim |\tilde{E}_\Delta|^2$ on approaching the transition.

(and hence a free spin), and $\tilde{E}_\Delta \rightarrow \pm\infty$. For $\tilde{E}_\Delta \rightarrow +\infty$, the $\mathcal{T}^z = -\frac{1}{2}$ pseudospin component (*ie.* the $(-)$ -parity TQD doublet) is frozen out, and we designate this as the ‘LM $(-)$ ’ FP; while for $\tilde{E}_\Delta \rightarrow -\infty$ the $\mathcal{T}^z = +\frac{1}{2}$ component is frozen out, corresponding to a LM $(+)$ FP.

The critical FP arises for $\tilde{E}_\Delta = 0$. In this case (see Sec. 6.3.1), a trivial rotation of the pseudospin axes gives the QCP Hamiltonian $H_{\text{red}}^{\text{QCP}} = H_L + 2J_{\text{mix}} \hat{\mathcal{T}}^z \hat{\mathbf{S}} \cdot (\hat{\mathbf{s}}_{L0} - \hat{\mathbf{s}}_{R0})$, with the quantum number $\mathcal{T}^z$ conserved and the Hilbert space thus separable into disjoint $\mathcal{T}^z = \pm\frac{1}{2}$ sectors. As discussed in Sec. 6.3.1, the CFP itself corresponds to the spin being quenched in a one-channel fashion by coupling to the L lead in the $\mathcal{T}^z = +\frac{1}{2}$ sector, and to the R lead for $\mathcal{T}^z = -\frac{1}{2}$. More formally, on writing $H_{\text{red}}^{\text{QCP}} = H_L + 2\hat{\mathcal{T}}^z \hat{\mathbf{S}} \cdot (J_{\text{mix}}^L \hat{\mathbf{s}}_{L0} - J_{\text{mix}}^R \hat{\mathbf{s}}_{R0})$ — with $J_{\text{mix}}^L = J_{\text{mix}}^R = J_{\text{mix}} > 0$ in the ‘bare’ $H_{\text{red}}^{\text{QCP}}$ — the CFP corresponds to $J_{\text{mix}}^L \rightarrow \infty$ and $J_{\text{mix}}^R = 0$ in the $\mathcal{T}^z = +\frac{1}{2}$ sector, with $J_{\text{mix}}^L = 0$ and $J_{\text{mix}}^R \rightarrow \infty$ for $\mathcal{T}^z = -\frac{1}{2}$.

Finally, for $\tilde{E}_\Delta \neq 0 \neq J_{\text{mix}}$, the higher lying component of the pseudospin is naturally frozen out on sufficiently low energy scales $T \ll |\tilde{E}_\Delta|$. Virtual excitations to the upper pseudospin sector still arise, however, and treating the mixing term Eq. 6.34a perturbatively (strictly valid for large $|\tilde{E}_\Delta|$) gives $H_{\text{red}}^{\text{eff}} = H_L + H_{\text{hyb}}^{\text{eff}}$, with

$$H_{\text{hyb}}^{\text{eff}} = \left(\frac{J_{\text{mix}}^2}{2E_\Delta} \right) \hat{\mathbf{S}} \cdot (\hat{\mathbf{s}}_{L0} + \hat{\mathbf{s}}_{R0}). \quad (6.35)$$

This is a model of 2CK form in the reduced Hilbert space of the lowest pseudospin component ($(+)$ -parity for $\tilde{E}_\Delta < 0$ and $(-)$ -parity for $\tilde{E}_\Delta > 0$), for which the ultimate stable FP is of course the infrared 2CK FP.

The overall low-energy FP structure of the reduced model is thus indeed that of

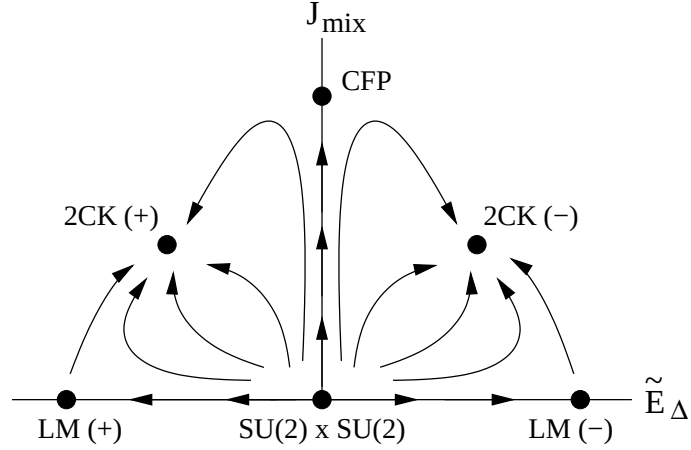


Figure 6.19: Schematic illustration of RG flow between the FPs (circles) of the reduced model. See text for discussion.

the full TQD model (we discuss its RG flow diagram below). On studying Eq. 6.34 directly with NRG the transition occurs as expected at $\tilde{E}_\Delta = 0$, and the above FPs are indeed observed *eg.* in the T -dependence of thermodynamics.

Fig. 6.18 shows the resultant 2CK scale T_K/D *vs.* $\tilde{E}_\Delta/D$ for systems with common $\rho J_{\text{mix}} = 0.075$. T_K is determined in the usual way from the entropy, and is found to be non-zero for any $\tilde{E}_\Delta \neq 0$ (Fig. 6.18).

We identify T_K^c as the crossover scale from the $SU(2) \times SU(2)$ FP to the CFP, and so $T_K^c/D \propto \exp(-1/\rho J_{\text{mix}}) = 10^{-6}$ (essentially corresponding to the maximum in T_K : see Fig. 6.18). The inset to Fig. 6.18 shows T_K/D *vs.* $|\tilde{E}_\Delta|/T_K^c$ on logarithmic axes. Just like Fig. 6.14 for the full TQD model, the point $\tilde{E}_\Delta = T_K^c$ can be seen to separate two distinct regimes. For $|\tilde{E}_\Delta| \gg T_K^c$, systems may be considered ‘deep’ in the 2CK phase (which situation constitutes the majority of the main panel of Fig. 6.18, and indeed the majority of the parameter space of Eq. 6.34). For $\tilde{E}_\Delta \ll T_K^c$ by contrast, systems flow close to the CFP, and are ‘near’ the transition. The vanishing T_K scale associated with the transition is found to be characterized by a power-law decay $T_K \sim |\tilde{E}_\Delta|^\nu$ with $\nu = 2$, as found in the full TQD model (Sec. 6.3.3). We also add that since the reduced model Eq. 6.34 lacks a direct coupling of form $\hat{\mathbf{S}} \cdot (\hat{\mathbf{s}}_{L0} + \hat{\mathbf{s}}_{R0})$ correlated to the pseudospin (*cf* Eq. 6.13), the variation of T_K is symmetric in $\tilde{E}_\Delta$, as evident in Fig. 6.18.

A schematic illustration of the RG flow is given in Fig. 6.19, in the $(\tilde{E}_\Delta, J_{\text{mix}})$ -plane. The FPs are indicated by circles, the arrows representing RG flow between them. At the highest temperatures, the system is always described by a free spin and a free pseudospin (the $SU(2) \times SU(2)$ FP, $J_{\text{mix}} = \tilde{E}_\Delta = 0$ in Eq. 6.34).

Considering now the case of $J_{\text{mix}} = 0$, the spin always remains free, but the upper pseudospin component is frozen out for any $\tilde{E}_\Delta \neq 0$, whence as $T \rightarrow 0$ the

system is described by either a (+) or (−) parity LM FP. By contrast, for $\tilde{E}_\Delta = 0$, any $J_{\text{mix}} \neq 0$ drives the system to the CFP as $T \rightarrow 0$. In the general case where $|\tilde{E}_\Delta| \neq 0$ and $J_{\text{mix}} \neq 0$, the system always flows ultimately to a 2CK FP (the parity of which depends on which component of the pseudospin lies lowest, *ie.* whether $\tilde{E}_\Delta > 0$ or < 0). In this case RG flow first approaches the LM FPs if $|\tilde{E}_\Delta| \gg T_K^c$, or the CFP for $|\tilde{E}_\Delta| \ll T_K^c$, before finally flowing to the appropriate stable 2CK FP.

And as evident from the results of Sec. 6.3 (*eg.* Fig. 6.13), the RG flows depicted schematically in Fig. 6.19 are just those arising at low-energies in the full TQD model, in the vicinity of, and at, the quantum phase transition.

6.4.1 Pseudospin properties

The reduced model, Eq. 6.34, provides a direct means of studying properties of the pseudospin itself, which we consider here. Throughout this section, we compare two cases with the same coupling $\rho J_{\text{mix}} = 0.075$, and both are chosen so as to have the same 2CK scale $T_K/D = 10^{-13}$. However, one is deep in the 2CK regime (with $\tilde{E}_\Delta/D = -10^{-3} \equiv 10^{+3}T_K^c$), while the other is close to the transition (with $\tilde{E}_\Delta/D = -10^{-10} \equiv 10^{-4}T_K^c$) — see Fig. 6.18.

While $\hat{T}^z$ is not a conserved quantity in Eq. 6.34, expectation values of it can be computed directly with NRG. Fig. 6.20 shows $\langle \hat{T}^z \rangle$ *vs.* T/D , with the top panel for $\tilde{E}_\Delta/D = -10^{-3}$, away from the transition (solid line), and the bottom panel for $\tilde{E}_\Delta/D = -10^{-10}$, close to the transition (dashed line).

Away from the transition, $\langle \hat{T}^z \rangle$ saturates rapidly to its $T = 0$ value of $\langle \hat{T}^z \rangle = 0.47$ on the scale of $\tilde{E}_\Delta$, indicating that the $\mathcal{T}^z = -\frac{1}{2}$ component of the pseudospin has largely been frozen out. The small degree of mixing of the $\mathcal{T}^z = \pm\frac{1}{2}$ components through Eq. 6.34a means that $\langle \hat{T}^z \rangle$ is close to its maximum value of $+\frac{1}{2}$ obtained in the large $|\tilde{E}_\Delta|$ limit.

In the bottom panel of Fig. 6.20 for the system close to the transition, the pseudospin components are near degenerate and we see that $\langle \hat{T}^z \rangle = 0.0018$ at $T = 0$. The degree of mixing is large, and so $\langle \hat{T}^z \rangle$ is naturally rather small. Indeed, for $T \gg T_K^c$ the pseudospin components are quasidegenerate and $\langle \hat{T}^z \rangle \simeq 0$. As the temperature is lowered, the system flows near the CFP and $\langle \hat{T}^z \rangle$ grows until the 2CK FP is reached for $T \approx T_K$.

In the inset we show the $T = 0$ value of $\langle \hat{T}^z \rangle$ *vs.* $|\tilde{E}_\Delta|/D$. A smooth crossover from $\langle \hat{T}^z \rangle \approx \frac{1}{2}$ to 0 occurs on the scale of $T_K^c/D = 10^{-6}$, with $\langle \hat{T}^z \rangle = 0$ precisely at the transition, indicative of the strict degeneracy of the pseudospin components for $\tilde{E}_\Delta$.

An obvious question arises: for $T \ll \tilde{E}_\Delta$, why is the upper pseudospin component not completely projected out, giving ultimately $\langle \hat{T}^z \rangle = \frac{1}{2}$ at $T = 0$ for any system not exactly at the transition? The answer is that the stable FP in the model for any

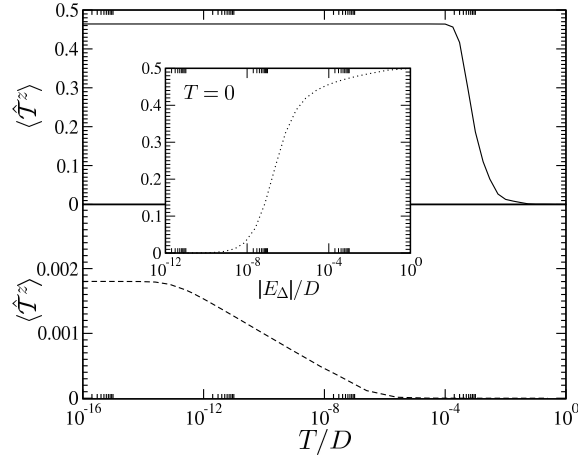


Figure 6.20: $\langle \hat{T}^z \rangle$ vs. T/D for $\rho J_{\text{mix}} = 0.075$ and $\tilde{E}_\Delta/D = -10^{-3}$ (top panel) and -10^{-10} (bottom panel). The inset shows the $T = 0$ variation of $\langle \hat{T}^z \rangle$ vs. $|\tilde{E}_\Delta|/D$.

non-zero $\tilde{E}_\Delta$ is the 2CK FP, and formation of this state via Eq. 6.35 necessitates virtual excitations to the upper lying pseudospin sector. Thus, even at $T = 0$ the $\hat{T}^\pm$ terms of $H_{\text{red}}^{\text{eff}}$ are operable and act to mix $\mathcal{T}^z = \pm \frac{1}{2}$ components.

We now turn to the expectation values $\langle \hat{T}^+ \rangle = \langle \hat{T}^- \rangle \equiv \langle \hat{T}^\pm \rangle$ in Fig. 6.21, which embody the degree of pseudospin mixing.

We consider first the inset, where the variation of $\langle \hat{T}^\pm \rangle$ at $T = 0$ is plotted vs. $|\tilde{E}_\Delta|$. We find that the inverse relationship $\langle \hat{T}^\pm \rangle \sim 1/|\tilde{E}_\Delta|$ holds over the entire range of $\tilde{E}_\Delta$. The degree of pseudospin mixing is naturally suppressed when the energy separation between the $\mathcal{T}^z = \pm \frac{1}{2}$ sectors is large, while mixing is favoured when the pseudospin components are near-degenerate. This can be thought of in terms of the energy penalty in making a virtual excitation to a state in the higher lying pseudospin sector, which is proportional to $|\tilde{E}_\Delta|$ (see Eq. 6.35). It is these virtual excitations which ultimately drive the system to the stable 2CK FP for $T \approx T_K$. For $T \ll T_K$ therefore, we expect $\langle \hat{T}^\pm \rangle$ to remain constant down to $T \rightarrow 0$.

We consider now the main panel of Fig. 6.21, where we show $\langle \hat{T}^\pm \rangle$ vs. T/D for the same systems as in Fig. 6.20: the solid line being away from the transition ($\tilde{E}_\Delta/D = -10^{-3}$), while the dashed line is close to the transition ($\tilde{E}_\Delta/D = -10^{-10}$).

The situation away from the transition is again straightforward: as the temperature is lowered, $\langle \hat{T}^\pm \rangle$ increases, and it is found that $\langle \hat{T}^\pm \rangle \sim 1/T$. On further decreasing the temperature however, the growth of $\langle \hat{T}^\pm \rangle$ is arrested on the scale $T \approx |\tilde{E}_\Delta|$, where it plateaus to its ultimate $T = 0$ value (see inset). The $|\tilde{E}_\Delta|$ scale of course corresponds to the temperature below which the upper pseudospin component is essentially frozen out (see Fig. 6.20), although mixing of the pseudospin components (described by $\langle \hat{T}^\pm \rangle$) remains finite (albeit small) down to $T = 0$.

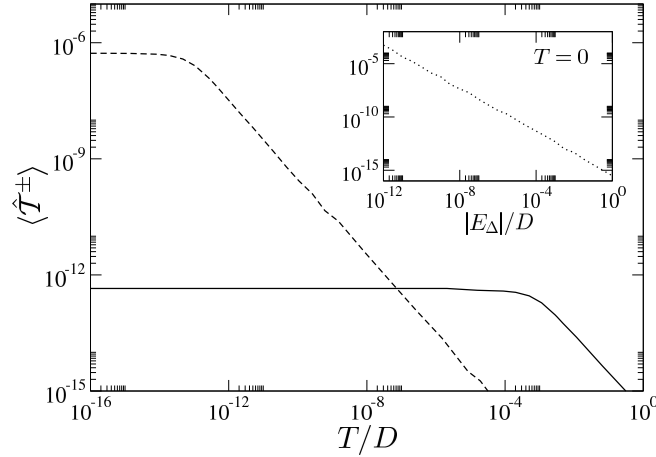


Figure 6.21: $\langle \hat{T}^+ \rangle = \langle \hat{T}^- \rangle \equiv \langle \hat{T}^\pm \rangle$ vs. T/D for the same systems as in Fig. 6.20. The inset again shows the $T = 0$ variation as a function of $|E_\Delta|/D$.

The dashed line for a system close to the transition shows different behaviour, even though both systems have the same T_K . Here, $\langle \hat{T}^\pm \rangle$ continues to grow down to $T \approx T_K$ (rather than $T \approx |\tilde{E}_\Delta|$ as for the solid line), below which it plateaus to its eventual $T = 0$ value. However, as we showed in the inset, $\langle \hat{T}^\pm \rangle \sim 1/|\tilde{E}_\Delta|$ at $T = 0$, and thus the variation of $\langle \hat{T}^\pm \rangle$ must take a different form: $\langle \hat{T}^\pm \rangle \sim T_K/(T \times |\tilde{E}_\Delta|)$. Near the transition, we established in Sec. 6.4 that $T_K \sim |\tilde{E}_\Delta|^2$ (as for the full TQD model), and so for $|\tilde{E}_\Delta| < T_K^c$ we can equivalently write $\langle \hat{T}^\pm \rangle \sim |\tilde{E}_\Delta|/T$, which is confirmed directly from NRG for the reduced model.

Again, reintroducing the term $(\frac{1}{2}J_A + J_B\hat{T}^z)\hat{\mathbf{S}} \cdot (\hat{\mathbf{s}}_{L0} + \hat{\mathbf{s}}_{R0})$ does not change the essential physics elucidated here, and so the reduced model Eq. 6.34 faithfully captures the novel behaviour of the full TQD model near the transition.

6.5 Summary

In this chapter, we have studied what is arguably the simplest two-channel device in which to understand the consequences of local frustration arising from internal degrees of freedom: a triple quantum dot ring, with dots mutually coupled by antiferromagnetic exchange interactions, and tunnel-coupled symmetrically to two metallic leads. While important aspects of related models have been considered before [65, 68, 85, 111, 114], the underlying physics is found to be even richer than hitherto uncovered.

Two distinct 2CK phases arise due to the mirror symmetry in the problem, each displaying classic non-Fermi liquid properties of the 2CK fixed point, below a characteristic two-channel Kondo scale (see Sec. 6.2), such as an entropy $S_{\text{imp}} = \frac{1}{2} \ln(2)$ and a spin susceptibility $\chi_{\text{imp}} \propto \ln(1/T)$. In particular, we studied the

single-particle spectrum $\pi\Gamma D_1(\omega) \equiv \pi\Gamma D_3(\omega)$ of the dots tunnel-coupled to the leads in Sec. 6.2.2, and demonstrated universal scaling collapse to the spectrum of a single-spin 2CK model. At the Fermi level in particular, we found at $T = 0$ that the spectrum reached *half* the unitarity limit, $\pi\Gamma D_1(0) = \frac{1}{2}$, yielding thereby a conductance through the terminal dots of $G_c/G_0 = \frac{1}{2}$.

But although two-channel Kondo physics predominates in the underlying parameter space, the parity-distinct nature of the 2CK phases means that a quantum phase transition between them occurs. The 2CK phases were shown in Sec. 6.3 to be separated by a quantum critical point, for which an effective low-energy model was derived (Sec. 6.1.2). Precisely at the transition, parity mixing of the quasi-degenerate local trimer states acts to destabilise the 2CK fixed points, and the critical fixed point is shown to consist of a free pseudospin together with effective *single-channel* spin quenching. At the transition, the system is shown to share many properties with the channel-anisotropic 2CK model — and indeed the conventional spin- $\frac{1}{2}$ Anderson model. But the L/R mirror symmetry of the setup necessitates that the strong-coupling Kondo singlet *and* the set of weak-coupling free conduction band states form symmetrically in each channel. This gives rise to some unusual physical properties not accessible in systems where orbital effects arising from the internal degrees of freedom of the device are absent. For example, we showed in Sec. 6.3 that a residual $T = 0$ entropy $S_{\text{imp}} = \ln(2)$ characterizes the quantum critical point (corresponding to the free pseudospin), but that $\chi_{\text{imp}} \propto 1/T_K^{1CK}$ is also observed, indicative of single-channel spin quenching. Indeed, the spectrum $\pi\Gamma D_1(\omega = 0) = \frac{1}{2}$ at the transition, but the low-frequency asymptotics again show that the Kondo resonance is not characteristic of the 2CK spectrum, but rather is typical of the Fermi liquid behaviour of the single-channel Anderson model, but with a halved amplitude symptomatic of the fact that the Kondo singlet forms with the left lead for only one of the two pseudospin sectors, while it forms in the right lead for the other. The behaviour of the full TQD model at the transition can thus in some sense be considered as a “quasi Fermi liquid”.

Driven by varying the interdot exchange couplings, occurring at the point of inherent magnetic frustration, and characterised by a nontrivial quantum critical point, the transition thus provides a striking example of the subtle interplay between internal spin and orbital degrees of freedom in coupled quantum dot systems.

CHAPTER 7

Larger quantum dot rings

In the previous chapter, we explored in detail the simplest structure to exhibit frustration: a triple quantum dot (TQD) ring. We demonstrated that, connected to two leads as in Fig. 6.1, two-channel Kondo (2CK) physics predominates in the mirror-symmetric systems considered, but that tuning the interdot couplings to the point of inherent magnetic frustration in the trimer leads to novel physical behaviour. The lowest states of the isolated trimer are a pair of doublets, which were shown to have different parity under exchange of dots $1 \leftrightarrow 3$. As a consequence of this symmetry, a level-crossing is permitted in the isolated TQD, which in turn results in the formation of two 2CK phases of distinct parity when the leads are attached. Thus, a quantum phase transition (QPT) occurs on varying the interdot exchange coupling, with a nontrivial critical point separating these phases. In the full model, it is the *overall* left $\leftrightarrow$ right parity (rather than the local $1 \leftrightarrow 3$ dot parity) that is conserved, and it was shown that mixing of the doublet states — acting thereby to switch the local dot parity — drives the transition.

There are three key properties of this TQD system which are responsible for the subtle physical behaviour elucidated in Chapter 6. Firstly, the ring must be constructed of an *odd* number of dots, so that the lowest states are a pair of doublets. Secondly, there must be an effective *antiferromagnetic* coupling between these doublets and the leads,¹ so that 2CK physics results when either state is the TQD ground state. Finally, the doublets must have different *parity* under left $\leftrightarrow$ right exchange, so that two distinct phases result, with a QPT separating them.

We extend the work of the previous chapter here to larger quantum dot ring models. In particular, we analyze larger odd-membered spin ring systems, showing that the above conditions are satisfied for rings of the same basic geometry as the TQD studied previously, and that analogous physical behaviour results.

¹The lowest state of an even ring is always a spin-singlet state, which decouples from the leads, and hence no effective Kondo coupling can result. As a consequence, Kondo physics is absent in such systems, and so we do not discuss even ring systems further here.

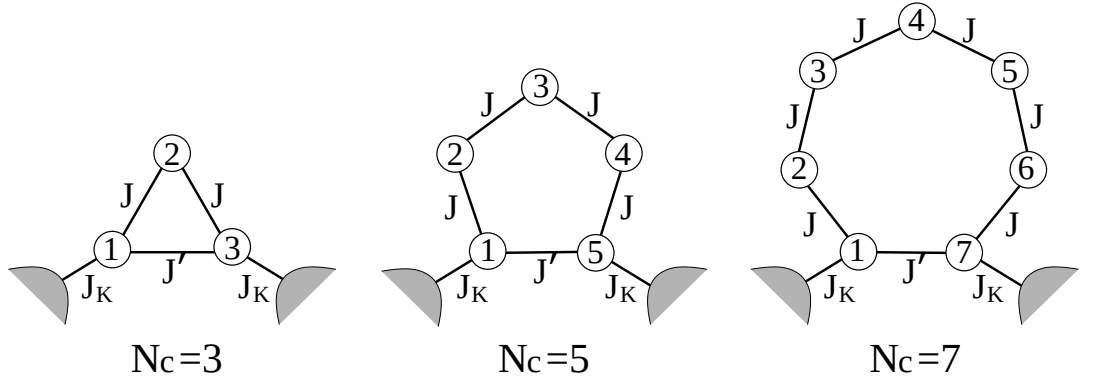


Figure 7.1: Schematic illustration of quantum dot rings connected to two leads. Only odd rings of size $N_c = 3, 5$ and 7 are shown.

7.1 Model and physical picture

In this chapter, we consider rings of odd numbers of dots connected to two leads, and investigate the evolution of properties as a function of interdot couplings. In the previous chapter, we studied a TQD, modelling dots 1 and 3 as Andersonian sites, tunnel-coupled to the leads. As the lowest-energy manifold of TQD states is the singly-occupied manifold, in a certain temperature window this model can be mapped onto a spin model. Therefore, here we choose to model larger ring systems as Heisenberg rings of *spins*, as this allows the generic behaviour of quantum dot rings to be understood simply, while retaining the essential physics of more realistic models.² In particular, we show that the underlying physics of a TQD spin ring is the same as that elucidated in Chapter 6.

As before, we focus specifically on systems tuned to mirror symmetry, with two neighbouring dots each connected to their own metallic lead, as illustrated in Fig. 7.1 for $N_c = 3, 5$ and 7 . The class of Hamiltonians we study are thus of the form $H = H_L + H_{\text{ring}}^{N_c} + H_K$. As usual, $H_L = \sum_{\alpha, \mathbf{k}, \sigma} \epsilon_{\mathbf{k}} a_{\alpha \mathbf{k} \sigma}^\dagger a_{\alpha \mathbf{k} \sigma}$ refers to the two equivalent non-interacting leads ($\alpha = L, R$), and

$$H_{\text{ring}}^{N_c} = J \left(\sum_{i=1}^{N_c-1} \hat{\mathbf{S}}_i \cdot \hat{\mathbf{S}}_{i+1} \right) + J' \hat{\mathbf{S}}_1 \cdot \hat{\mathbf{S}}_{N_c}, \quad (7.1)$$

$$H_K = J_K (\hat{\mathbf{S}}_1 \cdot \hat{\mathbf{S}}_{L0} + \hat{\mathbf{S}}_{N_c} \cdot \hat{\mathbf{S}}_{R0}),$$

where $\hat{\mathbf{S}}_i$ is a spin- $\frac{1}{2}$ operator for dot i and N_c is the total number of dots in the ring. $\hat{\mathbf{S}}_{L0}$ is the spin density of the left lead at dot 1, and similarly $\hat{\mathbf{S}}_{R0}$ is the spin density of the right lead at dot N_c , as previously defined in Eq. 3.2a.

²For a ring of a given size N_c comprising only spins, the dot Hilbert space is of dimension 2^{N_c} , rather than 4^{N_c} for rings of sites. Thus NRG calculations are much less expensive, which means in practice that more accurate results can be obtained for larger and more complicated systems.

7.1.1 Properties of the isolated rings

In the spirit of the approach adopted in the previous chapter, we consider first the rings detached from their leads. Studying and characterizing the states of the isolated rings is essential to obtain an understanding of the interplay between internal spin and orbital degrees of freedom of the quantum dot device, and hence the resulting Kondo physics on coupling to the leads.

The states of the isolated ring are of course simply the eigenstates of $H_{\text{ring}}^{N_c}$. For $N_c = 3$, these eigenstates are particularly simple objects, since (modulo an irrelevant constant) the dot Hamiltonian can be written in the form

$$H_{\text{ring}}^{N_c=3} = J\hat{\mathbf{S}}_2 \cdot \hat{\mathbf{S}}_{13} + \frac{1}{2}J'\hat{\mathbf{S}}_{13}^2 \quad (7.2)$$

where $\hat{\mathbf{S}}_{13} = (\hat{\mathbf{S}}_1 + \hat{\mathbf{S}}_3)$ is a conserved quantity describing the combined spin of the dots 1 and 3. This is precisely the Hamiltonian arising in the singly-occupied sector of Eq. 6.1 for the TQD tunnel-coupled to its leads, and hence the same states arise. In particular, the lowest doublets are given by Eq. 6.2, and as $\hat{\mathbf{S}}_{13}$ is a conserved quantity, dots 1 and 3 are either found in a singlet combination (the $|N_c = 3; +; S^z\rangle$ doublet) or a triplet combination (the $|N_c = 3; -; S^z\rangle$ doublet). Indeed, as was shown in Sec. 4.1.1, these states can be generated explicitly in terms of Clebsch-Gordon coefficients by vector coupling the total spin $\hat{\mathbf{S}} = (\hat{\mathbf{S}}_1 + \hat{\mathbf{S}}_2 + \hat{\mathbf{S}}_3)$ and the combined spin $\hat{\mathbf{S}}_{13}$ using Eq. 4.2, as both are conserved by $H_{\text{ring}}^{N_c=3}$.

The L/R mirror symmetry of $H_{\text{ring}}^{N_c}$ also implies that states of any ring can in addition always be labelled by their *parity*. As in Appendix A, we define an operator $\hat{P}_{i,j}$ which exchanges orbital labels on dots i and j . The overall parity operator, $\hat{P}_{\text{ring}}^{N_c}$, acting on the ring Hilbert space is then given by

$$\hat{P}_{\text{ring}}^{N_c} = \prod_{i=1}^{\frac{1}{2}(N_c-1)} \hat{P}_{i,(N_c+1-i)} \quad (7.3)$$

For any N_c therefore, $[H_{\text{ring}}^{N_c}, \hat{P}_{\text{ring}}^{N_c}] = 0$ immediately follows from Eq. 7.1, reflecting the invariance of the ring part of the Hamiltonian to exchange of left and right dot labels. We also note that $\hat{P}_{\text{ring}}^{N_c}$ is self-inverse (*ie.* $(\hat{P}_{\text{ring}}^{N_c})^2 = 1$) and so eigenvalues of it are naturally ± 1 only. Thus we will label the ring states according to parity such that $\hat{P}_{\text{ring}}^{N_c}|N_c; \pm; S^z; r\rangle = \pm|N_c; \pm; S^z; r\rangle$ (with r an index distinguishing different states with the same parity and S^z).

From Appendix A, Eq. A.12, it readily follows [150] that for a spin-only system (as appropriate for $H_{\text{ring}}^{N_c}$), $\hat{P}_{i,j}$ reduces to $\hat{P}_{i,j} = (1 - \hat{\mathbf{S}}_{ij}^2)$, and thus for $N_c = 3$ we obtain $\hat{P}_{\text{ring}}^{N_c=3} = \hat{P}_{1,3} \equiv (1 - \hat{\mathbf{S}}_{13}^2)$, recovering the expression used for the TQD in Chapter 6. Labelling the TQD states by parity is thus wholly equivalent to labelling

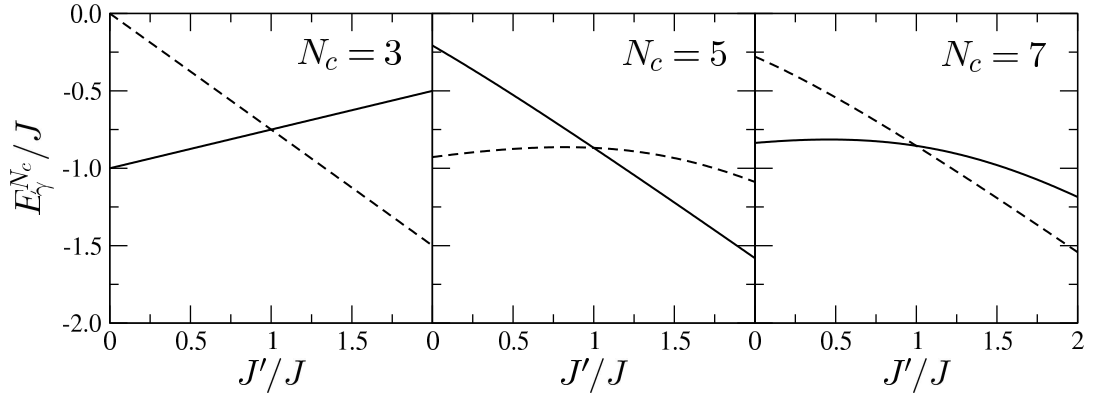


Figure 7.2: Variation in energy $E_\gamma^{N_c}/J$ of the lowest pair of doublets in isolated spin rings of size $N_c = 3, 5$ and 7 as a function of the dimensionless ratio of interdot couplings J'/J (see Fig. 7.1), as calculated from numerical diagonalization of $H_{\text{ring}}^{N_c}$. In each case there is a level crossing, with the $\gamma = -$ (odd) parity state (solid line) and the $\gamma = +$ (even) parity state (dashed line) being degenerate precisely at $J' = J$.

them by $\hat{\mathbf{S}}_{13}$.

For $N_c = 5$, Eq. 7.3 similarly gives $\hat{P}_{\text{ring}}^5 = \hat{P}_{1,5}\hat{P}_{2,4} \equiv (1 - \hat{\mathbf{S}}_{15}^2)(1 - \hat{\mathbf{S}}_{24}^2)$. We note that while eigenstates of $H_{\text{ring}}^{N_c=5}$ can of course be labelled by their parity through $\hat{P}_{\text{ring}}^5$, they *cannot* be specified by $\hat{\mathbf{S}}_{15}$ or $\hat{\mathbf{S}}_{24}$, as these are not conserved quantities. Indeed, as we discussed in Sec. 4.1.1 in the context of quantum dot chains, a simple description of the eigenstates for any $N_c > 3$ is not possible, since in general only the total ring spin $\hat{\mathbf{S}}$ is conserved, so no vector coupling scheme can be employed.

In general then, one must simply diagonalize $H_{\text{ring}}^{N_c}$ numerically, and here we focus on the low-lying states. For antiferromagnetic couplings ($J, J' > 0$), the lowest states of $H_{\text{ring}}^{N_c}$ are always a pair of doublets which are found³ to have different parity under $\hat{P}_{\text{ring}}^{N_c}$.

The different parity of the lowest doublets means that a level crossing is allowed by symmetry. By contrast an ‘avoided-crossing’ results if two states are described by the same quantum numbers for a complete set of mutually commuting operators. Here, the inherent magnetic frustration which must occur in odd rings when all interdot exchange couplings are equal implies that there is a degeneracy of the ground state at the point $J = J'$, and hence that the lowest states must have different symmetries.

That there is indeed a simple level-crossing of the $|N_c; \pm; S^z\rangle$ ring doublets⁴ is confirmed in Fig. 7.2, where we plot the energy $E_\gamma^{N_c}/J$ of these states as a function of the ratio of interdot couplings J'/J , for rings with $N_c = 3, 5$ and 7 . The separation in energy $E_\Delta^{N_c} = (E_+ - E_-)$ vanishes in each case at the point $J' = J$, so that the $|N_c; -; S^z\rangle$ doublet (odd parity; solid lines) and the $|N_c; +; S^z\rangle$ doublet (even parity;

³That the lowest doublets have different parity has been checked explicitly up to $N_c = 15$, and we suspect it is generally true for any N_c , although we do not have a proof *per se* of this.

⁴We consider the lowest doublet state of each parity $\gamma = \pm$ now, and hence drop the index r .

dashed lines) are indeed degenerate when the isolated ring is frustrated.

The nontrivial many-body behaviour of interest of course results on coupling the ring to the leads, as considered below.

7.1.2 Effective 2CK models of odd spin rings

In the following, we proceed analogously to Sec. 6.1.2, generalizing the results of the TQD to rings of arbitrary (odd) N_c . We are generically interested here (as in Chapter 6) in the regime where the interdot couplings J and J' are large compared with the (exponentially small) single-channel Kondo scale, $T_K^{1CK}/D \propto \exp(-1/\rho J_K)$, and will in fact consider explicitly $\max(J, J') > J_K$.

As the temperature is reduced, the higher lying states of the ring are successively projected out, and so only an *effective* coupling between the lower-lying states and the leads need enter a description of the system on these temperature/energy scales.

Specifically, for $E_{\Delta}^{N_c} < 0$, the $|N_c; +; S^z\rangle$ doublet is the ring ground state, while for $E_{\Delta}^{N_c} > 0$, $|N_c; -; S^z\rangle$ lies lowest. First we consider the situation when the doublets are not near-degenerate, well away from the point of frustration (which occurs at $E_{\Delta}^{N_c} = 0$, or equivalently $J' = J$: see Fig. 7.2). For temperatures $T \lesssim |E_{\Delta}^{N_c}|$ only the single lowest ring state $|N_c; \gamma; S^z\rangle$ need be retained, as all excited states are thermally inaccessible. Below, we construct an effective low-energy model valid in this regime, projecting into the reduced Hilbert space of the lowest doublet using

$$\hat{1}_{\pm}^{N_c} = \sum_{S^z} |N_c; \pm; S^z\rangle \langle N_c; \pm; S^z|, \quad (7.4)$$

for the appropriate $\gamma = +/ -$ ground state for any ring of size N_c . We will employ the Brillouin-Wigner expansion [122] of H , treating H_K as a perturbation to the states of $H_{\text{ring}}^{N_c}$, viz

$$\begin{aligned} H_{\text{eff}, \gamma}^{N_c} &= H_{\text{eff}, \gamma}^{N_c, 0} + H_{\text{eff}, \gamma}^{N_c, \text{I}} + H_{\text{eff}, \gamma}^{N_c, \text{II}} + \dots \\ &= \hat{1}_{\gamma}^{N_c} \left(H_{\text{ring}}^{N_c} + H_K + H_K (E_{\gamma}^{N_c} - H_{\text{ring}}^{N_c})^{-1} \hat{P} H_K + \dots \right) \hat{1}_{\gamma}^{N_c}, \end{aligned} \quad (7.5)$$

where $\hat{P} = \hat{1}_{\text{full}} - \hat{1}_{\gamma}^{N_c}$ is an operator which projects into the excited manifold of states, and $H_{\text{eff}, \gamma}^{N_c, 0} = \hat{1}_{\gamma}^{N_c} H_{\text{ring}}^{N_c} \hat{1}_{\gamma}^{N_c} = E_{\gamma}^{N_c} \hat{1}_{\gamma}^{N_c}$ is simply the energy of the ring ground state for $\gamma = +$ or $-$.

The first-order term, $H_{\text{eff}, \gamma}^{N_c, \text{I}}$, describes simply the projection of H_K onto the ring ground state $|N_c, \gamma; S^z\rangle$. This term might be expected to dominate the perturbation expansion, as the hierarchical structure of Eq. 7.5 implies a separation of energy scales. In Sec. 6.1.2 of Chapter 6, we considered this term alone for the TQD system, and so it is a natural place for us to begin the analysis of the larger rings.

To this end, we note that $H_{\text{eff}, \gamma}^{N_c, \text{I}} \equiv J_K (\hat{1}_{\gamma}^{N_c} \hat{\mathbf{S}}_1 \hat{1}_{\gamma}^{N_c} \cdot \hat{\mathbf{s}}_{L0} + \hat{1}_{\gamma}^{N_c} \hat{\mathbf{S}}_{N_c} \hat{1}_{\gamma}^{N_c} \cdot \hat{\mathbf{s}}_{R0})$ may be

alternatively written as

$$H_{\text{eff},\gamma}^{N_c, \text{I}} = \frac{1}{2} J_K \hat{\mathbf{1}}_\gamma^{N_c} (\hat{\mathbf{S}}_1 + \hat{\mathbf{S}}_{N_c}) \hat{\mathbf{1}}_\gamma^{N_c} \cdot (\hat{\mathbf{S}}_{L0} + \hat{\mathbf{S}}_{R0}), \quad (7.6)$$

using the symmetry⁵ $\hat{\mathbf{1}}_\gamma^{N_c} \hat{\mathbf{S}}_1 \hat{\mathbf{1}}_\gamma^{N_c} = \hat{\mathbf{1}}_\gamma^{N_c} \hat{\mathbf{S}}_{N_c} \hat{\mathbf{1}}_\gamma^{N_c}$. Eq. 7.6 is the generalized odd-ring analogue of Eq. 6.6 for the TQD studied in Chapter 6, and is similarly a model of 2CK form:

$$H_{\text{eff},\gamma}^{N_c, \text{I}} = J_{K\gamma}^{N_c, \text{I}} \hat{\mathbf{S}}_\gamma \cdot (\hat{\mathbf{S}}_{L0} + \hat{\mathbf{S}}_{R0}), \quad (7.7)$$

where $\hat{\mathbf{S}}_\gamma$ is the spin- $\frac{1}{2}$ operator representing the appropriate doublet $\gamma = +/ -$, which is independent of N_c , since it is only the magnitude of the effective coupling (embodied in $J_{K\gamma}^{N_c, \text{I}}$) that depends on the ring size: the underlying structure of the low-energy effective model is the same in all cases. As in Sec. 6.1.2, considering just the z -components of the spin, the effective coupling can be shown⁶ to be

$$J_{K\gamma}^{N_c, \text{I}} = \langle N_c; \gamma; +\frac{1}{2} | S_1^z + S_{N_c}^z | N_c; \gamma; +\frac{1}{2} \rangle J_K. \quad (7.8)$$

Provided $J_{K\gamma}^{N_c, \text{I}} > 0$ (*ie.* it is antiferromagnetic), 2CK physics is expected below a characteristic temperature/energy scale T_K , given as usual for a model of 2CK form (such as Eq. 7.7) from perturbative scaling [40] by

$$T_K \sim J_{K, \text{eff}} \exp(-1/\rho J_{K, \text{eff}}), \quad (7.9)$$

with the effective coupling $J_{K, \text{eff}} = J_{K\gamma}^{N_c, \text{I}} + \mathcal{O}(J_K^2)$ given to first-order by Eq. 7.8.

The same low-energy effective model results for all odd rings (away from the point of frustration at $J' = J$). Indeed, the structure of Eq. 7.7 is identical to that of the TQD tunnel-coupled to its leads, studied in the previous chapter. However, the effective couplings themselves depend on the specific details of the bare model. We examine these effective couplings, as calculated from Eq. 7.8, for various rings below. First however, we comment that ring parity is conserved in Eq. 7.7, with $[\hat{P}_{\text{ring}}^{N_c}, H_{\text{eff},\gamma}^{N_c, \text{I}}] = 0$. Thus, since the 2CK effective model Eq. 7.7 is valid for $E_\Delta^{N_c} \ll 0$ (where the ring parity is $(+)$ /even) and for $E_\Delta^{N_c} \gg 0$ (where the ring parity is $(-)$ /odd), a quantum phase transition between phases of distinct parity must occur as a function of $E_\Delta^{N_c}$ (and hence J'). This is considered in Sec. 7.3.

We return now to Eq. 7.8, and consider the variation of effective coupling $J_{K\gamma}^{N_c, \text{I}}/J_K$ as a function of J'/J for rings of size $N_c = 3, 5$ and 7 , as shown in Fig. 7.3. $J_{K\gamma}^{N_c, \text{I}}/J_K$ itself essentially describes the renormalization (to first order) in coupling between the lowest ring doublet state $|N_c, \gamma; S^z\rangle$ and the leads, as compared with a standard single-spin 2CK model with Kondo coupling J_K . In Fig. 7.3 we only plot

⁵This can be readily proved using the ring parity operator: see Eq. 7.14.

⁶That $\langle N_c; \gamma; S^z | S_1^z + S_{N_c}^z | N_c; \gamma; S^z \rangle \propto S^z$ is a general result of the $SU(2)$ spin symmetry of the problem, as discussed in Sec. 4.1.1.

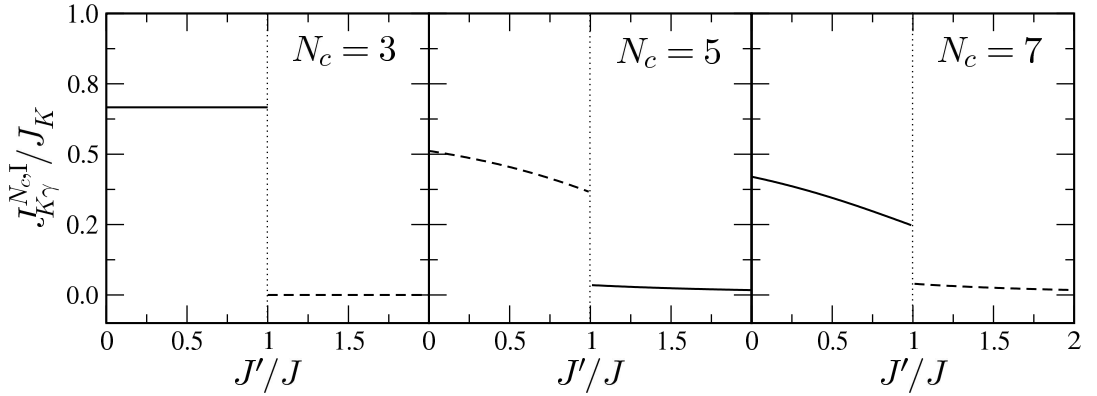


Figure 7.3: Evolution in the first-order effective coupling $J_{K\gamma}^{N_c, I}/J_K$, between the ring ground state and the attached leads (as calculated from Eq. 7.8) as a function of J'/J for rings of size $N_c = 3, 5$ and 7 . Solid lines are used for $\gamma = -$ while dashed lines indicate $\gamma = +$, as before. The odd parity ($-$) state is lowest for $E_\Delta > 0$, while the even parity state is the ring ground state for $E_\Delta < 0$.

$J_{K+}^{N_c, I}/J_K$ (shown as the dashed lines) when $|N_c; +; S^z\rangle$ is the ring ground state (*ie.* for $E_\Delta^{N_c} < 0$), while $J_{K-}^{N_c, I}/J_K$ (solid lines) are shown only when $|N_c; -; S^z\rangle$ is the ring ground state ($E_\Delta^{N_c} > 0$). Indeed, the perturbative results of Eq. 7.8 are only strictly valid in the large $|E_\Delta^{N_c}|$ limit.

We consider first the simplest ring, $N_c = 3$ (left panel of Fig. 7.3), to make connection with the work of Chapter 6. The TQD studied previously modelled dots 1 and 3 as Andersonian sites rather than spins (Eq. 6.1), but it was shown in Sec. 6.1.2 that this model maps onto the spin model considered here when the dots are essentially singly-occupied (Eq. 6.4 $\equiv$ Eq. 7.1 for $N_c = 3$). We revisit the $N_c = 3$ ring again here as the situation comprises a limiting case which can be simply understood in terms of the explicit form of the TQD states (Eq. 6.2). The physical picture in the case of the larger, more complicated rings is then clear in the context of these simple results.

The ring ground state effective coupling, $J_{K\gamma}^{N_c, I}$ (calculated from Eq. 7.8), and hence the Kondo scale on which the 2CK FP is reached (determined through Eq. 7.9), depends on the configuration of spins on the dots connected to the leads. In the TQD, the $|N_c = 3; -; S^z\rangle$ doublet (lowest for $J'/J < 1$) contains a pure triplet configuration of dots 1 and 3, and direct evaluation of Eq. 7.8 yields $J_{K-}^{N_c=3} = \frac{2}{3}J_K$ for all $J'/J < 1$ (see left panel of Fig. 7.3). This is of course precisely the result obtained in the $J' = 0$ case studied in Sec. 4.1.2 and for the TQD tunnel-coupled to its leads in Sec. 6.1.2. As the effective coupling is antiferromagnetic, Eq. 7.9 gives an exponentially small 2CK scale, $T_K \sim J_K \exp(-3/2\rho J_K)$, independent of J'/J .

By contrast, the $|N_c = 3; +; S^z\rangle$ doublet (the TQD ground state for $J'/J > 1$) has a singlet-locked combination of dots 1 and 3, which thus do not couple to the leads to first order and so $J_{K+}^{N_c=3} = 0$ for all $J'/J > 1$.

Turning now to the larger rings, evaluation of Eq. 7.8, using the numerically diagonalized eigenstates of $H_{\text{ring}}^{N_c}$, yields the effective coupling $J_{K\gamma}^{N_c, I}/J_K$; shown for $N_c = 5$ in the middle panel of Fig. 7.3 and $N_c = 7$ in the right panel. The behaviour is somewhat similar to that of the $N_c = 3$ case: for $J' < J$, the effective coupling is a significant fraction of the bare Kondo coupling J_K , while, for $J' > J$ it is near zero.

A key difference arise for larger rings, however. Since $\hat{\mathbf{S}}_{1N_c} = (\hat{\mathbf{S}}_1 + \hat{\mathbf{S}}_{N_c})$ is not a conserved quantity for $N_c = 5$ or 7 , the terminal dots are not found in pure singlet or triplet configurations. The resultant mixing of singlet and triplet states of the dots connected to the leads means that the limit of $J_{K\gamma}^{N_c, I}/J_K = \frac{2}{3}$ for $J' < J$ is not strictly satisfied for $N_c > 3$. The $J' = 0$ case was studied in Chapter 4, where it was found that the effective coupling diminished with increasing N_c . This is of course physically natural, since the longer the chain, the weaker the correlations between the terminal dots, which in turn results in a smaller effective coupling through Eq. 7.8. This is seen in Fig. 7.3, going from $N_c = 3 \rightarrow 5 \rightarrow 7$. Indeed, as J' is switched on and increased, the degree of singlet character in the configuration of dots 1 and N_c is expected to increase, as a direct antiferromagnetic interaction between them is now present. This is manifest in the general diminution of $J_{K\gamma}^{N_c, I}/J_K$ with increasing J' , as seen clearly in Fig. 7.3 for $N_c = 5$ and 7 .

Significantly, in the $J' > J$ regime, the terminal dots are no longer found in a pure singlet configuration for $N_c > 3$, and so $J_{K\gamma}^{N_c, I}/J_K > 0$ — although it remains rather small.

Before considering the behaviour of these system with NRG, we pause to comment on the physical implications of the above results. In the $J' < J$ regime, the behaviour of odd rings of any size is expected to be qualitatively similar to the $N_c = 3$ case — and indeed the TQD tunnel-coupled to leads which we studied extensively in Chapter 6 — since the same effective low-energy model Eq. 7.7 results in each case. The underlying stable FP is the 2CK FP: two-channel Kondo physics is expected below T_K , as given from Eq. 7.9, with the effective coupling calculable from Eq. 7.8, and shown for $N_c = 3, 5, 7$ in Fig. 7.3. While the effective coupling (and hence the T_K scale) varies with N_c and J' in this regime, universal behaviour of *eg.* the thermodynamics is expected in terms of T/T_K .

By contrast, the behaviour in the $J' > J$ regime appears to be quite different. In the $N_c = 3$ case, $J_{K+}^{N_c=3, I} = 0$ which, to this level of calculation, implies that the TQD decouples from the leads. The LM FP would now be stable, and the 2CK FP would not be reached for any $J' > J$, even as $T \rightarrow 0$. For $N_c = 5$ and 7 , a small antiferromagnetic effective coupling *does* result (due to the small degree of triplet character in the configuration of the terminal dots). However, this first-order effective coupling is extremely small, and so the Kondo scale (see Eq. 7.9) is essentially unobservable — even going to very high iteration numbers with NRG. For

example, in the $N_c = 5$ case, for a system with $J'/J = \frac{3}{2}$ (thereby deep in the $J' > J$ regime; see Fig. 7.3) and $\rho J_K = 0.1$ (with $\rho = 1/(2D)$ the density of lead states as usual), the Kondo scale as calculated via Eqs. 7.8 and 7.9 is $T_K/D \approx 10^{-175}$.

One might expect, however, that considering higher-order terms in the perturbation expansion, Eq. 7.5, could change qualitatively the simplistic physical picture described above. While the effective coupling (to first order) in the $J' > J$ regime is found to be very small (or zero) in spin rings, this is *not* because the bare energy scale J_K in Eq. 7.8 is small, but rather that the matrix elements themselves are small. The second-order term, $H_{\text{eff},\gamma}^{N_c, \text{II}}$, involves different matrix elements, as the excited states of the system are now involved (see Eq. 7.5). Thus, $J_{K\gamma}^{N_c, \text{II}}$ may make a significant contribution to the full effective coupling $J_{K,\text{eff}}$ in the $J' > J$ regime, and it is to this that we now turn.

We consider first the second-order term in the $J' > J$ regime for $N_c = 3$, as this is the simplest concrete example. Virtual excitations from the $|N_c = 3; +; S^z\rangle$ ground state to the higher lying $|N_c = 3; -; S^z\rangle$ doublet and the TQD quartet state are eliminated perturbatively in $H_{\text{eff},+}^{N_c=3, \text{II}}$ (see Eq. 7.5). The calculation itself is rather lengthy, but the result is again a simple 2CK model (neglecting RG irrelevant terms), of the form:

$$H_{\text{eff},+}^{N_c=3, \text{II}} = J_{K+}^{N_c=3, \text{II}} \hat{\mathbf{S}}_+ \cdot (\hat{\mathbf{s}}_{L0} + \hat{\mathbf{s}}_{R0}) \quad (7.10)$$

with the effective coupling to second order given by

$$J_{K+}^{N_c=3, \text{II}} = \frac{J_K^2}{6} \left(\frac{1}{E_{\Delta,Q}^{N_c=3}} - \frac{1}{E_{\Delta}^{N_c=3}} \right), \quad (7.11)$$

where $E_{\Delta,Q}^{N_c=3} = E_+^{N_c=3} - E_Q^{N_c=3} = -(J' + \frac{1}{2}J)$ is the energy difference between the $|N_c = 3; +; S^z\rangle$ ground state doublet and the quartet state, while $E_{\Delta}^{N_c=3} = E_+^{N_c=3} - E_-^{N_c=3} = J - J'$ is the energy difference between the two doublets, as before. As the calculation is valid only for $J' > J$ (*ie.* $E_{\Delta}^{N_c=3} < 0$), it is easily shown that the effective coupling given by Eq. 7.11 is always *antiferromagnetic*, but decreases rapidly as J' itself increases.

The second term of Eq. 7.11 corresponds to virtual excitations to the other doublet state of the TQD. This is the dominant contribution, since the doublets are the lowest pair of isolated ring states, and hence their energy separation $E_{\Delta}^{N_c}$ is always smallest. Indeed, it is readily shown that for any ring, the dominant contribution to $J_{K\gamma}^{N_c, \text{II}}$ in the $J' > J$ regime is proportional to $J_K^2/E_{\Delta}^{N_c}$, giving thereby a significant antiferromagnetic effective coupling between the lowest ring doublet and the leads, as in Eq. 7.11. The Kondo scale is again given by Eq. 7.9, but now with $J_{K,\text{eff}} = J_{K\gamma}^{N_c, \text{I}} + J_{K\gamma}^{N_c, \text{II}} + \mathcal{O}(J_K^3)$.

The above discussion indicates that 2CK physics predominates in *both* regimes $J' \ll J$ and $J' \gg J$ for any odd ring, although the Kondo scale T_K in the latter decreases rapidly with J' , indicative of the distinct nature of the effective coupling to second-order. As a consequence, deep in either phase, universality is expected, with the same underlying 2CK FP describing the behaviour of the system on the lowest temperature/energy scales.

We note that the above result is also perfectly consistent with the behaviour of the TQD tunnel-coupled to its leads, which we elucidated in Chapter 6. There we found using NRG that the underlying physics in both regimes, $J' \ll J$ and $J' \gg J$, was fundamentally similar, and described at the lowest temperature/energy scales by the 2CK FP. Indeed, a full $\mathcal{O}(V^2)$ Schrieffer-Wolff transformation [8, 17] for this system yields an effective low-energy model of 2CK form, with significant antiferromagnetic effective couplings, even in the $J' > J$ regime.

The effective models derived in this section are of course only valid well away from the point of frustration. As discussed above, two phases with distinct parity arise — with the overall L/R parity controlled by the local ring parity γ of the ground ring doublet $|N_c; \gamma; S^z\rangle$ for $J' \ll J$ and $J' \gg J$. A quantum phase transition must therefore result, but to understand the behaviour near this transition, both doublets must be retained in the ground state manifold. We consider that situation in Sec. 7.3 below, but first confirm the physical picture presented above by studying the full ring model (Eq. 7.1) directly with NRG for systems away from the point of frustration.

7.2 2CK phases of odd rings

In the previous section, we discussed the expected physical behaviour of odd rings of dots, described generically by Eq. 7.1. We derived perturbatively an effective low temperature/energy 2CK model, Eq. 7.7, which is valid away from the point of magnetic frustration (which occurs for $J' \approx J$). We argued that in the $J' < J$ regime, a substantial antiferromagnetic first-order effective coupling between the ring ground state and the leads arises, while in the $J' > J$ regime, the second-order term dominates, leading to an effective coupling that is again antiferromagnetic, but which rapidly diminishes on increasing J' . In both cases, however, the stable FP is the 2CK FP, which must describe the properties of such rings below T_K , itself given by Eq. 7.9.

In this section, we study Eq. 7.1 for $N_c = 3, 5$, and 7 with NRG [12, 13, 27] away from the point $J' = J$, where 2CK behaviour is expected to arise. For all calculations performed, we use an NRG discretization parameter $\Lambda = 3$ and retain typically $N_s \approx 4000$ states per iteration.

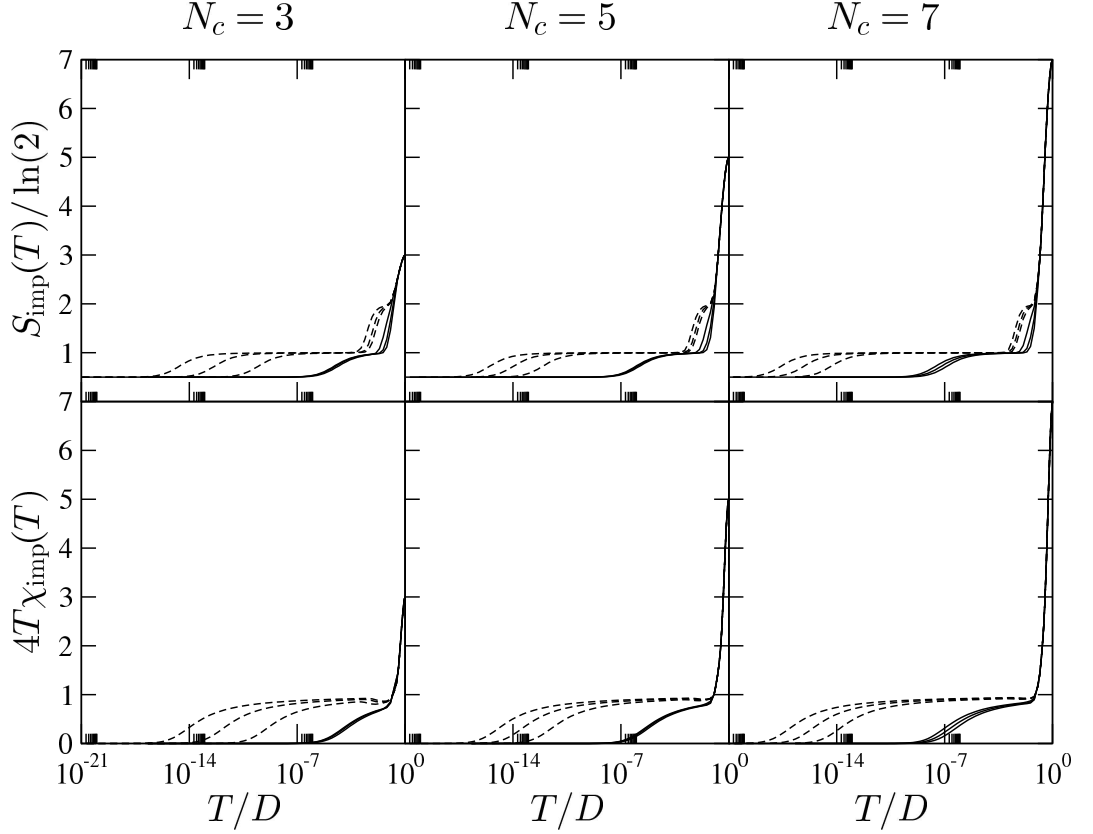


Figure 7.4: Thermodynamics for odd spin rings of size $N_c = 3, 5$, and 7 . Shown for fixed $\rho J_K = 0.15$ and $\rho J = 0.2$, varying $\rho J'$. Solid lines are for systems in the $J' < J$ regime, with $\rho J' = 0.05, 0.1$ and 0.15 , while dashed lines are for systems in the $J' > J$ regime, with $\rho J' = 0.21, 0.215$ and 0.22 (in order of decreasing T_K). The top row shows the entropy $S_{\text{imp}}(T)/\ln(2)$ while the bottom row shows the spin susceptibility $4T\chi_{\text{imp}}(T)$ both *vs.* T/D .

7.2.1 Thermodynamics

We consider first the ring contribution [12, 13, 27] to thermodynamic quantities, focusing specifically as usual on the entropy $S_{\text{imp}}(T)$ and the uniform spin susceptibility $T\chi_{\text{imp}}(T)$ (see Sec. 3.5).

In Fig. 7.4 we plot $S_{\text{imp}}(T)/\ln(2)$ on the top row and $4T\chi_{\text{imp}}(T)$ on the bottom row, both on a common temperature scale T/D . We compare rings of size $N_c = 3$ (left panels), 5 (middle panels), and 7 (right panels) for systems with fixed $\rho J_K = 0.15$ and $\rho J = 0.2$, varying $\rho J'$ in each case. Solid lines are for systems in the $J' < J$ regime, with $\rho J' = 0.05, 0.1$ and 0.15 , while dashed lines are for systems in the $J' > J$ regime, with $\rho J' = 0.21, 0.215$ and 0.22 (in order of decreasing T_K).

Considering first the left panels of Fig. 7.4 for $N_c = 3$, all systems plotted are described by the same FP at high temperatures $T \gg \max(J, J')$. The entropy of $S_{\text{imp}} = 3\ln(2)$ and the uniform spin susceptibility of $T\chi_{\text{imp}} = \frac{3}{4}$ are both characteristic of three uncoupled free spins (the FP Hamiltonian simply being H with $J = J' = J_K = 0$).

As the temperature is lowered, the higher lying ring states are successively projected out. In the $J' < J$ regime (solid lines), all but the lowest doublet state is projected out for $T < |E_{\Delta}^{N_c}|$, where the system is described by the effective model Eq. 7.7. For $T_K \ll T \ll J$, the system flows close to the LM FP, with a characteristic entropy of $S_{\text{imp}} = \ln(2)$ and a susceptibility which follows the Curie law for a free spin- $\frac{1}{2}$ object: $T\chi_{\text{imp}} = \frac{1}{4}$. The LM FP Hamiltonian in the reduced Hilbert space of the lowest doublet is then Eq. 7.7 with $J_{K\gamma}^{N_c, \text{I}} = 0$. The LM FP is unstable however, with the residual antiferromagnetic effective coupling driving the system to the 2CK FP below $T \sim T_K$, where the conduction electrons in the leads overscreen the lowest ring doublet. In all cases, the characteristic [43–45] 2CK $T = 0$ residual entropy of $S_{\text{imp}} = \frac{1}{2} \ln(2)$ results, while the susceptibility flows to $T\chi_{\text{imp}} = 0$. In addition, $\chi_{\text{imp}}(T)$ itself diverges logarithmically [43, 45, 46] below T_K (not shown), again typical of the approach to the 2CK FP.

In the $J' > J$ regime (dashed lines), the LM FP is also reached for $T \ll |E_{\Delta}^{N_c}|$, but as the $|N_c; \pm; S^z\rangle$ doublets are closer in energy for the systems shown, there is an appreciable temperature window $E_{\Delta}^{N_c} < T < \max(J, J')$ where the quartet state of the TQD has been projected out, but the two doublets remain quasidegenerate. As a result, there is a short plateau for which $S_{\text{imp}} = \ln(4)$, and $T\chi_{\text{imp}} = \frac{1}{4}$. Again, below T_K , the 2CK FP is reached, but as is evident from Fig. 7.4, the Kondo scale is much smaller in the $J' > J$ regime.

As J' is increased in the $J' < J$ regime, the T_K scale describing the crossover from the LM FP to the 2CK FP is seen to remain roughly constant, in agreement with the physical arguments presented in Sec. 7.1.2 and the evaluation of Eq. 7.8 for the $|N_c; -, S^z\rangle$ doublet ground state in the $N_c = 3$ case. By contrast, in the $J' > J$ regime, T_K is exponentially smaller, and decreases rapidly with increasing J' : again in accord with the perturbative analysis of the low-temperature behaviour of the model presented above. We analyse the evolution of the Kondo scale T_K with J' shortly, but first we consider the behaviour of the rings with $N_c = 5$ (middle panels) and $N_c = 7$ (right panels).

From a cursory inspection of Fig. 7.4, it is clear that the FP structure of the model for $N_c = 5$ and 7 is very similar to that of the $N_c = 3$ case (and indeed the TQD tunnel-coupled to leads, which we studied in the previous chapter: see Figs. 6.3 and 6.5). In all cases, systems flow to the LM FP on the scale of $T \sim |E_{\Delta}^{N_c}|$, with the characteristic [13] $S_{\text{imp}} = \ln(2)$ of a free spin, and a Curie law susceptibility $T\chi_{\text{imp}} = \frac{1}{4}$. Below T_K the 2CK FP is reached in all cases, and $S_{\text{imp}} = \frac{1}{2} \ln(2)$ is the residual entropy down to $T = 0$, while $T\chi_{\text{imp}} = 0$.

Only at *high* temperatures do the models with different N_c display different behaviour in the thermodynamics. However, in all cases the model is trivially described by N_c uncoupled free spins for $T > \max(J, J')$: again the FP Hamiltonian is just Eq. 7.1 with $J = J' = J_K = 0$. For a ring of size N_c , we thus obtain

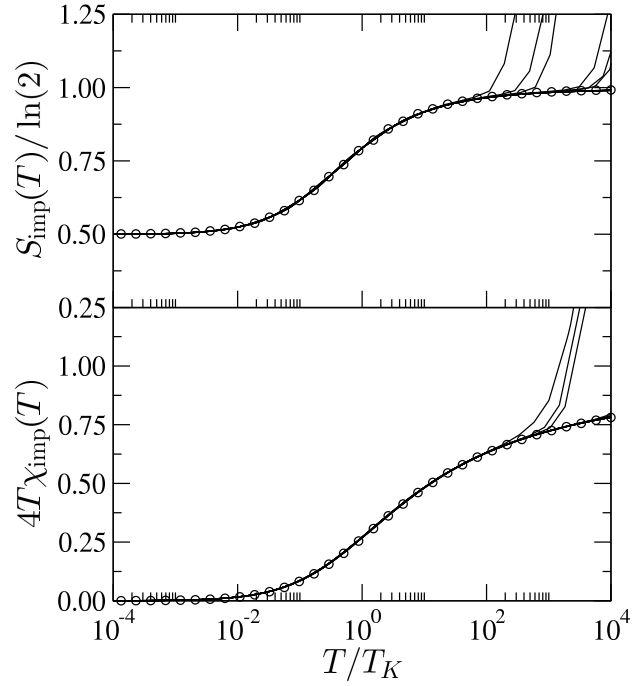


Figure 7.5: Thermodynamics for all systems presented in Fig. 7.4, demonstrating the universal collapse to a common curve when scaled in terms of T/T_K . As before, the top panel shows $S_{\text{imp}}(T)/\ln(2)$, while the bottom panel shows $4T\chi_{\text{imp}}(T)$. Also plotted for comparison is a single-spin 2CK model (open circles).

$$S_{\text{imp}} = N_c \ln(2), \text{ and } T\chi_{\text{imp}} = \frac{1}{4} N_c.$$

While all systems flow ultimately to the 2CK FP below T_K , this scale is itself dependent on N_c and J' through Eqs. 7.8 and 7.9. As N_c is increased, the T_K scale is seen to decrease, as expected from the variation of the effective ring ground state coupling presented in Fig. 7.3. As all systems presented in Fig. 7.4 flow from the LM FP to the 2CK FP, we expect universal behaviour to arise on scaling in terms of the Kondo temperature T_K . In Fig. 7.5 we show all the data of Fig. 7.4 for both $S_{\text{imp}}(T)/\ln(2)$ (top panel) and $4T\chi_{\text{imp}}(T)$ (bottom panel) *vs.* T/T_K , with the Kondo scale T_K determined in practice as usual [13] through $T_K\chi_{\text{imp}}(T_K) = 0.07$, and as such is a measure of the approach to the 2CK FP. Systems in both $J' < J$ and $J' > J$ regimes for $N_c = 3, 5$, and 7 collapse to a common universal curve. We also plot thermodynamics for a single-spin 2CK model (Eq. 2.24), scaled in terms of its Kondo temperature (open circles) for comparison. The exact agreement indicates that the underlying behaviour of the model for any⁷ odd N_c is that of the effective 2CK model Eq. 7.7.

⁷The scaling collapse has also been verified for $N_c = 9$ and 11 away from the transition, and the physically motivated arguments of Sec. 7.1.2 suggest that the 2CK FP is stable for all odd rings.

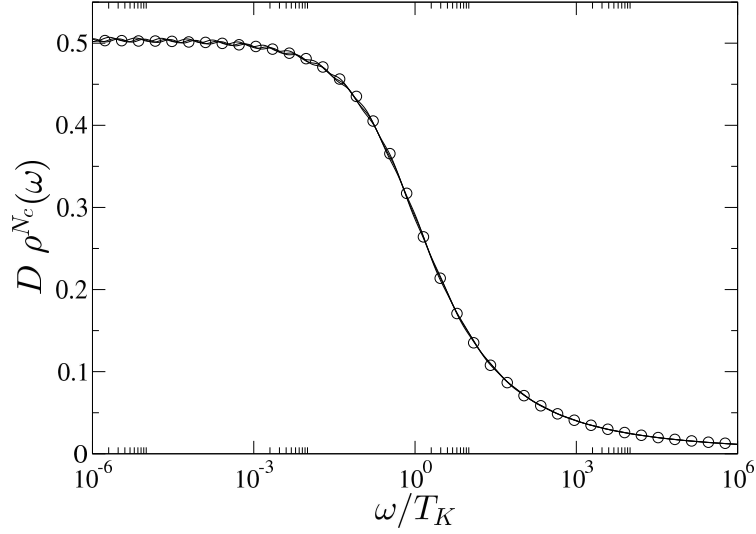


Figure 7.6: $T = 0$ Spectrum $D \rho^{N_c}(\omega)$ vs. ω/T_K for all systems presented in Fig. 7.4, showing the universal collapse to the scaling curve $D \rho^{2CK}(\omega)$ for the single-spin 2CK model (open circles).

7.2.2 Dynamics

We now consider briefly dynamics of the 2CK phases, focusing specifically on the $T = 0$ spectrum of dot 1. Proceeding analogously to the work in Secs. 3.6.3 and 4.2.2, we define the spectral density as $D \rho_L^{N_c}(\omega) = -\pi \rho_T \text{Im}\{t_L^{N_c}(\omega)\}$, with $t_L^{N_c}(\omega)$ the t -matrix for the left lead. But since the systems considered here have strict mirror symmetry, $t_L^{N_c}(\omega) = t_R^{N_c}(\omega) \equiv t^{N_c}(\omega)$. Thus $D \rho_L^{N_c}(\omega) = D \rho_R^{N_c}(\omega) \equiv D \rho^{N_c}(\omega)$, and a single spectrum results (as it must), irrespective of whether we consider the spin-scattering of left or right lead states due to the ring. As in Sec. 4.2.2, equations of motion methods [8, 139] yield straightforwardly $t^{N_c}(\omega)$, with the spectral density following as $\rho^{N_c}(\omega) = -\frac{\pi}{2}(\rho J_K)^2 \text{Im}\{G_L^{N_c}(\omega)\}$, with

$$G_L^{N_c}(\omega) = \langle\langle \hat{S}_1^- f_{L0\downarrow} + \hat{S}_1^z f_{L0\uparrow}; \hat{S}_1^+ f_{L0\downarrow}^\dagger + \hat{S}_1^z f_{L0\uparrow}^\dagger \rangle\rangle_\omega \quad (7.12)$$

where $f_{L0\sigma}^\dagger$ is an operator for the 0-orbital of the left Wilson chain (defined in Eq. 3.2), and $\hat{S}_1^\pm$ and $\hat{S}_1^z$ are spin- $\frac{1}{2}$ operators for dot 1.

We calculate $D \rho^{N_c}(\omega)$ as described in Sec. 3.6.3, using the highly accurate density matrix formulation of the NRG [20, 21, 27], and plot it vs. ω/T_K at $T = 0$ in Fig. 7.6 for all the systems presented for the thermodynamics in Fig. 7.4 (*ie.* we display the spectra for $N_c = 3, 5$ and 7 in both regimes $J' < J$ and $J' > J$). Rescaled in terms of their Kondo temperatures, T_K (determined in practice as usual from the thermodynamics as in Sec. 7.2.1), the data again collapse to the universal scaling spectrum of the single-spin 2CK model (plotted with open circles for comparison). Thus, the low- ω asymptotic form of the spectrum for odd spin rings (away from the

point of frustration) is:

$$D\rho^{N_c}(\omega) \underset{\frac{|\omega|}{T_K} \ll 1}{\sim} \frac{1}{2}[1 - a(|\omega|/T_K)^{\frac{1}{2}}] \quad (7.13)$$

with $a \simeq 0.47$, as we obtained for the TQD tunnel-coupled to the leads studied in the previous chapter, and which value is consistent with that found for the quadrupolar Anderson impurity model [108]⁸. Thus, we see low-frequency universal scaling of the dynamics⁹ for systems with different N_c and deep in either phase, where either $|N_c; \pm; S^z\rangle$ state is the ring ground state.

In the next section, we look at the situation when the ring is magnetically frustrated, and the $|N_c; \pm; S^z\rangle$ ring states are therefore close to degeneracy (near the point $J' = J$).

7.3 Frustration in odd rings

Deep in either regime $E_\Delta \ll 0$ or $E_\Delta \gg 0$, the effective 2CK model Eq. 7.7 is valid, and describes properties of the system in the reduced Hilbert space of the ground ring state $|N_c; \gamma; S^z\rangle$, with $\gamma = +$ or $-$ respectively. As these ring states have different parity, γ , and given that this ring parity is a conserved quantity in the low-energy effective model Eq. 7.7 (*ie.* $[\hat{P}_{\text{ring}}^{N_c}, H_{\text{eff}, \gamma}] = 0$), a quantum phase transition must occur on tuning J' .

Close to the point $J' = J$ when the ring is magnetically frustrated, the $|N_c; \pm; S^z\rangle$ doublets are near-degenerate, and both must be retained in the lowest manifold of ring states. We showed in Sec. 6.1.2 of Chapter 6 for the TQD tunnel-coupled to leads, that while overall left/right parity must always be conserved, a term which mixes the parity of the isolated *ring* states must enter the effective model near the point of frustration. In this section we show that this term — which is responsible for the QPT in that model — must be present in any odd ring of the same basic geometry (see Eq. 7.1 and Fig. 7.1). Thus, we expect that a QPT of the same *type* will be observed on tuning J' for any N_c . Below we study the transition with NRG for $N_c = 3, 5$ and 7 and confirm that this is indeed the case.

First however, we derive a low-energy effective model valid in the region of the transition, generalizing the approach of Sec. 6.1.2. As both of the lowest ring doublets must now be retained in the low-energy ring manifold of states, we define $\hat{1}^{N_c} = \hat{1}_+^{N_c} + \hat{1}_-^{N_c}$ (with $\hat{1}_\pm^{N_c}$ itself given in Eq. 7.4), and consider explicitly the first-

⁸The asymptotic form of the spectrum is in marked contrast to the $[1 - a'(|\omega|/T_K)^2]$ decay characteristic of the normal Fermi liquid FP in single-channel models [8, 27]

⁹We have also studied the dynamic susceptibility $\chi_1(\omega) = -\frac{1}{\pi} \text{Im}\{\langle\langle S_1^z; S_1^z \rangle\rangle_\omega\}$ for these systems, and again find low- ω scaling in terms of ω/T_K , recovering the universal curve presented in the inset to Fig. 6.9 of Chapter 6 for the TQD tunnel-coupled to its leads.

order term $H_{\text{eff}}^{N_c, \text{trans}} = \hat{1}^{N_c} H_K \hat{1}^{N_c}$.

Considerable simplification of the resulting algebra can be made by using $\hat{\mathbf{S}}_1 = \hat{P}_{\text{ring}}^{N_c} \hat{\mathbf{S}}_{N_c} \hat{P}_{\text{ring}}^{N_c}$ (which follows from Eq. 7.3), with the definition of the ring states $\hat{P}_{\text{ring}}^{N_c} |N_c; \gamma; S^z\rangle = \gamma |N_c; \gamma; S^z\rangle$, to obtain

$$\langle \gamma; S^z | \hat{\mathbf{S}}_1 | \gamma'; S^{z'} \rangle = \gamma \gamma' \langle \gamma; S^z | \hat{\mathbf{S}}_{N_c} | \gamma'; S^{z'} \rangle, \quad (7.14)$$

and hence $\hat{1}_\gamma \hat{\mathbf{S}}_1 \hat{1}_{\gamma'} = \gamma \gamma' \hat{1}_\gamma \hat{\mathbf{S}}_{N_c} \hat{1}_{\gamma'}$. Using this relation with H_K given in Eq. 7.1, it follows that

$$\begin{aligned} H_{\text{eff}}^{N_c, \text{trans}} = \sum_{\gamma=\pm} \frac{1}{2} J_K [\hat{1}_\gamma (\hat{\mathbf{S}}_1 + \hat{\mathbf{S}}_{N_c}) \hat{1}_\gamma \cdot (\hat{\mathbf{s}}_{L0} + \hat{\mathbf{s}}_{R0}) \\ + \hat{1}_\gamma (\hat{\mathbf{S}}_1 - \hat{\mathbf{S}}_{N_c}) \hat{1}_{-\gamma} \cdot (\hat{\mathbf{s}}_{L0} - \hat{\mathbf{s}}_{R0})] \\ + \hat{1}_\gamma E_\gamma. \end{aligned} \quad (7.15)$$

This is wholly equivalent to the effective model of the transition derived for the TQD tunnel-coupled to leads in the previous chapter, Eq. 6.10. The first term is simply one or other of Eq. 7.6 for $\gamma = +/ -$, leading thereby to a direct 2CK coupling of each of the lowest ring doublets $|N_c; \gamma; S^z\rangle$ to the lead combination $(\hat{\mathbf{s}}_{L0} + \hat{\mathbf{s}}_{R0})$, described by Eq. 7.7.

As in the previous chapter, Sec. 6.1.2, we introduce operators for real spin $\hat{\mathbf{S}}$ ($= \sum_\gamma \hat{\mathbf{S}}_\gamma$) and pseudospin $\hat{\mathcal{T}}$ for the local ring Hilbert space, similarly defined for arbitrary ring size N_c as

$$\hat{S}^z = \sum_{\gamma=\pm, S^z} |N_c; \gamma; S^z\rangle S^z \langle N_c; \gamma; S^z| \quad (7.16a)$$

$$\hat{T}^z = \sum_{\gamma=\pm, S^z} |N_c; \gamma; S^z\rangle \frac{1}{2} \gamma \langle N_c; \gamma; S^z| \quad (7.16b)$$

and

$$\hat{S}^\pm = \sum_\gamma |N_c; \gamma; \pm \frac{1}{2}\rangle \langle N_c; \gamma; \mp \frac{1}{2}| \quad (7.17a)$$

$$\hat{T}^\pm = \sum_{S^z} |N_c; \pm; S^z\rangle \langle N_c; \mp; S^z|. \quad (7.17b)$$

We note that while these operators act on different Hilbert spaces for the different rings, in every case they are fundamentally spin- $\frac{1}{2}$ operators, and thus we drop the label N_c . The ring doublets are each eigenstates of $\hat{S}^z$ and $\hat{T}^z$; in particular, the eigenvalues of $\hat{T}^z \equiv \frac{1}{2}(\hat{1}_+^{N_c} - \hat{1}_-^{N_c})$ correspond simply to (half) the parity of the appropriate doublet. By contrast, the doublets are interconverted via $\hat{T}^\pm |N_c; \mp; S^z\rangle = |N_c; \pm; S^z\rangle$, and as such $\hat{T}^\pm$ acts to switch the parity of the lowest

ring states.

In Sec. 6.1.2 of Chapter 6 we used the explicit form of the TQD states to recast Eq. 7.15 in terms of these spin and pseudospin operators. In fact, these transformations may be performed quite generally, as described in Appendix B, and it can then be shown for any odd N_c that Eq. 7.15 reduces to

$$\begin{aligned} H_{\text{eff}}^{\text{trans}} = & \left(\frac{1}{2} J_A^{N_c, \text{I}} + J_B^{N_c, \text{I}} \hat{T}^z \right) \hat{\mathbf{S}} \cdot (\hat{\mathbf{s}}_{L0} + \hat{\mathbf{s}}_{R0}) \\ & + J_{\text{mix}}^{N_c, \text{I}} (\hat{T}^+ + \hat{T}^-) \hat{\mathbf{S}} \cdot (\hat{\mathbf{s}}_{L0} - \hat{\mathbf{s}}_{R0}) \\ & + E_{\Delta}^{N_c} \hat{T}^z, \end{aligned} \quad (7.18)$$

and so the difference between rings of different size N_c only enters the low-energy description of the model through the effective couplings $J_A^{N_c, \text{I}}$, $J_B^{N_c, \text{I}}$ and $J_{\text{mix}}^{N_c, \text{I}}$, where

$$J_A^{N_c, \text{I}} = (J_{K+}^{N_c, \text{I}} + J_{K-}^{N_c, \text{I}}) \quad J_B^{N_c, \text{I}} = (J_{K+}^{N_c, \text{I}} - J_{K-}^{N_c, \text{I}}) \quad (7.19)$$

and from Appendix B, Eq. B.12, we obtain

$$J_{K\gamma}^{N_c, \text{I}} = \langle N_c; \gamma; \frac{1}{2} | \hat{S}_1^z + \hat{S}_{N_c}^z | N_c; \gamma; \frac{1}{2} \rangle J_K, \quad (7.20a)$$

$$J_{\text{mix}}^{N_c, \text{I}} = \langle N_c; \gamma; \frac{1}{2} | \hat{S}_1^z - \hat{S}_{N_c}^z | N_c; -\gamma; \frac{1}{2} \rangle J_K. \quad (7.20b)$$

$J_{K\gamma}^{N_c, \text{I}}$ is simply the first-order coupling for the $\gamma = +/ -$ ring doublets, derived also in Sec. 7.1.2, Eq. 7.8, while $J_{\text{mix}}^{N_c, \text{I}}$ embodies the strength of the pseudospin mixing term. We comment briefly here that a full second-order calculation could also be performed in the vicinity of the transition, but that an effective low-energy model of exactly the same form as Eq. 7.18 results¹⁰. Only the effective couplings are renormalized; the second-order terms make a significant contribution to the total effective coupling in the $J' > J$ regime only, as discussed in Sec. 7.1.2.

We note that while $J_{\text{mix}}^{N_c, \text{I}} = \frac{1}{\sqrt{3}} J_K \simeq 0.577 J_K$ is constant for $N_c = 3$, in general it depends on J'/J and N_c through Eq. 7.20 (although it is always found to be antiferromagnetic). Specifically, for $J'/J = 1$ (at the point of frustration in the isolated rings), numerical evaluation of Eq. 7.20 gives $J_{\text{mix}}^{N_c, \text{I}} \simeq 0.507 J_K$ for $N_c = 5$ and $\simeq 0.452 J_K$ for $N_c = 7$.

In Sec. 7.1.1 we discussed the symmetry of the isolated rings, showing that $[H_{\text{ring}}^{N_c}, \hat{P}_{\text{ring}}^{N_c}] = 0$. But this parity is *not* a conserved quantity in the full model¹¹: instead it is the *overall* left $\leftrightarrow$ right parity which is in general conserved. We define

$$\hat{P}_{L,R}^{N_c} = \hat{P}_{\text{ring}}^{N_c} \prod_{\mathbf{k}} \hat{P}_{L\mathbf{k}, R\mathbf{k}}, \quad (7.21)$$

¹⁰In fact, additional RG irrelevant terms also enter, but the essential physics is not altered qualitatively by these contributions.

¹¹The low-energy effective model Eq. 7.7 does conserve ring parity, although this description is not valid near the transition

which simultaneously permutes the ring spins, and exchanges left and right lead states, such that $[H, \hat{P}_{L,R}^{N_c}] = 0$ for any N_c . So, even though on their own the pseudospin mixing terms have odd parity in the sense that $\hat{P}_{\text{ring}}^{N_c} \hat{T}^\pm = -\hat{T}^\pm \hat{P}_{\text{ring}}^{N_c}$, the second line of Eq. 7.18 remains *even* overall, as the spin itself couples to the *odd* (antisymmetric) lead combination $\hat{\mathbf{S}}_{L0} - \hat{\mathbf{S}}_{R0}$.

Thus, this term generically enters the low-energy effective model for rings of this geometry (see Fig. 7.1 and Eq. 7.1) near the point of frustration. We showed in Chapter 6 that this term is responsible for a QPT in the TQD, and so the same behaviour is expected here. Indeed, the effective model Eq. 7.18 was studied directly with NRG in Sec. 6.4, varying the effective couplings $J_A^{N_c, \text{I}}$, $J_B^{N_c, \text{I}}$ and $J_{\text{mix}}^{N_c, \text{I}}$ independently. It was shown that the same underlying FP structure results, provided the couplings $J_{K\gamma}^{N_c, \text{I}}$ and $J_{\text{mix}}^{N_c, \text{I}}$ are *antiferromagnetic*, which is readily confirmed from Eq. 7.20. Since it is only these effective couplings that change with N_c (rather than the structure of the effective Hamiltonian itself), fundamentally similar physics is expected near the transition for any odd ring.

The behaviour in the vicinity of the point of frustration is thus anticipated to be analogous to that elucidated in Sec. 6.3 of the previous chapter, and we confirm this directly with NRG below.

7.3.1 Spin-spin correlation functions

To understand the effect of magnetic frustration in the full ring model (Fig. 7.1 and Eq. 7.1), we examine first the evolution of spin-spin correlation functions between the dots, as J' is varied. Away from the transition, pseudospin mixing terms are suppressed (by the term $E_\Delta^{N_c} \hat{T}^z$ in Eq. 7.18), and so local properties of the ring are expected to be characteristic of either $|N_c; +; S^z\rangle$ for $E_\Delta^{N_c} \ll 0$ or $|N_c; -; S^z\rangle$ for $E_\Delta^{N_c} \gg 0$.

In the isolated rings ($J_K = 0$), a level crossing of these lowest doublets occurs at $J' = J$, and hence a discontinuity in $\langle \hat{\mathbf{S}}_i \cdot \hat{\mathbf{S}}_j \rangle$ must arise at $T = 0$. In the vicinity of the degeneracy point of the model, however, the effective model Eq. 7.18 describes the low-temperature behaviour of the system. As this model contains pseudospin mixing terms which act to interconvert the lowest doublets, local properties of the ring in this regime cannot be characteristic of $|N_c; +; S^z\rangle$ or $|N_c; -; S^z\rangle$ alone, and so the full model must display different behaviour in the frustrated region.

In Figs. 7.7–7.9, we present the $T = 0$ spin-spin correlators between neighbouring dots of the ring, calculated using NRG for the full model Eq. 7.1. In Fig. 7.7 we show the simplest ($N_c = 3$) case, and consider the evolution of $\langle \hat{\mathbf{S}}_1 \cdot \hat{\mathbf{S}}_2 \rangle \equiv \langle \hat{\mathbf{S}}_3 \cdot \hat{\mathbf{S}}_2 \rangle$ (left panel) and $\langle \hat{\mathbf{S}}_1 \cdot \hat{\mathbf{S}}_3 \rangle$ (right panel) as a function of $\rho J'$. The dotted lines show the same functions calculated for the isolated trimer, as determined below.

The parity of a ring state (see Appendix A and Sec. 7.1.1) can be defined through

$\gamma = \langle N_c; \gamma; S^z | \hat{P}_{\text{ring}}^{N_c} | N_c; \gamma; S^z \rangle$, which for $N_c = 3$ may be simply written as $\gamma = \langle N_c = 3; \gamma; S^z | (-\frac{1}{2} - 2\hat{\mathbf{S}}_1 \cdot \hat{\mathbf{S}}_3) | N_c = 3; \gamma; S^z \rangle$, and hence we obtain $\langle N_c = 3; \gamma; S^z | \hat{\mathbf{S}}_1 \cdot \hat{\mathbf{S}}_3 | N_c = 3; \gamma; S^z \rangle = -\frac{1}{4}(1 + 2\gamma)$. Thus in the isolated TQD, for $J' < J$ (where $|N_c = 3; -; S^z\rangle$ is the ground state), $\langle \hat{\mathbf{S}}_1 \cdot \hat{\mathbf{S}}_3 \rangle = \frac{1}{4}$, while for $J' > J$ (where $|N_c = 3; +; S^z\rangle$ is now lowest), $\langle \hat{\mathbf{S}}_1 \cdot \hat{\mathbf{S}}_3 \rangle = -\frac{3}{4}$ (and as calculated directly in Sec. 6.1.1).

As $|N_c = 3; \gamma; S^z\rangle$ is a *doublet* state for either $\gamma = +/ -$ and each dot comprising the ring is a spin- $\frac{1}{2}$ object, a sum rule relates the spin-spin correlators in the TQD: $\langle N_c = 3; \gamma; S^z | \hat{\mathbf{S}}_1 \cdot \hat{\mathbf{S}}_2 | N_c = 3; \gamma; S^z \rangle = -\frac{1}{8}(3 + 4\langle N_c = 3; \gamma; S^z | \hat{\mathbf{S}}_1 \cdot \hat{\mathbf{S}}_3 | N_c = 3; \gamma; S^z \rangle) = \frac{1}{4}(\gamma - 1)$. Thus for $J' < J$ (when $|N_c = 3; -; S^z\rangle$ lies lowest) $\langle \hat{\mathbf{S}}_1 \cdot \hat{\mathbf{S}}_2 \rangle = -\frac{1}{2}$, while $\langle \hat{\mathbf{S}}_1 \cdot \hat{\mathbf{S}}_2 \rangle = 0$ for $J' > J$, as $|N_c = 3; +; S^z\rangle$ is now the ground TQD state.

In the full model, ring parity is of course not conserved, and so the above calculations are not strictly valid. However, well away from the point of frustration, the effective model Eq. 7.7 describes the low-temperature behaviour of the system, and $[H_{\text{eff},\gamma}^{N_c=3}, \hat{P}_{\text{ring}}^{N_c=3}] = 0$. Thus, the isolated ring correlators calculated above represent the limiting behaviour deep in either regime: $J' \ll J$ or $J' \gg J$. This is confirmed in Fig. 7.7, by comparing $\langle \hat{\mathbf{S}}_i \cdot \hat{\mathbf{S}}_j \rangle$ calculated from NRG for the full model (solid lines), and for the isolated TQD (dotted lines).

In fact, the behaviour of $\langle \hat{\mathbf{S}}_i \cdot \hat{\mathbf{S}}_j \rangle$ for the full model is very close to that of the isolated ring for the vast majority of the parameter space. Only for $J' \approx J$, are there significant deviations: the solid line crosses over very rapidly between the limiting values shown by the dotted line. This indicates that $|E_{\Delta}^{N_c=3}|$ does not have to be very far away from zero before the physical picture is essentially that of the effective 2CK model Eq. 7.7 (where ring parity *is* conserved).

Figs. 7.8 and 7.9 similarly show neighbouring spin-spin correlators $\langle \hat{\mathbf{S}}_i \cdot \hat{\mathbf{S}}_j \rangle$ at $T = 0$ vs. $\rho J'$ for the same parameters as in Fig. 7.7, but for $N_c = 5$ and 7 respectively. In these models, the behaviour for the isolated ring is more complicated as the ring parity cannot be directly related to the spin-spin correlators. However, $\langle \hat{\mathbf{S}}_i \cdot \hat{\mathbf{S}}_j \rangle$ may be computed directly from the eigenstates of $H_{\text{ring}}^{N_c}$, and these are again plotted as the dotted lines. Away from $J' = J$, we again see excellent agreement between the correlators of the full model calculated by NRG (solid lines) and those for the isolated rings. In all cases in Figs. 7.8 and 7.9 however, the full model shows a rapid crossover between the limiting behaviour described by the isolated ring.

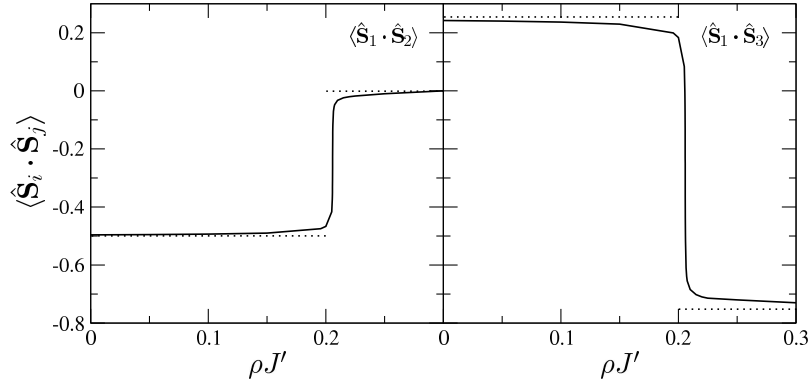


Figure 7.7: Spin-spin correlation functions for $N_c = 3$. Shown for fixed $\rho J = 0.2$ and $\rho J_K = 0.15$ at $T = 0$ are $\langle \hat{\mathbf{S}}_1 \cdot \hat{\mathbf{S}}_2 \rangle \equiv \langle \hat{\mathbf{S}}_3 \cdot \hat{\mathbf{S}}_2 \rangle$ (left panel) and $\langle \hat{\mathbf{S}}_1 \cdot \hat{\mathbf{S}}_3 \rangle$ (right panel) all *vs.* $\rho J'$. The dotted lines correspond to the same functions calculated for the isolated ring.

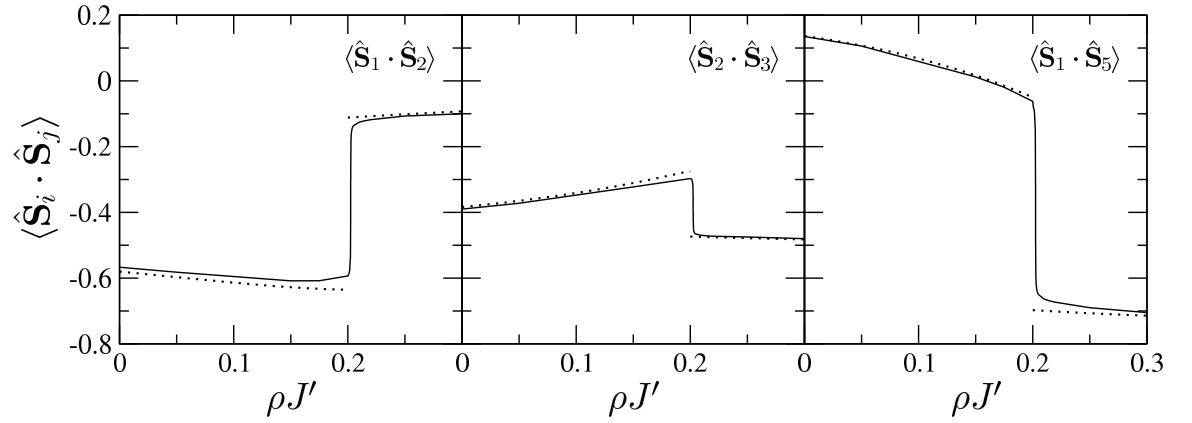


Figure 7.8: Spin-spin correlation functions for $N_c = 5$ at $T = 0$, with the same parameters as Fig. 7.7: $\langle \hat{\mathbf{S}}_1 \cdot \hat{\mathbf{S}}_2 \rangle \equiv \langle \hat{\mathbf{S}}_5 \cdot \hat{\mathbf{S}}_4 \rangle$ (left panel), $\langle \hat{\mathbf{S}}_2 \cdot \hat{\mathbf{S}}_3 \rangle \equiv \langle \hat{\mathbf{S}}_4 \cdot \hat{\mathbf{S}}_3 \rangle$ (middle panel), and $\langle \hat{\mathbf{S}}_1 \cdot \hat{\mathbf{S}}_5 \rangle$ (right panel). The dotted lines are again for the isolated ring.

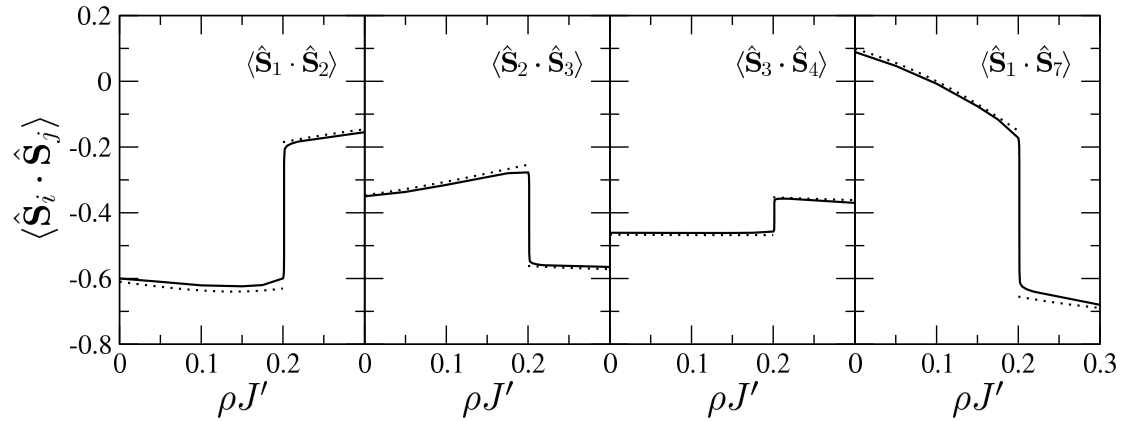


Figure 7.9: Spin-spin correlation functions for $N_c = 7$ at $T = 0$, with the same parameters as Fig. 7.7: $\langle \hat{\mathbf{S}}_1 \cdot \hat{\mathbf{S}}_2 \rangle \equiv \langle \hat{\mathbf{S}}_7 \cdot \hat{\mathbf{S}}_6 \rangle$ (left panel), $\langle \hat{\mathbf{S}}_2 \cdot \hat{\mathbf{S}}_3 \rangle \equiv \langle \hat{\mathbf{S}}_6 \cdot \hat{\mathbf{S}}_5 \rangle$ (centre-left), $\langle \hat{\mathbf{S}}_3 \cdot \hat{\mathbf{S}}_4 \rangle \equiv \langle \hat{\mathbf{S}}_5 \cdot \hat{\mathbf{S}}_4 \rangle$ (centre-right) and $\langle \hat{\mathbf{S}}_1 \cdot \hat{\mathbf{S}}_7 \rangle$ (right panel). The dotted lines are again for the isolated ring.

Finally, we compare the panels on the far right of Figs. 7.7–7.9, which show the evolution of $\langle \hat{\mathbf{S}}_1 \cdot \hat{\mathbf{S}}_{N_c} \rangle$ with $\rho J'$. The arguments presented above indicate that in either regime $J' \ll J$ or $J' \gg J$, $\langle \hat{\mathbf{S}}_1 \cdot \hat{\mathbf{S}}_{N_c} \rangle$ is essentially constant for $N_c = 3$, and characterizes either the triplet or singlet combination of spins 1 and N_c . For $N_c = 5$ and 7 however, $\langle \hat{\mathbf{S}}_1 \cdot \hat{\mathbf{S}}_{N_c} \rangle$ decreases as $\rho J'$ increases, as expected from the increased singlet character of the spins, favoured by antiferromagnetic J' (see Fig. 7.1). As N_c itself increases, the triplet character of the dot combination 1 and N_c decreases in the $J' \ll J$ regime, but increases in the $J' \gg J$ regime. These trends are also reflected in the effective coupling (to first order) between the lowest ring state and the leads, as shown previously in Fig. 7.3, and discussed in Sec. 7.1.2. In fact, comparison of the variation of $\langle \hat{\mathbf{S}}_1 \cdot \hat{\mathbf{S}}_{N_c} \rangle$ and $J_{K\gamma}^{N_c, I}/J_K$ with $\rho J'$ and N_c shows a qualitative similarity for this reason.

In Figs. 7.10–7.12 we show a magnification of the same data for $N_c = 3, 5$ and 7 in the region of frustration, $J' \approx J$. Two striking features are immediately obvious from these figures. Firstly, the evolution of each of the spin-spin correlators, $\langle \hat{\mathbf{S}}_i \cdot \hat{\mathbf{S}}_j \rangle$, is *continuous* as $\rho J'$ is varied (unlike the case for the isolated rings). Secondly, all correlators (for neighbouring dots) cross at a *single point* in each case. The point when all of the correlators are equal is of course the point of complete local magnetic frustration in the ring; the value $J' \equiv J'_c$ at this point is naturally renormalized slightly from the degeneracy point of the doublets in the isolated ring, disconnected from the leads. For $\rho J = 0.2$ and $\rho J_K = 0.15$ as used in these figures, we find that $\rho J'_c = 0.20576\dots$ for $N_c = 3$, $\rho J'_c = 0.20246\dots$ for $N_c = 5$ and $\rho J'_c = 0.20135\dots$ for $N_c = 7$.

We shall see in the next section that there is a quantum critical point at $\tilde{E}_\Delta = J'_c - J' = 0$ for each of $N_c = 3, 5$ and 7, separating the 2CK phases of distinct ground state parity, studied above in Sec. 7.2. We also confirm that this transition is of exactly the same type as that present in the TQD system when tunnel-coupled to its leads, which we studied in Chapter 6.

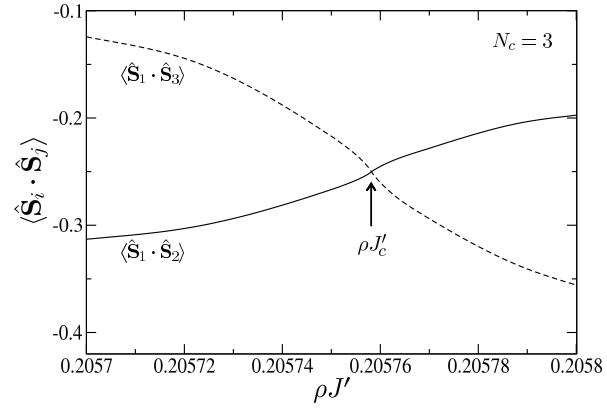


Figure 7.10: Spin-spin correlation functions $\langle \hat{\mathbf{S}}_i \cdot \hat{\mathbf{S}}_j \rangle$ vs. $\rho J'$ at $T = 0$ for $N_c = 3$ with the same parameters as in Fig. 7.7. Shown is a magnification in the frustrated region. $\rho J'_c \simeq 0.20576\dots$ is defined as the point where the correlators cross.

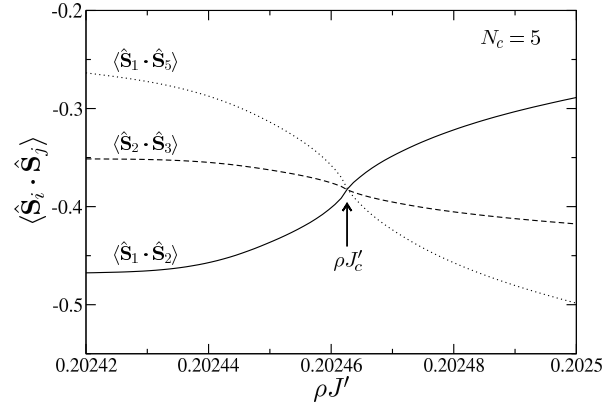


Figure 7.11: Spin-spin correlation functions $\langle \hat{\mathbf{S}}_i \cdot \hat{\mathbf{S}}_j \rangle$ vs. $\rho J'$ at $T = 0$ for $N_c = 5$ with the same parameters as in Fig. 7.7. Shown is a magnification in the frustrated region. $\rho J'_c \simeq 0.20246\dots$ is defined as the point where the correlators cross.

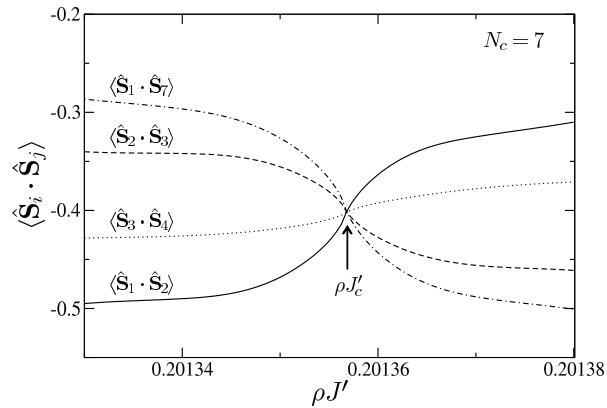


Figure 7.12: Spin-spin correlation functions $\langle \hat{\mathbf{S}}_i \cdot \hat{\mathbf{S}}_j \rangle$ vs. $\rho J'$ at $T = 0$ for $N_c = 7$ with the same parameters as in Fig. 7.7. Shown is a magnification in the frustrated region. $\rho J'_c \simeq 0.20135\dots$ is defined as the point where the correlators cross.

7.3.2 Thermodynamics of the transition

We now turn to thermodynamics in the vicinity of the transition, focusing on the ring contribution to the entropy $S_{\text{imp}}(T)$ for odd rings, obtained via NRG for the full model. First we comment that the expected behaviour is that of the TQD tunnel-coupled to leads, which we studied in Chapter 6.

A low-temperature effective Hamiltonian of the same form (Eq. 7.18 or Eq. 6.13) describes generically the behaviour of odd rings of spins, with two leads exchange-coupled to neighbouring dots (see Fig. 7.1 and Eq. 7.1). The magnitude of the effective couplings $J_{K\gamma}^{N_c, \text{I}}$ and $J_{\text{mix}}^{N_c, \text{I}}$ do depend on the ring size N_c and the ratio J'/J , as obtained via Eq. 7.20, but these couplings are always *antiferromagnetic*. We showed in Sec. 6.4 of the previous chapter that the underlying physics and FP structure of the model (and indeed the nature of the transition itself), is independent of $J_{K\gamma}^{N_c, \text{I}}$ and $J_{\text{mix}}^{N_c, \text{I}}$ (provided they are antiferromagnetic). Thus, the same behaviour as that discussed in Secs. 6.3 and 6.4 is indeed expected here.

In Sec. 6.3, we showed that the transition occurred at the point of complete magnetic frustration in the TQD, $\tilde{E}_\Delta = (J'_c - J') = 0$ (as can be understood from the form of the low-energy effective model for the transition, Eq. 7.18, and discussed in Sec. 6.3.1). Thus, in practice we determine J'_c as the point where all of the spin-spin correlators become equal at $T = 0$, as shown in Figs. 6.11 and 7.10–7.12. However, the transition will of course also be manifest in the behaviour of the thermodynamics, as shown below.

The $\mathcal{T}^z = \pm \frac{1}{2}$ components of the pseudospin are degenerate precisely at the transition, but in either $\mathcal{T}^z$ sector, the real spin $\hat{\mathbf{S}}$ couples *asymmetrically* to left and right channels, which is known to destabilise the 2CK FP [40, 45, 46, 49, 124]. The critical FP (CFP) is thus essentially a ‘doubled’ version of the SC FP, with the ring spin fully quenched below a characteristic single-channel scale $T_K^{1CK} \equiv T_K^c$ by the lead to which it is more strongly coupled (see Sec. 6.3.1). For $\mathcal{T}^z = +\frac{1}{2}$ the left lead screens the spin and the right lead decouples, while for $\mathcal{T}^z = -\frac{1}{2}$ the situation is reversed, and the right lead screens the spin. Without comment on non-universal energy scales $T \sim \max(J, J')$, the entropy at the quantum critical point (QCP) is thus expected to be $S_{\text{imp}}^{QCP}(T) = \ln(2) + S_{\text{imp}}^{1CK}(T)$, where the explicit $\ln(2)$ refers to the free pseudospin at the transition and $S_{\text{imp}}^{1CK}(T)$ is the entropy obtained for a standard single-spin 1CK model with $T_K^{1CK} = T_K^c$ (see Sec. 6.3.1). In the vicinity of the transition, RG flow is expected near the CFP for $|\tilde{E}_\Delta| \ll T_K^c$. But ultimately, the upper component of the pseudospin is frozen out as T is lowered further, and the 2CK FP is reached for $T \sim T_K$, with T_K itself vanishing as $J' \rightarrow J'_c$, characteristic of the transition.

In Fig. 7.13 we show the evolution of the entropy with temperature near the transition for different odd rings. In all cases we study the full model Eq. 7.1 via

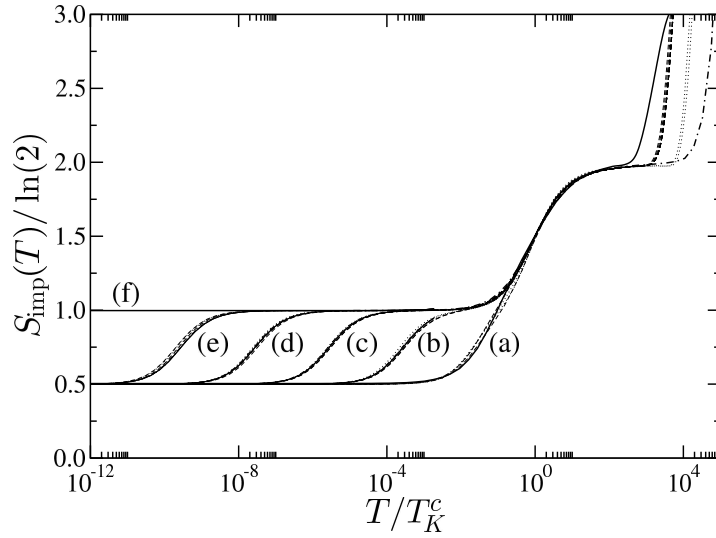


Figure 7.13: Entropy $S_{\text{imp}}(T)$ vs. T/T_K^c for $N_c = 3$ (solid lines), 5 (dashed lines) and 7 (dotted lines). Shown for common fixed $\rho J = 0.2$ and $\rho J_K = 0.15$, with $\rho J'$ varied through $\tilde{E}_\Delta = (J'_c - J') = \pm \lambda T_K^c$, with $\lambda = 10^n$ and $n = 0, -1, -2, -3, -4$ [lines (a–e)] progressively approaching the transition [$\lambda = 0$, line (f)]. Also plotted for comparison (dot-dashed lines) is the entropy for the TQD model tunnel-coupled to leads studied in Chapter 6, with $\tilde{U} = 7 = -2\tilde{\epsilon}$ and $\rho J = 0.1$, varying $\rho J'$ as above.

NRG, and present results for $\rho J = 0.2$ and $\rho J_K = 0.15$, varying $\rho J'$ as before. To compare models with different N_c as the transition is approached, we rescale the temperature axis in terms of $T_K^{1CK} \equiv T_K^c$, which describes the flow to the CFP. In practice (and as used in the previous chapter) we will define this scale via $T_K^c \chi_{\text{imp}}(T_K^c) = 0.07$ at the point of the transition, $J' = J'_c$. Thus, T_K^c obviously depends on the value of $\rho J'_c$, which we determined in Figs. 7.10–7.12 as the point of complete magnetic frustration in the rings.

Thus, in Fig. 7.13 we show $S_{\text{imp}}(T)$ vs. T/T_K^c , with $\rho J'$ varied via $\tilde{E}_\Delta = (J'_c - J') = \pm \lambda T_K^c$, where $\lambda = 10^n$ and $n = 0, -1, -2, -3, -4$, [lines (a–e)] progressively approaching the transition [$\lambda = 0$, line (f)] from either side. We consider explicitly $N_c = 3$ (solid lines), 5 (dashed lines) and 7 (dotted lines), and also plot as the dot-dashed lines the entropy for the TQD tunnel-coupled to its leads, which we presented in Fig. 6.13 of the previous chapter (for $\tilde{U} = 7 = -2\tilde{\epsilon}$ and $\rho J = 0.1$, varying $\rho J'$ as above, and again rescaled in terms of its T_K^c).

Fig. 7.13 immediately indicates the existence of a QPT in each ring, through the vanishing Kondo scale, T_K (defined as before via $S_{\text{imp}}(T_K) = 0.55$, suitably between $\ln(2)$ and $\frac{1}{2} \ln(2)$, and hence characterizing the flow to the ultimate stable 2CK FP of the model for any non-zero $\tilde{E}_\Delta$). Lines (a), corresponding to $J' = J'_c \pm T_K^c$, represent the limiting case, with the entropy flowing from $\ln(4)$, characteristic of the free spin and free pseudospin $SU(2) \times SU(2)$ FP, directly to the 2CK FP (see Sec. 6.3.1).

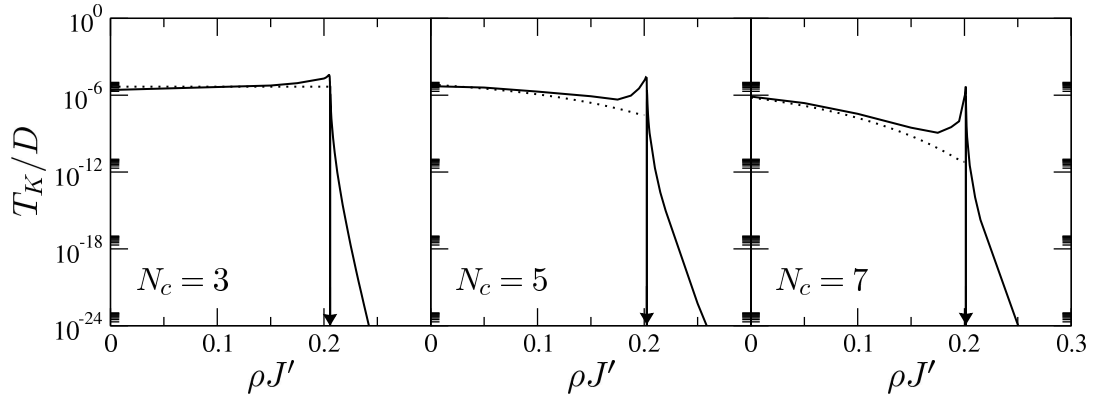


Figure 7.14: Variation of the Kondo scale T_K as measured from the entropy (defined through $S_{\text{imp}}(T_K) = 0.55$). Plotted is T_K/D vs. $\rho J'$ for common fixed $\rho J = 0.2$ and $\rho J_K = 0.15$, for rings of size $N_c = 3$ (left panel), 5 (middle panel) and 7 (right panel). Also plotted as dotted lines are the the Kondo scales obtained from perturbative scaling in the $J' < J$ regime, with $\rho J_{K\gamma}$ from Eq. 7.8 used in Eq. 7.9.

For $|\tilde{E}_\Delta| \gg T_K^c$, the RG flow in the vicinity of the CFP is not observed; the upper component of the pseudospin is simply frozen out for $T < |\tilde{E}_\Delta|$, so that the 2CK FP is only reached via the usual LM FP. This situation was discussed in Sec. 7.2 and shown explicitly in Fig. 7.4 for rings away from the transition.

Lines (b–e) successively approach the transition, and the 2CK scale is seen clearly to diminish, with T_K itself vanishing for $\lambda = 0$, line (f). For systems close to the transition ($|\tilde{E}_\Delta| < T_K^c$), the evolution of the entropy is seen to be common to all rings with the same $\tilde{E}_\Delta$ for $T \ll \max(J, J')$, demonstrating a universality in the low-temperature behaviour.

We note briefly that as N_c is varied, other thermodynamic quantities, such as $T\chi_{\text{imp}}(T)$ or $\chi_{\text{imp}}(T)$ itself, show the same behaviour as that examined in Sec. 6.3 of Chapter 6, and hence the underlying physics is fundamentally that of the TQD model.

Indeed, $T_K \equiv T_K(\tilde{E}_\Delta)$ is characterized by the same power-law decay in all cases

$$T_K \stackrel{J' \rightarrow J'_c \pm}{\sim} \mathcal{A} |J'_c - J'|^\nu \quad : \nu = 2 \quad (7.22)$$

with critical exponent $\nu = 2$ and common amplitudes $\mathcal{A}$ on approaching the transition from either side. This is the same result as established in Sec. 6.3 for the TQD tunnel-coupled to leads, and hence the transition is shown to be of the same fundamental type.

In Fig. 7.14 we plot the variation of the 2CK scale over a wide range of $\rho J'$, for systems with common $\rho J = 0.2$ and $\rho J_K = 0.15$ as usual. We also show a magnified view in the region of the transition in Fig. 7.15, discussed shortly.

First we consider the general behaviour shown in Fig. 7.14, where we plot T_K/D

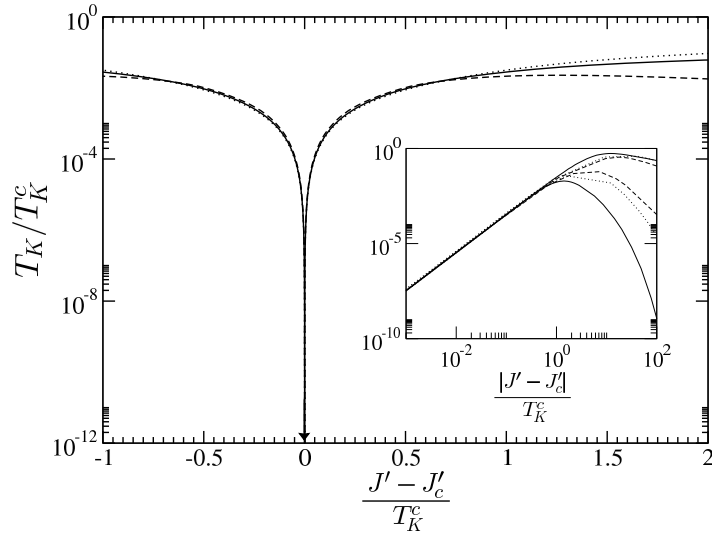


Figure 7.15: Variation of the 2CK scale T_K/T_K^c vs. $(J' - J_c)/T_K^c$ in the vicinity of the transition, plotted for the same systems as in Fig. 7.14, with $N_c = 3$ (solid line), 5 (dashed line) and 7 (dotted line). The inset shows the data on a log-log scale, demonstrating the power-law decay $T_K \propto |J' - J_c|^2$ for $|J' - J_c| \ll T_K^c$.

vs. $\rho J'$ for $N_c = 3$ (left panel) 5 (middle panel) and 7 (right panel), wherein three distinct regimes of behaviour can be immediately seen for each N_c . For $J' \ll J$, there is a modest variation in T_K ; the precise variation determined by NRG (solid lines) agrees very well in this limit with the Kondo scale obtained from perturbative scaling (dotted lines), using the first-order effecting coupling $J_{K\gamma}^{N_c, I}$ Eq. 7.8 in Eq. 7.9.

For $J' \gg J$ by contrast, the Kondo scale drops off very rapidly, as expected from the second-order effective coupling dominant in this regime, which itself diminishes as $J_{K\gamma}^{N_c, II} \propto J_K^2/E_\Delta^{N_c}$ (as discussed in Sec. 7.1.2).

Finally and most importantly, is the region in the vicinity of the transition, where T_K vanishes. This is shown in more detail in Fig. 7.14, where a magnification is shown. We plot T_K/T_K^c vs. $(J' - J_c)/T_K^c$ so as to compare rings of different N_c (which naturally have different values of T_K^c and ρJ_c). As usual, the solid line refers to $N_c = 3$, the dashed to $N_c = 5$ and the dotted to $N_c = 7$. As expected from the collapse of the entropy to a common form in Fig. 7.13 for different values of N_c , here we see that the variation of T_K close to the transition follows the same quadratic form, as given in Eq. 7.22. This behaviour is most easily seen in the inset, where the same results are plotted on a log-log scale, all data collapsing onto a single line of slope $\nu = 2$ for $|J' - J_c| \ll T_K^c$.

The common form of the thermodynamics for rings of different sizes, and the same power-law decay of T_K in the region of the transition, demonstrates that the low-temperature properties and FP structure of these rings is fundamentally alike. In the next section, we examine briefly dynamics near the transition, again showing

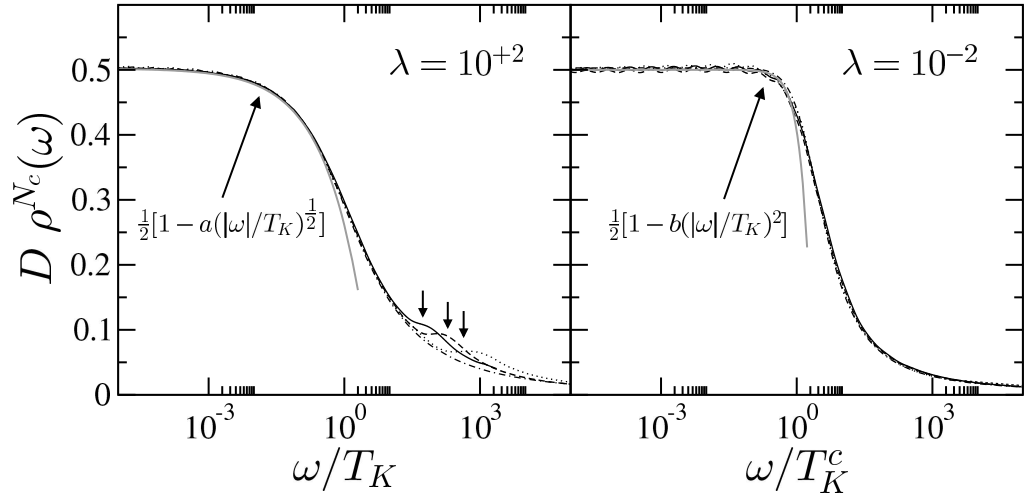


Figure 7.16: $T = 0$ spectrum $D\rho^{N_c}(\omega)$ for rings with $N_c = 3$ (solid lines) 5 (dashed lines) and 7 (dotted lines). Shown for $\rho J = 0.2$, $\rho J_K = 0.15$ as before, but with $\tilde{E}_\Delta = (J'_c - J') = -\lambda T_K^c$. Left panel: $D\rho^{N_c}(\omega)$ vs. ω/T_K for $\lambda = 10^{+2}$, away from the transition. Vertical arrows indicate the point at which $\omega = |\tilde{E}_\Delta|$ for the three rings. The dot-dashed line is for a single-spin 2CK model $D\rho^{2CK}(\omega)$. Right panel: $D\rho^{N_c}(\omega)$ vs. ω/T_K^c for $\lambda = 10^{-2}$, close to the transition. The dot-dashed line here is *half* the spectrum for a single-channel Kondo model, $\frac{1}{2}D\rho^{1CK}(\omega)$. The asymptotic low- ω behaviour, described by Eqs. 7.13 and 7.23, is shown as the grey line in each regime.

that the same behaviour arises for the general class of odd spin rings as does for the TQD tunnel-coupled to leads, studied in Chapter 6.

7.3.3 Dynamics

We now turn to dynamics near the transition, as before studying the spectrum $D\rho^{N_c}(\omega)$. We focus on the universality of the behaviour evident in these systems, noting that away from the transition, the spectrum typical of a single-spin 2CK model is expected at low- ω (as shown in Fig. 7.6), while precisely at the transition, the CFP controls the behaviour of the spectrum at low- ω .

In Fig. 7.16 we plot the $T = 0$ spectrum $D\rho^{N_c}(\omega)$ for rings with $N_c = 3$ (solid lines), 5 (dashed lines) and 7 (dotted lines) and common $\rho J = 0.2$, $\rho J_K = 0.15$, varying $\rho J'$ via $\tilde{E}_\Delta = (J'_c - J') = -\lambda T_K^c$. We consider first the left panel, where we show $D\rho^{N_c}(\omega)$ vs. ω/T_K for $\lambda = 10^{+2}$. These systems are thus “deep” in the 2CK phase, since RG flow is not observed near the CFP (the limiting case being $\lambda = 1$, corresponding to line (a) in Fig. 7.13). Indeed, for $|\omega| \ll T_K$ the expected square-root asymptotic behaviour of Eq. 7.13 for the 2CK model is recovered for each ring (see comparison to grey line).

The behaviour of the spectrum is well-described by the scaling spectrum of the single-spin 2CK model $D\rho^{2CK}(\omega)$ (shown as the dot-dashed line), with departure from it only occurring on the high- ω non-universal scale of $|\tilde{E}_\Delta|$. An intermediate

peak in the spectrum centred on $|\omega| = |\tilde{E}_\Delta|$ (indicated with the vertical arrows in the left panel of Fig. 7.16) is observed for each system. For $N_c = 3, 5$ and 7 , these peaks appear at different values of ω/T_K , despite the common λ , simply because T_K naturally depends on N_c .

The right panel of Fig. 7.16 shows $D\rho^{N_c}(\omega)$ vs. ω/T_K^c for $\lambda = 10^{-2}$, and hence corresponds to systems close to the transition (see Figs. 7.13 and 7.15). The 2CK FP must describe the system for $|\omega| \ll T_K$, but we note that $T_K \ll T_K^c$ for systems with $\lambda = 10^{-2}$. Thus, there is a significant window $T_K \ll |\omega| \ll T_K^c$, where the CFP controls the behaviour of the spectrum, and so the resonance itself, occurring at $|\omega| \sim T_K^c$, is characteristic of the flow to the CFP. The low- ω behaviour is found to be

$$D\rho_{QCP}^{N_c}(\omega) \stackrel{T_K \ll |\omega| \ll T_K^c}{\sim} \frac{1}{2}[1 - b(|\omega|/T_K^c)^2] \quad (7.23)$$

which form is asymptotically common to that of the spectrum $\pi\Gamma D_1(\omega)$ for the TQD tunnel-coupled to its leads at the transition, as studied in Sec. 6.3.4. This quadratic behaviour is also that obtained [8] approaching the strong coupling Fermi liquid FP of the single-channel Anderson (or Kondo) model, but with a halved amplitude. As discussed in Sec. 6.3.4, this can be understood from the nature of the CFP itself. The ring spin is wholly quenched by strong coupling to a single lead in a given $\mathcal{T}^z$ sector (reflecting channel anisotropy at the QCP — see Sec. 6.3.1 and Eq. 6.31). But this screening only occurs via coupling to either given lead in a *single* pseudospin sector. Since both sectors are degenerate precisely at the transition, $D\rho_{QCP}^{N_c}(\omega = 0) = \frac{1}{2}$ results. This physical picture is confirmed in the right panel of Fig. 7.16, where for comparison we plot as the dot-dashed line *half* the spectrum for a single-channel Kondo model, $\frac{1}{2}D\rho^{1CK}(\omega)$, the agreement being essentially perfect.

For $|\omega| \ll T_K$, the asymptotic form of the approach to the 2CK FP (Eq. 7.13) is recovered, but for $|\omega| \ll T_K^c$, Eq. 7.23 gives $D\rho^{N_c}(\omega) \approx \frac{1}{2}$, which is common to the low- ω behaviour near the 2CK FP, and so the entire spectrum for $\lambda = 10^{-2}$ is essentially indistinguishable from that of the QCP spectrum itself (see Sec. 6.3.4).

Finally, we comment briefly on the situation between the limiting cases shown in the left and right panels of Fig. 7.16. For $10^{-2} \lesssim \lambda \lesssim 10^{+2}$, the spectra correspond to the crossover cases, where neither scaling spectrum shown in Fig. 7.16 applies, since the non-universal scale of $|\tilde{E}_\Delta|$ is now comparable to the Kondo scale T_K^c .

7.4 Summary

In this chapter, we have considered the behaviour of a general class of odd rings of dots, modelled as spins, and coupled symmetrically to two metallic leads (see Fig. 7.1 and Eq. 7.1). This work generalizes the results of Chapter 6, where we focused specifically on a triple quantum dot, tunnel-coupled to its leads.

When disconnected from the leads, we showed in Sec. 7.1.1 that all odd rings become magnetically frustrated when all interdot couplings J and J' are tuned to coincidence. This is manifest in particular through the degeneracy of the ground state, which at the point of frustration, comprise a pair of doublet states. The level crossing of these doublet states as a function of J' is permitted by their distinct *parity*, resulting directly from the mirror symmetry of the setup. In Sec. 7.3.1, we show that on coupling to the leads, all odd rings can again be tuned to the point of inherent local magnetic frustration, occurring at a slightly renormalized ratio of interdot couplings compared with the isolated rings.

In Sec. 7.2, we consider the behaviour of systems away from the point of frustration, developing specifically in Sec. 7.1.2 a low-energy effective 2CK model. Using NRG, we demonstrate the underlying universality in this regime of all odd rings, showing that the behaviour is described ubiquitously by the 2CK FP on the lowest temperature/energy scales. In particular we examined the temperature-dependence of thermodynamics, and the frequency-dependence of the spectrum.

The mirror symmetry of the model implies that the many-body states of the system can be classified according to an overall ‘left/right’ parity. Indeed, the low-energy effective models derived well away from the point of frustration conserve local ring parity, and it is shown that *two* distinct 2CK phases therefore result. As a consequence, a quantum phase transition must occur on tuning the interdot couplings.

In Sec. 7.3 we considered the case near the point of frustration in these systems, and developed a generic low-energy effective model to describe the behaviour in this regime. Near the point of degeneracy of the isolated ring ground state doublets (which occurs at $J' = J$), we showed that an extra term in the effective model arises, acting to switch the local ring parity. This term drives the quantum phase transition, and results in a novel critical fixed point which in turn controls the behaviour of the system in the vicinity of the transition. In Secs. 7.3.2 and 7.3.3, we study the transition and the critical fixed point, again focusing on the universality that arises in all odd rings. In particular, we show that the resulting low temperature/energy physics is that of the TQD tunnel-coupled to its leads, which we studied in detail in Chapter 6.

The behaviour of these systems arises fundamentally as a consequence of the geometry and symmetry of the setup, common to all rings studied so far. In the next chapter, we take a different geometry for the TQD, and demonstrate that markedly different physical behaviour is accessible.

CHAPTER 8

Alternative geometries for the TQD

In this chapter we revisit the spin ring TQD, but consider a different geometry. Maintaining mirror symmetry, there is only one other possible configuration for a two-channel TQD model, and that is one in which both leads are coupled to dot 2. The setup is illustrated schematically in Fig. 8.1, and represents a natural two-channel extension of the work studied in Ref. [64].

Below, we show that markedly different physical behaviour results in this system as a result of the different geometry and symmetry of the model. Specifically, an effective *ferromagnetic* coupling [62, 64] between the lowest TQD doublet state and the leads can be generated, which in turn results in a novel two-channel version of the standard ferromagnetic Kondo model. However, a transition to an antiferromagnetically-coupled 2CK phase is also shown to arise, with the transition itself characterized by a simple first-order level crossing. We argue below that the latter is necessitated on the grounds of symmetry, which is shown to be of a different class from that of the ring models studied in Chapters 6 and 7.

The Hamiltonian we study is $H = H_L + H_{\text{tri}} + H_K$, where as usual $H_L = \sum_{\alpha, \mathbf{k}, \sigma} \epsilon_{\mathbf{k}} a_{\alpha \mathbf{k} \sigma}^\dagger a_{\alpha \mathbf{k} \sigma}$ refers to the two equivalent non-interacting leads ($\alpha = A, B$), and

$$\begin{aligned} H_{\text{tri}} &= J \hat{\mathbf{S}}_2 \cdot (\hat{\mathbf{S}}_1 + \hat{\mathbf{S}}_3) + J' \hat{\mathbf{S}}_1 \cdot \hat{\mathbf{S}}_3, \\ H_K &= J_K \sum_{\alpha=A,B} \hat{\mathbf{S}}_2 \cdot \hat{\mathbf{s}}_{\alpha 0}, \end{aligned} \tag{8.1}$$

where as before $\hat{\mathbf{S}}_i$ is a spin- $\frac{1}{2}$ operator for dot i and $\hat{\mathbf{s}}_{\alpha 0}$ is the spin density of either lead $\alpha = A, B$ at dot 2 (as defined in Eq. 3.2).

We have deliberately refrained from using ‘left’ and ‘right’ labels in the above definitions, as the symmetry of the model is different from that studied previously, and we shall see that this has important implications for the behaviour of the system. In particular, inspection of Eq. 8.1 immediately indicates that swapping the leads

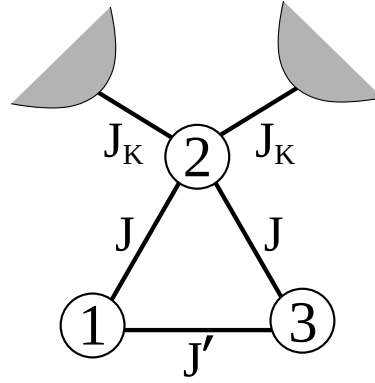


Figure 8.1: Schematic illustration of the TQD, exchange coupled to two leads at dot 2.

(permuting the labels A and B) leaves the full Hamiltonian unchanged, as does swapping dots 1 and 3.

As in Sec. 6.1, the combined spin of dots 1 and 3 is a conserved quantity of the isolated TQD Hamiltonian, since the latter can be written equivalently as $H_{\text{tri}} = J\hat{\mathbf{S}}_2 \cdot \hat{\mathbf{S}}_{13} + \frac{1}{2}J'\hat{\mathbf{S}}_{13}^2$ where $\hat{\mathbf{S}}_{13} = (\hat{\mathbf{S}}_1 + \hat{\mathbf{S}}_3)$. Recalling from Eq. 7.3 and Appendix A that for a system of spins, $\hat{P}_{1,3} = (1 - \hat{\mathbf{S}}_{13}^2)$ exchanges $1 \leftrightarrow 3$ dot labels, it is then clear that the isolated TQD also conserves local parity: $[\hat{P}_{1,3}, H_{\text{tri}}] = 0$. Importantly, however, $\hat{\mathbf{S}}_{13}$ — and hence $\hat{P}_{1,3}$ — is also now conserved in the *full* Hamiltonian, Eq. 8.1, since neither H_K nor H_L contain operators for dots 1 or 3. This situation is thus qualitatively distinct from that arising for the TQD studied in Chapter 6 or the $N_c = 3$ case of Eq. 7.1 in Chapter 7, where the Hamiltonian was shown to be invariant to *simultaneous* exchange of left $\leftrightarrow$ right leads *and* dots $1 \leftrightarrow 3$. Thus the Hilbert space of Eq. 8.1 separates into disjoint sectors of different TQD parity.

The states of the isolated TQD are of course the same as those for the $N_c = 3$ case of Eq. 7.1 in Chapter 7 (which are themselves simply the states in the singly-occupied manifold of the TQD studied in Chapter 6). For $J' < J$ the lowest TQD state is an odd ($-$) parity doublet, $|-, S^z\rangle$, while for $J' > J$ the TQD ground state is the even ($+$) parity doublet, $|+, S^z\rangle$ (see Eq. 6.2). The ground state parity $\gamma = +/-$ of the full many body system, obtained when the leads are attached, is thus carried by the parity of the ring ground state $|\gamma; S^z\rangle$. A quantum phase transition *must* therefore occur between these states of distinct parity.

However, the nature of this transition must be very different from that studied in Chapters 6 and 7: we showed that the phase transition in those models (Eqs. 6.1 or 7.1) was driven by a term in the low-energy effective model which acts to switch states of different local ring parity. But these terms must be strictly absent *by symmetry* in the model considered here, since the local TQD parity is a conserved quantity in the full model Eq. 8.1. We can therefore conclude that the transition

between the phases of distinct TQD parity in this model must be a simple level-crossing transition.

In the next section, we derive perturbatively an effective low-energy model, and discuss the expected behaviour in each of the phases, and near the transition itself.

8.1 Effective model and physical picture

Adopting a similar approach to Sec. 7.3, we derive a low-energy effective model applicable for temperatures $T \ll \max(J, J')$. We consider the generic case where we retain both $|\pm; S^z\rangle$ doublets in the ground TQD manifold of states, which is thus valid both deep in either phase, and in the region of the transition. The energy separation of the TQD doublets is $E_\Delta \equiv (E_+ - E_-) = (J - J')$, and can be arbitrarily small, vanishing at the point of degeneracy $J' = J$ (see Secs. 6.1.1 and 7.1.1). We thus define the unity operator for the local (dot) Hilbert space, viz:

$$\hat{1} = \sum_{\gamma=\pm} \sum_{S^z} |\gamma; S^z\rangle \langle \gamma; S^z| \equiv \hat{1}_+ + \hat{1}_-. \quad (8.2)$$

To first order in J_K an effective low-energy model is then obtained simply by projecting onto the reduced Hilbert space of the lowest pair of doublets. The resultant Hamiltonian to first order, $H_{\text{eff}} = \hat{1} H \hat{1}$, follows as

$$\begin{aligned} H_{\text{eff}} &= H_L + \hat{1}_+ E_+ + \hat{1}_- E_- + J_K \sum_{\alpha=A,B} \hat{1} \hat{\mathbf{S}}_2 \hat{1} \cdot \hat{\mathbf{s}}_{\alpha 0} \\ &\equiv H_L + \frac{1}{2} E_\Delta (\hat{1}_+ - \hat{1}_-) + J_K \sum_{\substack{\alpha=A,B \\ \gamma=\pm}} \hat{1}_\gamma \hat{\mathbf{S}}_2 \hat{1}_\gamma \cdot \hat{\mathbf{s}}_{\alpha 0} \end{aligned} \quad (8.3)$$

where the cross terms involving $\hat{1}_\gamma \hat{\mathbf{S}}_2 \hat{1}_{-\gamma}$ vanish by symmetry, since the $|\pm; S^z\rangle$ states have distinct parity and so cannot be interconverted. Another way of viewing this result is to note that the singlet or triplet configuration of the spins on dots 1 and 3 cannot be interconverted simply by spin exchange processes between the leads and dot 2. Using the definition of the doublets $|\gamma; S^z\rangle$ in Eq. 6.2 (or more generally from Appendix B), it is straightforward to show that

$$H_{\text{eff}} = H_L + \frac{1}{2} E_\Delta (\hat{1}_+ - \hat{1}_-) + \sum_{\substack{\alpha=A,B \\ \gamma=\pm}} J_{K\gamma} \hat{\mathbf{S}}_\gamma \cdot \hat{\mathbf{s}}_{\alpha 0} \quad (8.4)$$

where $\hat{\mathbf{S}}_\gamma$ is a spin- $\frac{1}{2}$ operator for the appropriate $\gamma = +/ -$ TQD doublet state, and the effective first-order coupling is given by

$$J_{K\gamma} = 2 \langle \gamma; \frac{1}{2} | \hat{S}_2^z | \gamma; \frac{1}{2} \rangle J_K \quad (8.5)$$

Direct evaluation of Eq. 8.5 using the definition of the doublets $|\gamma; S^z\rangle$, Eq. 6.2, gives $J_{K-} = -\frac{1}{3}J_K$ while $J_{K+} = +J_K$.

As discussed in Refs. [62, 64] in the context of single-channel models, this is a striking result: in the $J' < J$ regime, the effective coupling between the $|-, S^z\rangle$ TQD ground state and the leads is *ferromagnetic* ($J_{K-} < 0$), despite all the bare interdot couplings being antiferromagnetic. By contrast, in the $J' > J$ regime, where $|+, S^z\rangle$ is the TQD ground state, the effective coupling is equal to the bare coupling, $J_{K+} \equiv J_K$ — and hence is *antiferromagnetic*. This can be understood from the structure of the $|+, S^z\rangle$ doublet itself: the dots 1 and 3 are locked up in a singlet configuration, thereby leaving the spin on dot 2 essentially free¹. Thus, in the $J' > J$ regime, the spin on dot 2 effectively couples to the two leads antiferromagnetically and symmetrically, with dots 1 and 3 playing no role.

We now discuss briefly the expected behaviour of the model when deep in either regime: $J' \ll J$ or $J' \gg J$. In either case, the doublet lying higher in energy is projected out for $T \ll |E_\Delta|$ (by the middle term of Eq. 8.4), leaving only a single spin- $\frac{1}{2}$ object, coupled symmetrically to two leads. At low enough temperatures then, Eq. 8.4 reduces to a model of 2CK form, but the effective couplings are given by $J_{K\gamma}$ for whichever doublet $\gamma = +/ -$ lies lowest. For $J' \ll J$, a two-channel version of the ferromagnetic Kondo effect [8, 62, 64] is expected, with the TQD spin becoming asymptotically free as $T \rightarrow 0$ and so the stable FP is simply the LM FP. A residual entropy [13] $S_{\text{imp}}(T=0) = \ln(2)$ and Curie law [13] magnetic spin susceptibility $T\chi_{\text{imp}}(T) = \frac{1}{4}$ then results. The system here is an example of a “singular Fermi liquid” [134], reflected in the nonanalyticity of leading irrelevant logarithmic corrections to the fixed point [127, 134]. Precisely at the Fermi level however, both leads are completely decoupled from the TQD.

For $J' \gg J$ by contrast, the Kondo coupling to each lead is antiferromagnetic, and so the LM FP is destabilised. The 2CK FP then controls the $T \rightarrow 0$ behaviour, describing the non-Fermi liquid ground state in which the TQD spin is overscreened by the lead/conduction electrons in both leads below a characteristic [40] Kondo scale

$$T_K \sim J_{K+} \exp(-1/\rho J_{K+}). \quad (8.6)$$

We stress here that there is a single, fixed Kondo scale in the model, since $J_{K+} \equiv J_K$ is fixed by virtue of the singlet configuration of dots 1 and 3 in the ground state $|+, S^z\rangle$ doublet throughout this phase (see Eq. 8.5). Thus we expect a residual entropy [43–45] $S_{\text{imp}}(T=0) = \frac{1}{2} \ln(2)$ and $T\chi_{\text{imp}}(T=0) = 0$, with $\chi_{\text{imp}}(T)$ itself diverging logarithmically below T_K [43, 45, 46].

The $|E_\Delta|$ scale, however, can be arbitrarily small, as there is a level crossing of

¹The spin- $\frac{1}{2}$ operator for the $|+, S^z\rangle$ state could thus equivalently be written $\hat{\mathbf{S}}_+ \equiv \hat{\mathbf{S}}_2 \hat{1}_{13}$, where $\hat{1}_{13}$ is a unity operator acting on the Hilbert space of dots 1 and 3 only.

states with distinct parity in the full model. Since the effective model Eq. 8.4 reduces to a single-spin 2CK model only for $T \ll |E_\Delta|$, this implies that the temperature scale characterizing the flow to the ultimate stable FP of the model (be it either the 2CK FP or the LM FP), may itself be arbitrarily small.

Indeed, since the fixed points for the two stable phases are distinct, a quantum phase transition must occur on tuning J' through the critical value $J'_c \simeq J$. This is also consistent with the argument presented above that a transition must occur because of the distinct ground state parity associated with each phase. We study the transition with NRG below, but first recast Eq. 8.4 in terms of spin- $\frac{1}{2}$ operators for real spin $\hat{\mathbf{S}} (= \sum_\gamma \hat{\mathbf{S}}_\gamma)$ and pseudospin $\hat{\mathcal{T}}$ for the local dot Hilbert space, defined in Eqs. 6.11 and 6.12. Recalling that $\hat{\mathcal{T}}^z = \frac{1}{2}(\hat{1}_+ - \hat{1}_-)$ — and hence $\hat{\mathcal{T}}^z|\pm; S^z\rangle = \pm\frac{1}{2}|\pm; S^z\rangle$ — it follows that $[\hat{\mathcal{T}}^z, H] = 0$, since TQD parity is conserved. Thus, terms involving $\hat{\mathcal{T}}^\pm$, which thereby act to mix the components of the pseudospin, cannot enter the effective model. Finally, we use $\hat{\mathbf{S}} = \sum_\gamma \hat{\mathbf{S}}_\gamma$, and obtain

$$H_{\text{eff}} = H_L + \frac{1}{3}J_K(1 + 4\hat{\mathcal{T}}^z)\hat{\mathbf{S}} \cdot (\hat{\mathbf{s}}_{A0} + \hat{\mathbf{s}}_{B0}) + E_\Delta\hat{\mathcal{T}}^z. \quad (8.7)$$

The term E_Δ is equivalent to a magnetic field acting on the pseudospin, favouring the $|-; S^z\rangle$ doublet for $E_\Delta > 0$ and $|+; S^z\rangle$ for $E_\Delta < 0$. In the full model, the $|\gamma; S^z\rangle$ doublets are degenerate and the ring is inherently magnetically frustrated when no magnetic field acts on the pseudospin: $\tilde{E}_\Delta = (J'_c - J') = 0$ with $J'_c \approx J$ naturally renormalized slightly from its bare value for the isolated ring.

We note that the structure of Eq. 8.7 is similar to that of Eq. 6.13 studied in Chapter 6, except the effective couplings are different, and the $\hat{\mathcal{T}}^\pm$ terms are absent here by symmetry. As a result, one expects the resulting low-temperature/energy behaviour of the system to be rather different, as discussed above, and as demonstrated using NRG below.

In Fig. 8.2 we plot the variation of the $T = 0$ spin-spin correlation functions $\langle \hat{\mathbf{S}}_1 \cdot \hat{\mathbf{S}}_2 \rangle \equiv \langle \hat{\mathbf{S}}_3 \cdot \hat{\mathbf{S}}_2 \rangle$ (solid lines) and $\langle \hat{\mathbf{S}}_1 \cdot \hat{\mathbf{S}}_3 \rangle$ (dashed lines) *vs.* $\rho J'$, for systems with common fixed $\rho J = 0.1$ and $\rho J_K = 0.075$, calculated for the full model via NRG. The inset shows a magnification in the region of the transition, $J' \approx J$. The behaviour of these correlators is very different from that presented in Figs. 6.11 and 7.7–7.12, where leads were attached to neighbouring dots of the ring, rather than to the same dot, as studied here (see Fig. 8.1 and Eq. 8.1). In those systems, $\langle \hat{\mathbf{S}}_i \cdot \hat{\mathbf{S}}_j \rangle$ approached the limiting values for the isolated rings asymptotically for $J' \ll J$ and $J' \gg J$. But closer to the transition, significant deviations were observed, and indeed a continuous crossover in the vicinity of $J' \approx J$ occurs in all cases. Evidently from Fig. 8.2, the $T = 0$ correlators show a *discontinuity*, as is expected for a level-crossing transition.

We consider first the behaviour of $\langle \hat{\mathbf{S}}_1 \cdot \hat{\mathbf{S}}_3 \rangle$ (dashed lines). The key difference between this model and those studied in Chapters 6 and 7 is that here the ring parity

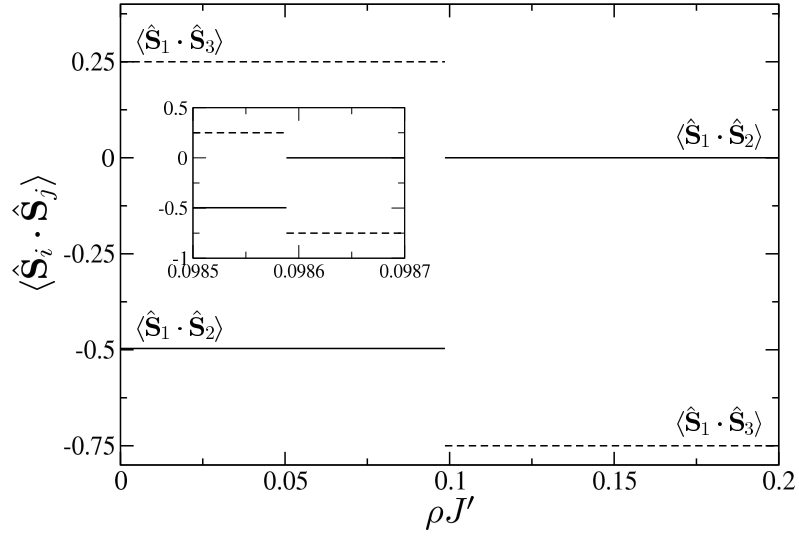


Figure 8.2: Spin-spin correlation functions $\langle \hat{\mathbf{S}}_1 \cdot \hat{\mathbf{S}}_2 \rangle \equiv \langle \hat{\mathbf{S}}_3 \cdot \hat{\mathbf{S}}_2 \rangle$ (solid line) and $\langle \hat{\mathbf{S}}_1 \cdot \hat{\mathbf{S}}_3 \rangle$ (dashed line) at $T = 0$ for $\rho J = 0.1$ and $\rho J_K = 0.075$, varying $\rho J'$. The inset shows a magnification in the region of the discontinuity.

$\hat{P}_{1,3}$ is a conserved quantity in the *full* Hamiltonian Eq. 8.1, not just in the isolated ring. The ground state parity at $T = 0$ is given by $\gamma = \langle \hat{P}_{1,3} \rangle \equiv \langle -\frac{1}{2} - 2\hat{\mathbf{S}}_1 \cdot \hat{\mathbf{S}}_3 \rangle$, and so we obtain $\langle \hat{\mathbf{S}}_1 \cdot \hat{\mathbf{S}}_3 \rangle = -\frac{1}{4}(1 + 2\gamma)$. The spin-spin correlator for dots 1 and 3 thus jumps discontinuously from $+\frac{1}{4}$ to $-\frac{3}{4}$ as the ground state parity switches from $\gamma = -$ (for $J' < J'_c$) to $\gamma = +$ (for $J' > J'_c$). This is the exact behaviour seen to occur from the dashed line in Fig. 8.2, with the value of $\rho J'_c = 0.09858\dots$ defined in practice as the point of the discontinuity.

Perhaps more interestingly, $\langle \hat{\mathbf{S}}_1 \cdot \hat{\mathbf{S}}_2 \rangle$ (solid line) also shows a discontinuity at $\rho J'_c$. This too might be expected for a level-crossing transition, yet the combined spin of dots 1 and 2 is *not* conserved. However, $\langle \hat{\mathbf{S}}_1 \cdot \hat{\mathbf{S}}_2 \rangle \equiv \langle \hat{\mathbf{S}}_3 \cdot \hat{\mathbf{S}}_2 \rangle = \frac{1}{2} \langle \hat{\mathbf{S}}_{13} \cdot \hat{\mathbf{S}}_2 \rangle$, and as $\hat{\mathbf{S}}_{13} = (\hat{\mathbf{S}}_1 + \hat{\mathbf{S}}_3)$ changes discontinuously across the transition, it is natural to expect that $\langle \hat{\mathbf{S}}_1 \cdot \hat{\mathbf{S}}_2 \rangle$ is also discontinuous. In the isolated ring, the total TQD spin is conserved, and at $T = 0$ the ground state is one or other of the doublets $|\gamma; S^z\rangle$, so a simple sum rule $\langle \hat{\mathbf{S}}_1 \cdot \hat{\mathbf{S}}_2 \rangle = -\frac{1}{8}(3 + 4\langle \hat{\mathbf{S}}_1 \cdot \hat{\mathbf{S}}_3 \rangle) = \frac{1}{4}(\gamma - 1)$ immediately follows. Thus a discontinuity in the isolated TQD is guaranteed, with $\langle \hat{\mathbf{S}}_1 \cdot \hat{\mathbf{S}}_2 \rangle$ jumping from $-\frac{1}{2}$ to 0 as the ground state switches from $\gamma = -$ to $\gamma = +$. In fact, we see that this is precisely the behaviour of $\langle \hat{\mathbf{S}}_1 \cdot \hat{\mathbf{S}}_2 \rangle$ in the full model, when the leads are attached.

We now consider the case precisely at the transition itself, when $\tilde{E}_\Delta = 0$, and the $\mathcal{T}^z = \pm\frac{1}{2}$ components of the pseudospin are degenerate. At ‘high’ temperatures (but for $T < \max(J', J)$, so that the TQD quartet state is projected out), the real spin and pseudospin are both free, and hence this $SU(2) \times SU(2)$ FP is simply described by Eq. 8.7 with $J_K = 0$ and $E_\Delta = 0$. As there are no pseudospin mixing terms, the $\mathcal{T}^z = \pm\frac{1}{2}$ sectors are strictly disjoint. In the $\mathcal{T}^z = -\frac{1}{2}$ sector, the spin

remains free down to $T \rightarrow 0$ as the effective coupling here is ferromagnetic, and so the LM FP [13] characterizes the low-temperature properties in this sector. The LM FP Hamiltonian is thus simply Eq. 8.7 with $J_K = 0$ and $\tilde{E}_\Delta = +\infty$.

However, in the $\hat{T}^z = +\frac{1}{2}$ sector, the LM FP (which here corresponds to Eq. 8.7 with $J_K = 0$ and $\tilde{E}_\Delta = -\infty$) is unstable since the effective coupling is antiferromagnetic. Thus the TQD spin is overscreened [40] below the 2CK scale, T_K , in this sector. The $T \rightarrow 0$ behaviour is then characteristic of the 2CK FP.

As both $\mathcal{T}^z = \pm\frac{1}{2}$ are degenerate at the transition, the transition FP (TFP) thus comprises both the overscreened 2CK state *and* the free local moment. The TFP is not as such a ‘critical’ FP, as it consists simply of a combination of the stable FPs for the distinct phases infinitesimally close to the TFP ($J' \rightarrow J'_c \pm$).

However, the TFP should have clear and rather unusual signatures in thermodynamic quantities such as entropy and uniform spin susceptibility. The residual ($T = 0$) entropy of the 2CK FP [43–45] is $S_{\text{imp}}^{2CK} = \frac{1}{2} \ln(2) \equiv \ln(\sqrt{2})$, and hence the degeneracy of the state can in some sense be thought of as being $\sqrt{2}$. At the TFP, we have both this 2CK state in the $\mathcal{T}^z = +\frac{1}{2}$ sector, and a free, doubly-degenerate spin- $\frac{1}{2}$ in the $\mathcal{T}^z = -\frac{1}{2}$ sector, for which [13] $S_{\text{imp}}^{LM} = \ln(2)$, and so the total entropy is expected to be

$$S_{\text{imp}}^{TFP}(T = 0) = \ln(2 + \sqrt{2}) \approx 1.772 \times \ln(2). \quad (8.8)$$

Likewise, for $\mathcal{T}^z = +\frac{1}{2}$, the spin susceptibility at $T = 0$ for the 2CK FP is [43, 45, 46] $T\chi_{\text{imp}}^{2CK} = 0$, while for $\mathcal{T}^z = -\frac{1}{2}$, the free spin gives a Curie law [13] $T\chi_{\text{imp}}^{LM} = \frac{1}{4}$. The TFP susceptibility is thus

$$T\chi_{\text{imp}}^{TFP}(T = 0) = \frac{2 \times \frac{1}{4} + \sqrt{2} \times 0}{2 + \sqrt{2}} = \frac{1}{2}(2 + \sqrt{2})^{-1} \approx 0.146, \quad (8.9)$$

which is readily understood as the mean $\langle (S^z)^2 \rangle$ for the degenerate LM and 2CK states.

We turn finally to the case of non-zero $\tilde{E}_\Delta$. As discussed above, away from the transition, the $SU(2) \times SU(2)$ FP describes the behaviour of the system for $|\tilde{E}_\Delta| < T < \max(J, J')$, but for $T \ll |\tilde{E}_\Delta|$, the upper component of the pseudospin is simply frozen out, and the system flows to either the 2CK FP (for $\tilde{E}_\Delta > 0$) or the LM FP (for $\tilde{E}_\Delta < 0$).

Close to the transition, however, the system flows near to the TFP when the pseudospin sectors are quasidegenerate, which occurs in the temperature window $T_\Delta \ll T \ll T_K$, where T_Δ is a scale which vanishes in a characteristic way as the transition is approached. Decreasing the temperature below T_Δ , we expect the upper pseudospin sector to be projected out as before, with the system ultimately being described by the 2CK or LM FPs for $T \ll T_\Delta$.

In the next section, we present thermodynamics for the full model calculated with NRG, demonstrating that the above physical picture does indeed describe the low-temperature behaviour of systems close to the transition.

8.2 Thermodynamics

In this section, we examine the TQD contribution to the entropy, $S_{\text{imp}}(T)$, and uniform spin susceptibility, $T\chi_{\text{imp}}(T)$. As before, the temperature dependence of such quantities allows the underlying FP structure and the relevant energy scales of the model to be determined [13, 27].

In Fig. 8.3 we plot $S_{\text{imp}}(T)$ (top panel) and $T\chi_{\text{imp}}(T)$ (bottom panel), both *vs.* a common temperature scale T/D (and $2D$ is the conduction bandwidth as usual). Shown are data for common fixed $\rho J = 0.1$ and $\rho J_K = 0.075$, varying $\rho J'$. A single Kondo scale can thus be defined², as T_K does not vary with $\rho J'$ ($J_{K+} = J_K$: see Eqs. 8.4–8.7) and corresponds to the characteristic scale below which the $|+; S^z\rangle$ doublet (or equivalently, the TQD spin- $\frac{1}{2}$ in the $\mathcal{T}^z = +\frac{1}{2}$ sector) is overscreened by antiferromagnetic coupling to the leads. Specifically, we find $T_K/D = 6 \times 10^{-7}$ (indicated with a vertical arrow in Fig. 8.3), and we give $\rho J'$ in terms of this scale, varying it via $\tilde{E}_\Delta = (J'_c - J') = \pm \lambda T_K$, with $\lambda = 10^n$ and $n = +5, +3, +1, 0, -1, -3, -5$ [lines (a–g)] approaching the transition itself [$\lambda = 0$, line (h)] from both sides. All systems with $\tilde{E}_\Delta > 0$ (solids lines) are in the LM phase, while systems with $\tilde{E}_\Delta < 0$ (dotted lines) are in the 2CK phase.

We consider first the evolution of the entropy in the top panel of Fig. 8.3. At the highest temperatures ($T \gg \max(J, J')$) each of the spins of the TQD are essentially free, and an entropy $S_{\text{imp}} = 3 \ln(2)$ naturally results. Lines (a) are for systems far away from the transition, with $\tilde{E}_\Delta = +10^5 \times T_K$ ‘deep’ in the LM phase, while $\tilde{E}_\Delta = -10^5 \times T_K$ is ‘deep’ in the 2CK phase. As the temperature is lowered, all but the lowest TQD doublet is projected out: the $E_\Delta \hat{\mathcal{T}}^z$ pseudospin magnetic field term of Eq. 8.7 ensures that only the lowest component of the pseudospin is thermally accessible for $T \ll |E_\Delta|$. For $\tilde{E}_\Delta > 0$, the LM FP is the stable FP, and thus a residual entropy $S_{\text{imp}} = \ln(2)$ persists down to $T = 0$ [solid line (a)]. By contrast, for $\tilde{E}_\Delta < 0$, the LM FP is unstable, the effective antiferromagnetic coupling between the lowest TQD doublet and the leads in the $\mathcal{T}^z = +\frac{1}{2}$ sector now driving the system to the 2CK FP below T_K . The residual entropy is now that characteristic [43–45] of the 2CK FP, and $S_{\text{imp}} = \frac{1}{2} \ln(2)$ at $T = 0$ [dotted line (a)].

For systems with smaller $|\tilde{E}_\Delta|$, a new FP is observed, corresponding to the situation where the TQD quartet is projected out, but the doublets are quasidegenerate. This is illustrated by lines (b,c) (for $|\tilde{E}_\Delta| = 10^3 \times T_K$ and $10 \times T_K$ respectively),

² T_K here is defined in practice through the spin susceptibility as $T_K \chi_{\text{imp}}(T_K) = 0.07$ for a system with $J' = 2J$, thereby representatively ‘deep’ in the 2CK phase

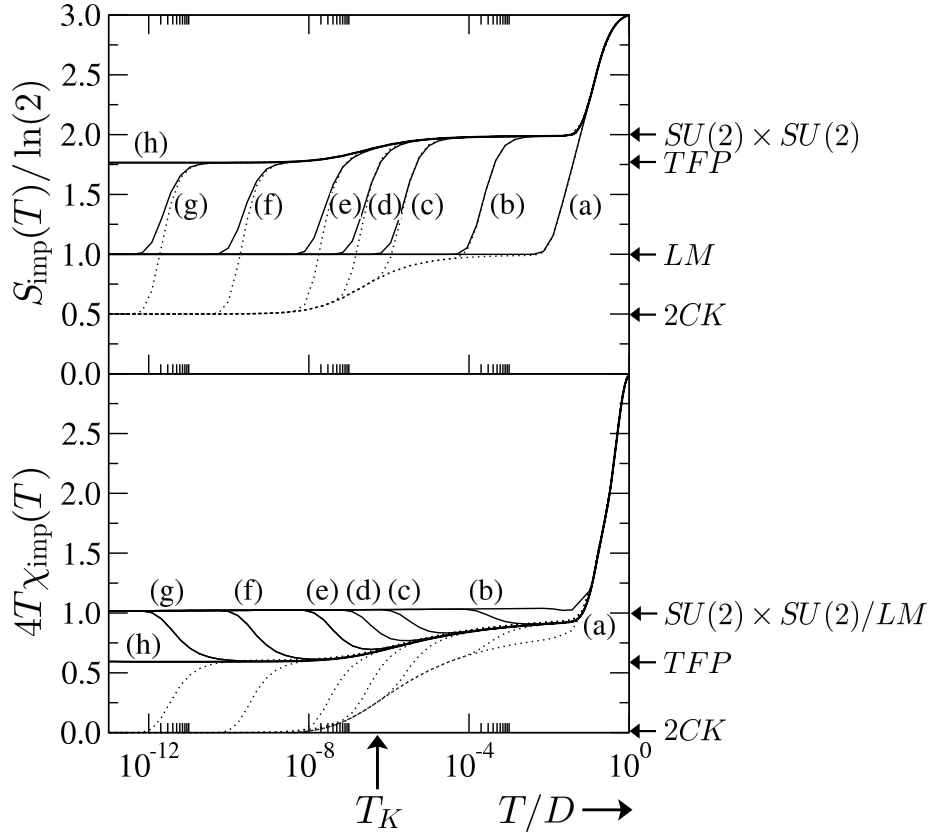


Figure 8.3: Thermodynamics in the vicinity of the transition. The top panel shows the entropy $S_{\text{imp}}(T)$ and the bottom panel shows the spin susceptibility $T\chi_{\text{imp}}(T)$, both *vs.* a common temperature scale T/D . In both panels, systems with common fixed $\rho J = 0.1$ and $\rho J_K = 0.075$ are plotted, varying $\rho J'$ via $\tilde{E}_\Delta = (J'_c - J') = \pm \lambda T_K$, and $\lambda = 10^n$ with $n = +5, +3, +1, 0, -1, -3, -5$ [lines (a–g)] approaching the transition [$\lambda = 0$, line (h)] from both the LM phase ($\tilde{E}_\Delta > 0$, solid lines) and from the 2CK phase ($\tilde{E}_\Delta < 0$, dotted lines).

where the entropy shows a distinctive plateau at $S_{\text{imp}} = 2\ln(2)$ in the temperature window $|\tilde{E}_\Delta| < T < \max(J, J')$. This is the ‘ $SU(2) \times SU(2)$ ’ FP described in Sec. 8.1, where the TQD spin and pseudospin are essentially free. Naturally, the system is described by this FP down to lower and lower temperatures as $|\tilde{E}_\Delta|$ decreases, since the components of the pseudospin are closer in energy [as in line (c)]. As the temperature is lowered further, however, the higher-lying component of the pseudospin is frozen out: for $T \ll |\tilde{E}_\Delta|$, $T^z = +\frac{1}{2}$ is no longer accessible for $\tilde{E}_\Delta > 0$ while $T^z = -\frac{1}{2}$ is projected out for $\tilde{E}_\Delta < 0$. The situation then is the same as for lines (a): the spin remains free in the LM phase (solid lines), and $S_{\text{imp}} = \ln(2)$ results as $T \rightarrow 0$, but in the 2CK phase (dotted lines) the TQD spin undergoes the 2CK effect below T_K and so $S_{\text{imp}} = \frac{1}{2}\ln(2)$ as $T \rightarrow 0$.

The obvious question is: what happens when the energy separation of the pseudospin components is reduced further; in particular so that $|\tilde{E}_\Delta| \leq T_K$? We argued in Sec. 8.1 that systems in this regime should flow close to the transition FP, before

crossing over to either the LM or 2CK FPs on a scale T_Δ . We define this scale in practice through $S_{\text{imp}}(T_\Delta) = \frac{3}{2} \ln(2)$, chosen so as to describe the energy scale where RG flow away from the unstable TFP occurs. Systems then flow directly to the ultimate stable FP which characterizes the phase.

Lines (d–e) are in the region where RG flow in the vicinity of the TFP is first observed, while lines (f–g) approach the transition much more closely, and so are well described by the TFP over an increasingly wide temperature window. Therefore, lines (d) for $\tilde{E}_\Delta = \pm T_K$ represents the borderline case, separating systems ‘away’ from the transition ($|\tilde{E}_\Delta| > T_K$) where no evidence of the TFP is observed, and systems ‘near’ the transition ($|\tilde{E}_\Delta| < T_K$) where the TFP strongly affects the behaviour of the thermodynamics in the temperature window $T_\Delta < T < T_K$. However, in each case (d–g), the upper component of the pseudospin is eventually projected out below $T \sim T_\Delta$, and the systems flow directly to either the LM FP ($\tilde{E}_\Delta > 0$) or the 2CK FP ($\tilde{E}_\Delta < 0$).

This is a non-trivial result: in the LM phase, the TQD spin in the $\mathcal{T}^z = +\frac{1}{2}$ sector undergoes the 2CK effect *even though it is not the ground state*, and then the many-body 2CK state is destroyed and projected out below T_Δ . Near the transition, 2CK physics is thus observed at finite temperatures in the LM phase, even though at $T = 0$ the system is a ‘singular Fermi liquid’ [127, 134], unlike the ground state in the 2CK phase which is a non-Fermi liquid [40, 49].

The scale T_Δ vanishes as the transition is approached, so that the TFP entropy of $S_{\text{imp}} = \ln(2 + \sqrt{2})$ (see Eq. 8.8) persists over a progressively wider temperature range [see lines (f,g)], and indeed is the $T = 0$ residual entropy at the transition itself [line (h)]. We study *how* the scale T_Δ vanishes below, as this is characteristic of the transition, but first examine briefly the bottom panel of Fig. 8.3, where we study the uniform spin susceptibility, $T\chi_{\text{imp}}(T)$, for the same systems.

The above behaviour is of course likewise manifest in the evolution of $T\chi_{\text{imp}}(T)$ approaching the transition. Again, behaviour common to all systems (a–h) is observed at high temperatures, with $T\chi_{\text{imp}} = \frac{3}{4}$ characteristic of three uncoupled free spins- $\frac{1}{2}$. As the temperature is decreased, the quartet state is rapidly projected out. Indeed, for lines (a), the LM FP is now reached directly, as the upper pseudospin component is also projected out. The free TQD spin gives rise to a Curie law susceptibility $T\chi_{\text{imp}} = \frac{1}{4}$, which remains the behaviour as $T \rightarrow 0$ in the LM phase, but $T\chi_{\text{imp}} = 0$ for $T \ll T_K$ in the 2CK phase [43, 45, 46].

For lines (b–h), the $SU(2) \times SU(2)$ FP is observed at intermediate temperatures $\max(T_K, |\tilde{E}_\Delta|) < T < \max(J, J')$, as was seen clearly from the $S_{\text{imp}} = 2 \ln(2)$ plateau in the entropy. However, a Curie law susceptibility $T\chi_{\text{imp}} = \frac{1}{4}$ still results, as the free pseudospin does not contribute to the magnetic susceptibility (which can be understood as the mean $\langle (S^z)^2 \rangle$).

For lines (b,c), below $T \sim |\tilde{E}_\Delta|$ the upper pseudospin component is frozen out,

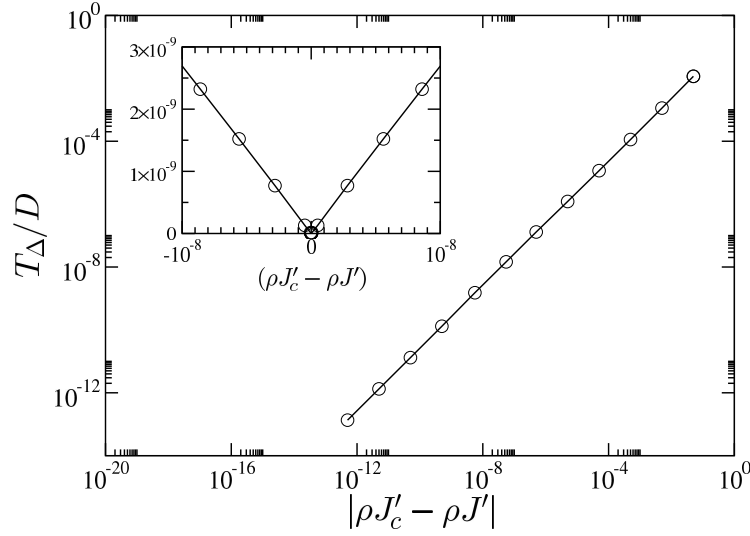


Figure 8.4: Variation of the vanishing T_Δ scale approaching the transition (at $\rho J'_c = 0.09856\dots$), for fixed $\rho J = 0.1$ and $\rho J_K = 0.075$. We plot T_Δ/D vs. $|\rho J'_c - \rho J'|$ on logarithmic axes over a wide range of values of $\rho J'$, demonstrating the linear decay $T_\Delta \propto |J'_c - J'|$. The scale decays symmetrically from either side of the transition (see inset, where the data are plotted on linear axes).

and systems then flow to either the LM FP for $\tilde{E}_\Delta > 0$ (solid lines) or to the 2CK FP below T_K for $\tilde{E}_\Delta < 0$ (dotted lines).

Lines (d–g) progressively approach the transition more closely, and thus flow near the TFP over a wider temperature range $T_\Delta < T < T_K$. Below $T \sim T_\Delta$, the higher lying pseudospin component is again projected out. Line (h), describing the transition itself ($\tilde{E}_\Delta = 0$), remains at the TFP as $T \rightarrow 0$, and so $T\chi_{\text{imp}}(T \rightarrow 0) = \frac{1}{2}(2 + \sqrt{2})^{-1}$ (see Eq. 8.9).

In Fig. 8.4 we show the variation of the T_Δ scale for fixed $\rho J' = 0.1$ and $\rho J_K = 0.075$, plotted as T_Δ/D vs. $|\rho J'_c - \rho J'| \equiv |\rho \tilde{E}_\Delta|$ on logarithmic axes. We define T_Δ as before from the thermodynamics via $S_{\text{imp}}(T_\Delta) = \frac{3}{2} \ln(2)$, and as such can be determined arbitrarily far away from the transition (see Fig. 8.3). Physical arguments presented in Sec. 8.1, and the thermodynamics studied with NRG in Fig. 8.3, indicate that $T_\Delta \rightarrow 0$ as $|\tilde{E}_\Delta| \equiv |J'_c - J'| \rightarrow 0\pm$. Fig. 8.4 shows that the scale vanishes *linearly*:

$$T_\Delta \stackrel{J' \rightarrow J'_c \pm}{\sim} \mathcal{A} |J'_c - J'|^\nu \quad : \nu = 1, \quad (8.10)$$

with common amplitudes $\mathcal{A}$ on approaching J'_c from either side, as seen clearly in the inset to Fig. 8.4, where the data are plotted on a linear scale. Thus, $T_\Delta \propto |\tilde{E}_\Delta|$, confirming as expected that the transition is characterized by a simple level-crossing. The higher lying pseudospin component is projected out below $T \sim |\tilde{E}_\Delta|$ as would

be naively expected from the pseudospin magnetic field term³ $\tilde{E}_\Delta \hat{T}^z$ in the low-energy effective Hamiltonian Eq. 8.7, even though the state being projected out is the many-body 2CK state for $\tilde{E}_\Delta > 0$. Indeed, Fig. 8.4 shows that the T_Δ scale corresponding to this process is proportional to $|\tilde{E}_\Delta|$, in either the large or the small $|\tilde{E}_\Delta|$ regime, supporting the argument that the transition is characterized by a simple level crossing.

8.3 Dynamics

The physical picture of the transition is clear from the thermodynamics presented in the previous section. For $J' < J'_c$, the model is described by the LM FP at the lowest temperatures, while for $J' > J'_c$, the 2CK FP is stable, and describes the behaviour of the system below $T \sim T_K$, which is itself fixed throughout the phase. A quantum phase transition between these phases occurs as $\rho J'$ is tuned through its critical value $\rho J'_c$, and is characteristic of a level-crossing transition (see Eq. 8.10 and Fig. 8.4). The TFP itself comprises both the LM and 2CK states, as reflected in the entropy and spin susceptibility at the transition (see Eqs. 8.8 and 8.9). In this section we examine dynamics of the model in each phase, and in the vicinity of the transition.

We focus initially on the $T = 0$ spectrum $D \rho_2(\omega)$, which we relate to the t-matrix $t_\alpha(\omega)$ for lead $\alpha = A, B$ through $D \rho_2(\omega) = -\pi \rho_T \text{Im}\{t_\alpha(\omega)\}$, as in Secs. 3.6.3 and 4.2.2 (and $\rho_T = N\rho = N/(2D)$ is the total density of states, where N is the total number of orbitals/ $\mathbf{k}$ -states in the lead). By symmetry, $t_A(\omega) = t_B(\omega) \equiv t(\omega)$, and using equation of motion methods [8, 139], it is then straightforward to show that $t(\omega) = \frac{J_K^2}{4N} G_{s,2}(\omega)$, with $G_{s,2}(\omega) = \langle \langle \hat{S}_2^- f_{A0\downarrow} + \hat{S}_2^z f_{A0\uparrow}; \hat{S}_2^+ f_{A0\downarrow}^\dagger + \hat{S}_2^z f_{A0\uparrow}^\dagger \rangle \rangle_\omega$, and $f_{A0\sigma}^\dagger$ is an operator for the ‘0’-orbital of the $\alpha = A$ Wilson chain (see Eq. 3.2), while $\hat{S}_2^-$ is a spin lowering operator for dot 2.

In Fig. 8.5 we show the $T = 0$ spectrum $D \rho_2(\omega)$ *vs.* ω/D for all systems plotted for the thermodynamics in Fig. 8.3. At $T = 0$, the 2CK FP describes all systems for any $\tilde{E}_\Delta < 0$, and hence the spectrum for a single-spin 2CK model (see Sec. 3.6.3) is expected. This is indeed seen to be the case, as all lines labelled ‘ $\tilde{E}_\Delta < 0$ ’ in Fig. 8.5 are perfectly coincident over the entire frequency range shown. The spectrum for a single-spin 2CK model (chosen to have the same T_K) is also plotted for comparison (dashed line), and agrees essentially perfectly, as expected.

By contrast, the LM FP describes the $T = 0$ behaviour of all systems for $\tilde{E}_\Delta > 0$. As each lead decouples, the spectrum characteristic [64, 127] of the ferromagnetic Kondo model is then expected. In Fig. 8.5, all spectra in the LM phase (lines labelled ‘ $\tilde{E}_\Delta > 0$ ’) again coincide at $T = 0$. This is most clearly seen in the inset,

³As previously discussed, $\tilde{E}_\Delta$ is renormalized slightly from its bare value E_Δ in the full model

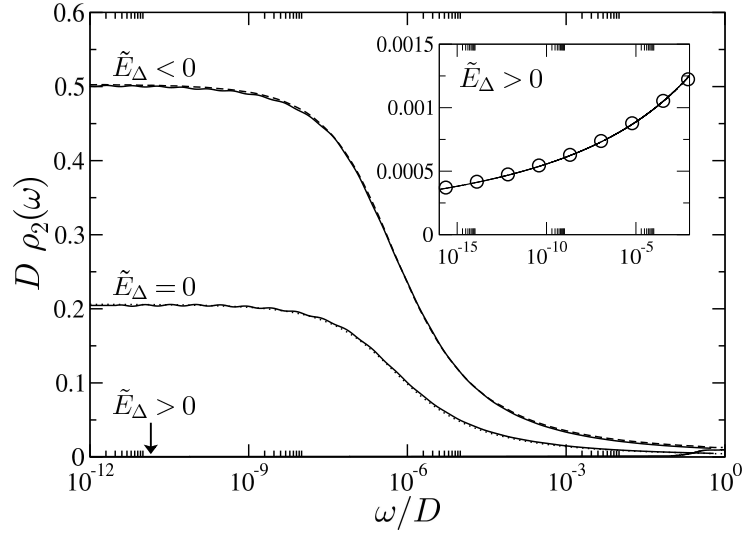


Figure 8.5: $T = 0$ local spectrum $D \rho_2(\omega)$ for dot 2 *vs.* ω/D for the same systems as plotted for the thermodynamics in Fig. 8.3. All of the systems in the 2CK phase ($\tilde{E}_\Delta < 0$) collapse onto the same curve, characteristic of the spectrum for the single-spin 2CK model (dashed line). All systems in the LM phase ($\tilde{E}_\Delta > 0$) again collapse onto a single curve. A magnification of the low-frequency behaviour in the LM phase is shown in the inset, fitted to a line of the form $D \rho_2(\omega) = a / \ln^2(|\omega|/T_0)$ (circles). The transition itself is also shown ($\tilde{E}_\Delta = 0$), and plotted for comparison (dotted line) is Eq. 8.11.

where a magnification of the low- ω behaviour is shown. In the single-channel ferromagnetic Kondo model⁴, it is known [127] that this low- ω behaviour is described by $D \rho^{1CK}(\omega) \sim a / \ln^2(|\omega|/T_0)$, reflecting the slow approach to the single-channel LM FP characterized by marginally irrelevant logarithmic corrections [127, 134]. This is manifestly also the behaviour of the spectrum at $T = 0$ in the two-channel LM phase of the TQD model, and demonstrated explicitly by the agreement with the circles in the inset to Fig. 8.5.

Finally, we consider the case of the transition itself, $\tilde{E}_\Delta = 0$, where even at $T = 0$, the TFP describes the behaviour of the system. From the physical picture discussed above, the spectrum naturally follows from the Lehmann representation [8] as

$$D \rho_2^{TFP}(\omega) = \frac{2 \times D \rho_2^{LM}(\omega) + \sqrt{2} \times D \rho_2^{2CK}(\omega)}{2 + \sqrt{2}}, \quad (8.11)$$

where $D \rho_2^{LM}(\omega)$ and $D \rho_2^{2CK}(\omega)$ are the spectra obtained in the LM and 2CK phases of the model, and the $\sqrt{2}$ factor arises from the unusual degeneracy of the non-Fermi liquid 2CK state [49] (most obviously seen in the entropy at the 2CK FP, $S_{\text{imp}} = \frac{1}{2} \ln(2) \equiv \ln(\sqrt{2})$). From Eq. 8.11, we would expect $D \rho_{K,2}^{TFP}(\omega =$

⁴The single-channel ferromagnetic Kondo model is the low-energy effective model in the LM phase of a TQD with a single lead connected to dot 2, and has been studied in Ref. [64], where the same low- ω behaviour was shown to arise.

$0) = \frac{1}{2}(1 + \sqrt{2})^{-1} \approx 0.207$, which is indeed shown to be the case in Fig. 8.5. To confirm this picture, we also plot Eq. 8.11 explicitly, which reproduces the TFP spectrum essentially perfectly, as shown for comparison by the dotted line. The low- ω asymptotic behaviour is thus of the form:

$$D \rho_2^{TFP}(\omega) \stackrel{\frac{|\omega|}{T_K} \ll 1}{\sim} \frac{1}{2}(1 + \sqrt{2})^{-1} \times [1 - a(|\omega|/T_K)^{\frac{1}{2}}]. \quad (8.12)$$

We comment briefly that while the TFP spectrum is only obtained precisely *at* the transition for $T = 0$, it is also recovered at *higher* temperatures as we move away from the transition. Specifically, for $T_\Delta \ll T \ll T_K$, the $T^z = \pm \frac{1}{2}$ components are quasidegenerate, and so the spectrum should be essentially that of the TFP spectrum, Eq. 8.11 — and this has been confirmed directly using NRG. Thus, *warming* a system in the ferromagnetically coupled LM phase produces a revival of the antiferromagnetic 2CK effect.

8.4 Summary

In this Chapter, we have considered an alternative geometry for the TQD, in which both leads are connected to the same dot. Maintaining mirror symmetry necessitates coupling the leads to dot 2 (see Fig. 8.1). We showed in Sec. 8.1 that markedly different physics results for two distinct reasons. Firstly, the effective coupling between the lowest TQD state and the leads switches from being *ferromagnetic* to *antiferromagnetic* as J' is tuned. As different stable FPs arise in each case, a quantum phase transition must result. For $J' < J'_c$, the TQD decouples from the leads, with the LM FP being stable. Thus, this TQD system allows to study a novel variant of the single-channel ferromagnetic Kondo model, in which the lowest TQD doublet is now coupled to two leads by an effective ferromagnetic coupling. It is found that the approach to the FP is again characterized by marginally irrelevant logarithmic corrections, indicating that systems in this phase are also ‘singular’ Fermi liquids. By contrast, for $J' > J'_c$, the effective antiferromagnetic coupling destabilises the LM FP and the non-Fermi liquid 2CK ground state is formed on the lowest temperature/energy scales.

A transition is also found on varying J' in the TQD studied in Chapters 6 and 7, but the effective coupling is always antiferromagnetic, and so the transition occurs instead between two 2CK phases of distinct parity.

The second key difference is that a local $1 \leftrightarrow 3$ parity is conserved in this model, meaning that the transition can only be a strict level-crossing transition. This was confirmed directly from NRG by establishing that the scale vanishes *linearly* near the transition, $T_\Delta \propto |J'_c - J'|$. In addition, the nature of the TFP itself indicates a

level-crossing transition: the TFP is a simple combination of the stable FPs for each phase (and as confirmed from the NRG energy level structure at the TFP). Again, this is in stark contrast to the situation when leads are attached to dots 1 and 3 (see Chapters 6 and 7), because such models, only *overall* left $\leftrightarrow$ right parity is conserved, and it is found that the local $1 \leftrightarrow 3$ parity is in fact mixed at the transition, leading thereby to a genuine quantum critical point. The Kondo scale was in that case found to vanish quadratically as the transition is approached, $T_K \propto |J'_c - J'|^2$, indicating the non-trivial nature of the QPT.

Thus we have shown that geometry and symmetry play important roles in determining the nature of the underlying Kondo physics, and its subtle interplay with the internal degrees of freedom of quantum dot devices. Much of the behaviour which results can be in fact determined and understood from simple physical and perturbative scaling arguments, although the exact solution of these models can still only be achieved at present by NRG.

CHAPTER 9

Summary

In this thesis, we have studied systems of coupled quantum dots in a two-channel environment. The work is motivated in part by significant recent experimental developments, which now allow for the controlled construction of complex nanodevices comprising arrays of several dots. In particular, the interdot couplings, geometry and capacitance of such systems can be fine-tuned, allowing access to a diverse range of strongly correlated electron behaviour.

Coupled dot systems allow to study the competition between orbital and spin degrees of freedom in a nanodevice, and the effect this subtle interplay has on Kondo physics. While the classic single-channel spin- $\frac{1}{2}$ Kondo effect — in which a localized spin is fully screened by coupling to itinerant conduction electrons — has been known to occur in metals with magnetic impurities since the 1960s, and indeed in single quantum dots since the late 1990s, the possibility of generating fascinating variants with coupled quantum dots has led to a resurgence of interest in the field.

Various non-Fermi liquid phases and novel phase transitions have been much studied theoretically; in particular the two-channel Kondo (2CK) model, proposed by Nozières and Blandin, is a prime example where *overscreening* of a spin- $\frac{1}{2}$ object by coupling to *two* independent leads at low temperatures gives rise to a state that cannot be described simply in terms of non-interacting conduction electron quasiparticles, even at the Fermi level.

As discussed in Chapter 2, the 2CK effect is extremely delicate, being destabilised by charge-transfer between the leads and asymmetry in the couplings. But notwithstanding the considerable technical difficulties that result, Potok *et al* have recently demonstrated unambiguous 2CK physics (at least at finite temperatures).

In this thesis, we consider theoretically a range of different two-channel systems with strict suppression of interlead charge transfer. In Chapters 4 and 5, we consider the behaviour of chains of dots, with a metallic lead connected to each end; while in Chapters 6–8 we study rings of dots. Throughout, we have used physically motivated

arguments and perturbative techniques to obtain analytical results and low-energy effective models, which in turn allow the underlying physical behaviour to be simply understood. We have also employed numerical renormalization group (NRG) methods (which were introduced and extended to the present application in Chapter 3) to obtain essentially exact results for both thermodynamic and dynamical properties of the models.

We now summarize the key findings of the thesis.

In Chapters 4 and 5, we consider a general class of models in which a chain of N_c quantum dots is coupled to two leads (see Eq. 4.1 and Fig. 4.1). Specifically, we study a Heisenberg chain of *spins* (with an interdot exchange coupling J), where the terminal dots are each coupled to their own metallic lead (with $J_{K\alpha}$ the exchange coupling to lead $\alpha = L, R$).

In Chapter 4, we study chiefly the regime in which the interdot coupling is large — specifically $J > \max(J_{KL}, J_{KR})$. In this regime, a low-energy effective model can be derived perturbatively, in terms of which the underlying physical behaviour of chains of different length can be simply understood. We show in Sec. 4.1.2 that the higher lying chain eigenstates become thermally inaccessible at low temperatures $T \ll J$, and so only the ground chain state need be retained in order to describe the system on low temperature/energy scales. Since the lowest state of an odd-length chain is always a *doublet*, the low-energy effective model obtained by projecting onto this state is of 2CK form, as shown in Sec. 4.1. Thus, *all* odd chains are described by the same effective model, and so a universality in the low-temperature properties is expected. Indeed, the effective *antiferromagnetic* Kondo coupling that arises for any odd N_c implies that on the lowest energy scales, mirror-symmetric systems are ubiquitously described by the 2CK fixed point (FP).

This is confirmed by direct NRG calculations in Sec. 4.2, where both thermodynamic (Sec. 4.2.1) and dynamical (Sec. 4.2.2) properties of such systems are studied in detail. In all cases we find as expected that systems exhibit the characteristic $T = 0$ residual entropy $S_{\text{imp}} = \frac{1}{2} \ln(2)$, while below T_K , the uniform spin susceptibility is shown to diverge logarithmically: $\chi_{\text{imp}}(T) \sim \ln(T_K/T)$. Indeed, the universality arising on rescaling the thermodynamics in terms of the Kondo scale T_K is shown explicitly for odd chains — in particular demonstrating the collapse to the standard single-spin 2CK scaling curves.

The $T = 0$ scaling spectrum $D\rho^{N_c}(\omega)$ *vs.* ω/T_K is also determined for odd chains (see Sec. 4.2.2). Both the high- ω and low- ω asymptotic behaviour is established, as given in Eqs. 4.17 and 4.18. In all cases, at the Fermi level $\omega = 0$, the spectrum reaches *half* the unitarity limit, as consistent with work on the related two-channel models.

In Sec. 4.3, we go on to consider the case where the mirror symmetry is broken. The 2CK FP is known to be the critical point of the channel-anisotropic 2CK

model, so in general a strong-coupling Fermi-liquid state is formed on the lowest temperature/energy scales for the single-spin model. We show that the same behaviour results for all odd chains, and again demonstrate the universality arising in such systems on rescaling in terms of an effective *single*-channel Kondo scale. A transition between phases where the residual chain doublet state is fully screened by conduction electrons in either the left or the right leads is studied for odd chains, and a universal description of the low-temperature/energy behaviour of all such systems is developed.

By contrast, in the large interdot coupling limit, the lowest state of an even chain is a spin-*singlet* (see Sec. 4.1.1), which simply decouples from the rest of the system for $T \ll J$.

In Chapter 5, we turn to the case of small interdot coupling. It is found from NRG that for odd chains of any length, decreasing J for mirror-symmetric systems still results in inherently *two-channel* physics on the lowest energy/temperature scales. Physical arguments and perturbative scaling techniques were employed for the $N_c = 3$ trimer case in Sec. 5.1.1, and it was shown that for $J < T_K^{1CK}$ an effective 2CK model again results (with T_K^{1CK} the single-channel Kondo scale below which the spin of the terminal dots is quenched by their attached lead in the $J = 0$ limit).

Thus, for any finite antiferromagnetic interdot coupling, mirror-symmetric systems must be controlled by the 2CK FP on the lowest temperatures. This physical picture was tested directly with NRG in Sec. 5.1.2, where we confirmed the mapping of the full model for $N_c = 3, 5$ and 7 onto the effective 2CK model at low temperatures, examining both thermodynamics and dynamics in detail. Indeed, the variation of the underlying 2CK scale, T_K^{2CK} , as a function of J (derived from scaling arguments in Eq. 5.11) was tested and confirmed in Fig. 5.4.

In Sec. 5.2, we considered even chains with small interdot couplings, focusing initially on the 2IK model in the case where the mirror symmetry of the model is broken. The large and small J limits of the model clearly indicate the presence of a quantum phase transition in the model (and indeed for any even chain system). Applying similar arguments to those presented in Sec. 5.1, we derived an effective model (Eq. 5.16) to describe the transition in Sec. 5.2.1, and argued that the same effective model describes the transition of all even chains.

Since the effective model in the asymmetric 2IK model is a channel-anisotropic 2CK model, we show that the transition and the nature of the critical point can again be simply understood. The physical picture is confirmed using NRG for the full 2IK model, where we examine both thermodynamics (Fig. 5.7) and dynamics (Fig. 5.9) in detail. Specifically, we study the variation of the Kondo scale in the vicinity of the transition (Fig. 5.8), and confirm the analytic prediction of the critical coupling strength (Fig. 5.10).

In Chapters 4 and 5, we have thus comprehensively studied the behaviour of

chains of dots coupled to two leads, in all parameter regimes of interest. We used perturbative techniques and scaling arguments to derive low-energy effective models for such systems, which provided a clear physical picture of the expected low-temperature and low-energy behaviour. In all cases, we showed that the fundamental physics can be related to that of the single-spin 2CK model for odd chains, or the 2IK model for even chains. In the latter case, we also showed that the transition which occurs on tuning the interdot coupling can also be thought of in terms of an effective channel-anisotropic 2CK model.

The underlying universality that arises in all such systems comprising chains of dots coupled to two leads can be understood in terms of their common fixed point structure. Clear signatures of these FPs can be seen in both thermodynamics and dynamics calculated directly using NRG — and the energy scales corresponding to RG flow between them can be easily identified. However, we have tried to stress throughout this thesis that the fundamental physical behaviour of the full model can often be related to the behaviour of simpler low-energy effective models which can be derived perturbatively. The details of the full model then enter only through the *effective* parameters.

Markedly different physics is however accessible in ring structures, where the inherent magnetic frustration of such systems plays an important role. This was the focus of Chapters 6–8, where we showed that unusual phases and novel phase transitions result.

In Chapter 6 we studied what is arguably the simplest two-channel device in which to understand the consequences of local frustration arising from internal degrees of freedom: a triple quantum dot ring. We considered a system where the dots were mutually coupled by antiferromagnetic exchange interactions, but tunnel-coupled symmetrically to two metallic leads (see Fig. 6.1 and Eq. 6.1).

Two distinct 2CK phases arise in such a ring due to the mirror symmetry in the problem, with each displaying classic non-Fermi liquid properties of the 2CK FP, as found for the odd chains of dots. In particular, we studied the single-particle spectrum $\pi\Gamma D_1(\omega) \equiv \pi\Gamma D_3(\omega)$ of the dots tunnel-coupled to the leads in Sec. 6.2.2, and demonstrated universal scaling collapse to the spectrum of a single-spin 2CK model established in Sec. 3.6.3. At the Fermi level, we found at $T = 0$ that the spectrum reached *half* the unitarity limit, $\pi\Gamma D_1(0) = \frac{1}{2}$, yielding thereby a zero-bias conductance through the terminal dots of $G_c/G_0 = \frac{1}{2}$ (with $G_0 = 2e^2/h$ the conductance quantum).

The above behaviour is in fact anticipated from the low-energy effective 2CK model which we derived perturbatively for systems deep in either 2CK phase. But although 2CK physics predominates in the underlying parameter space, the parity-distinct nature of the phases means that a quantum phase transition between them must occur.

The 2CK phases were shown in Sec. 6.3 to be separated by a quantum critical point, for which an effective low-energy model was derived (Sec. 6.1.2). Precisely at the transition, parity mixing of the quasidegenerate local trimer states acts to destabilise the 2CK fixed points, and the critical fixed point is shown to consist of a free pseudospin together with effective *single-channel* spin quenching. At the transition, the system shares many properties with the channel-anisotropic 2CK model — and indeed the conventional spin- $\frac{1}{2}$ Anderson model. But the L/R mirror symmetry of the setup necessitates that the strong-coupling Kondo singlet *and* the set of weak-coupling free conduction band states form symmetrically in each channel. This gives rise to some unusual physical properties not accessible in systems where orbital effects arising from the internal degrees of freedom of the device are absent.

We showed in Sec. 6.3 that a residual $T = 0$ entropy $S_{\text{imp}} = \ln(2)$ characterizes the quantum critical point (corresponding to the free pseudospin), but that $\chi_{\text{imp}} \propto 1/T_K^{1CK}$ is also observed, and is indicative of single-channel spin quenching. Indeed, the spectrum $\pi\Gamma D_1(\omega = 0) = \frac{1}{2}$ at the transition, but the low-frequency asymptotics again show that the Kondo resonance is *not* characteristic of the 2CK spectrum, but rather is typical of the Fermi liquid behaviour of the single-channel Anderson model (with a halved amplitude).

Driven by varying the interdot exchange couplings, occurring at the point of inherent magnetic frustration, and characterised by a nontrivial quantum critical point, the transition thus provides a striking example of the subtle interplay between internal spin and orbital degrees of freedom in coupled quantum dot systems.

This work was extended in Chapter 7, where we went on to consider other odd rings of the same basic geometry (see Fig. 7.1 and Eq. 7.1), now focusing specifically on Heisenberg rings of *spins*.

We showed in Sec. 7.1.2 that the $N_c = 3$ spin ring must share common low-temperature/energy behaviour with the triple quantum dot tunnel-coupled to leads studied in Chapter 6, since the effective models for each are of the same form. While the effective parameters are shown to be somewhat different, the underlying physical behaviour and fixed point structure that results (see Secs. 7.2 and 7.3) is equivalent. Indeed, the same effective model also results for *all* odd rings, and so the same basic behaviour is expected — including the two 2CK phases of distinct parity and the transition between them. Both thermodynamic and dynamical properties of rings with $N_c = 3, 5, 7$ were studied directly with NRG, confirming this physical picture.

The behaviour of these systems arises fundamentally as a consequence of the geometry and symmetry of the setup, common to all rings studied in Chapters 6 and 7. In Chapter 8, we consider a different geometry for the TQD, and demonstrate that markedly different physical behaviour results. Fig. 8.1 and Eq. 8.1 describe a model in which two leads are attached at dot 2. Strict suppression of interlead charge transfer necessitates here that dot 2 is modelled as a spin, and we consider a setup

explicitly tuned to mirror symmetry, as with the ring systems studied previously.

We showed in Sec. 8.1 that markedly different physics must result in this system. While two parity-distinct phases again result, we demonstrate that the symmetry of the model means that this parity is now carried by the *local* trimer states alone. This results in a simple level-crossing transition, the nature of which is shown to be rather different from that considered previously. A low-energy effective model is developed to describe the transition, and it is found that the effective coupling between the ground trimer doublet and the two leads is *ferromagnetic* in one phase, but is *antiferromagnetic* in the other. Both are separately accessible on tuning the interdot couplings, and the transition FP is shown to comprise a simple combination of the two stable FPs of the model.

In the antiferromagnetically-coupled phase, the usual 2CK FP is stable, as demonstrated in both thermodynamic and dynamical properties of such systems at low temperatures/energies, which are naturally characteristic of the non-Fermi liquid 2CK ground state. By contrast, for an effective ferromagnetic coupling, the slow approach to the stable LM FP is characterized by leading irrelevant logarithmic corrections, as evidenced most clearly in the low-frequency behaviour of the spectrum. But at the Fermi level $\omega = 0$, the trimer is shown to be completely decoupled from the leads; meaning in particular that the phase is a ‘singular Fermi liquid’.

Near the transition, even in the LM phase, the antiferromagnetically-coupled trimer doublet may still undergo the 2CK effect, leading to an overscreened non-Fermi liquid state — even though it is not the ground state. On the lowest temperature scales, however, this many-body state must be destroyed and projected out, leaving a simple unscreened free spin on the decoupled trimer. Interestingly therefore, *warming* a system in the ferromagnetically-coupled LM phase gives rise to a revival of the antiferromagnetic 2CK effect.

The symmetry of the triple quantum dot ring studied in Chapter 8 implies that there is a strict separation of the Hilbert space of the problem. As such, the role of frustration in such systems is strikingly different from that studied in Chapters 6 and 7, where a genuine quantum critical point arises.

The results and analysis presented in Chapters 4–8 thus illustrate clearly that while non-trivial many-body Kondo physics only results on coupling a nanodevice to metallic leads, the underlying spin and orbital degrees of freedom of the *isolated* device — and the subtle interplay between the two which is governed by the geometry and symmetry of the setup — has a profound effect on the resulting physical behaviour. Specifically, we demonstrate that a wide range of strongly correlated electron behaviour arises when coupled dots are connected to two leads, with both non-Fermi liquid two-channel Kondo phases and novel phase transitions being accessible.

APPENDIX A

Permutation operators and symmetry

In this appendix we consider two symmetries which play an important role in two-channel coupled quantum dot systems: up/down spin symmetry and left/right mirror symmetry. Here we derive the explicit forms of operators which permute up $\leftrightarrow$ down spins or left $\leftrightarrow$ right sites, and which allow one to determine a definite *parity* for a given state.

A.1 Spin symmetry

We define first even (e) and odd (o) orbitals for a given site i , obtained by the canonical transformation

$$c_{i,e}^\dagger = \frac{1}{\sqrt{2}}(c_{i\uparrow}^\dagger + c_{i\downarrow}^\dagger), \quad (\text{A.1a})$$

$$c_{i,o}^\dagger = \frac{1}{\sqrt{2}}(c_{i\uparrow}^\dagger - c_{i\downarrow}^\dagger), \quad (\text{A.1b})$$

which preserves the usual fermionic anticommutation relations. Exchanging $\uparrow \leftrightarrow \downarrow$ spins clearly has no effect on $c_{i,e}^\dagger$, but by contrast $c_{i,o}^\dagger \leftrightarrow -c_{i,o}^\dagger$. With $\hat{n}_{i,o} = c_{i,o}^\dagger c_{i,o}$ the number operator for the odd-orbital, we define a parity operator

$$\hat{P}_{i,\uparrow\downarrow} = 1 - 2\hat{n}_{i,o}. \quad (\text{A.2})$$

$\hat{P}_{i,\uparrow\downarrow}$ is self-adjoint and involutory ($\hat{P}_{i,\uparrow\downarrow}^2 = 1$) and hence has eigenvalues ± 1 only. Specifically, it is clear from Eq. A.2 that $P_{i,\uparrow\downarrow} = +1$ for $n_{i,o} = 0$ but $P_{i,\uparrow\downarrow} = -1$ for $n_{i,o} = 1$. Combining Eqs. A.1 and A.2 it follows that

$$[\hat{P}_{i,\uparrow\downarrow}, c_{i,e}^\dagger] = 0, \quad (\text{A.3a})$$

$$\{\hat{P}_{i,\uparrow\downarrow}, c_{i,o}^\dagger\} = 0, \quad (\text{A.3b})$$

and hence using Eq. A.1 we obtain

$$\hat{P}_{i,\uparrow\downarrow} c_{i,\uparrow}^\dagger = c_{i,\downarrow}^\dagger \hat{P}_{i,\uparrow\downarrow}, \quad (\text{A.4a})$$

$$\hat{P}_{i,\uparrow\downarrow} c_{i,\downarrow}^\dagger = c_{i,\uparrow}^\dagger \hat{P}_{i,\uparrow\downarrow}, \quad (\text{A.4b})$$

showing that $\hat{P}_{i,\uparrow\downarrow}$ does indeed permute up and down spin labels. Using Eq. A.1 in Eq. A.4 it is straightforward to show that

$$\hat{P}_{i,\uparrow\downarrow} = \hat{S}_i^+ + \hat{S}_i^- + 1 - \hat{n}_i, \quad (\text{A.5})$$

where $\hat{S}_i^\pm$ is the spin raising/lowering operator for site i , and $\hat{n}_i = \hat{n}_{i\uparrow} + \hat{n}_{i\downarrow}$ is the total number operator (with $\hat{n}_{i\sigma} = c_{i\sigma}^\dagger c_{i\sigma}$ as usual).

For a system of *spins*, $\hat{n}_i = 1$ by construction, and the physically obvious result for the up/down spin permutation operator is then simply $\hat{P}_{i,\uparrow\downarrow} = \hat{S}_i^+ + \hat{S}_i^-$.

Hamiltonians with overall $SU(2)$ spin symmetry are invariant to exchanging all spins $\uparrow \leftrightarrow \downarrow$. The relevant permutation operator is thus one in which all ‘up’ and ‘down’ spins are swapped simultaneously:

$$\hat{P}_{\uparrow\downarrow} = \prod_i \hat{P}_{i,\uparrow\downarrow} \quad (\text{A.6})$$

for all sites i , and hence $[H, \hat{P}_{\uparrow\downarrow}] = 0$. States can of course be classified according to this spin parity, but as $\hat{P}_{\uparrow\downarrow}$ clearly does not commute with the operator $\hat{S}^z$ (describing the total z -component of the spin), states of H written as $|S^z, r\rangle$ cannot also be eigenstates of $\hat{P}_{\uparrow\downarrow}$. However, $\hat{P}_{\uparrow\downarrow}$ does commute with the total spin $\hat{\mathbf{S}}$, and so it can be shown from Eq. A.4 that

$$\hat{P}_{\uparrow\downarrow} |\mu; S, S^z, r\rangle = \mu |\mu; S, -S^z, r\rangle, \quad (\text{A.7})$$

where $\mu = \pm 1$ only, since $\hat{P}_{\uparrow\downarrow}^2 = 1$.

A.2 Mirror symmetry

A similar approach may be adopted to construct an operator $\hat{P}_{i,j}$ which permutes site labels i and j for an arbitrary pair of orbitals. Again, we transform canonically to an even and odd orbital basis, defined through

$$c_{e\sigma}^\dagger = \frac{1}{\sqrt{2}}(c_{i\sigma}^\dagger + c_{j\sigma}^\dagger), \quad (\text{A.8a})$$

$$c_{o\sigma}^\dagger = \frac{1}{\sqrt{2}}(c_{i\sigma}^\dagger - c_{j\sigma}^\dagger), \quad (\text{A.8b})$$

Exchanging the labels $i \leftrightarrow j$ clearly has no effect on $c_{e\sigma}^\dagger$, but $c_{o\sigma}^\dagger \leftrightarrow -c_{o\sigma}^\dagger$. With the total odd orbital number operator $\hat{n}_o = \hat{n}_{o\uparrow} + \hat{n}_{o\downarrow}$, and $\hat{n}_o = c_{o\sigma}^\dagger c_{o\sigma}$, we thus define

$$\hat{P}_{i,j} = 2(\hat{n}_o - 1)^2 - 1. \quad (\text{A.9})$$

$\hat{P}_{i,j}$ is again self-adjoint and involutory ($\hat{P}_{i,j}^2 = 1$ being readily confirmed), so that eigenvalues of it are ± 1 only, and we obtain $P_{i,j} = +1$ for $n_o = 0, 2$ but $P_{i,j} = -1$ for $n_o = 1$. Combining Eqs. A.8 and A.9 it follows that

$$[\hat{P}_{i,j}, c_{e\sigma}^\dagger] = 0, \quad (\text{A.10a})$$

$$\{\hat{P}_{i,j}, c_{o\sigma}^\dagger\} = 0, \quad (\text{A.10b})$$

and hence using Eq. A.8 we obtain

$$\hat{P}_{i,j} c_{i\sigma}^\dagger = c_{j\sigma}^\dagger \hat{P}_{i,j}, \quad (\text{A.11a})$$

$$\hat{P}_{i,j} c_{j\sigma}^\dagger = c_{i\sigma}^\dagger \hat{P}_{i,j}, \quad (\text{A.11b})$$

and so $\hat{P}_{i,j}$ does indeed permute the i and j labels. Using Eq. A.8 in Eq. A.9 it is then straightforward (if lengthy) to show that

$$\begin{aligned} \hat{P}_{i,j} = & 2(\hat{\mathbf{I}}_i \cdot \hat{\mathbf{I}}_j - \hat{\mathbf{S}}_i \cdot \hat{\mathbf{S}}_j) + \sum_{k=\{i,j\},\sigma} \frac{1}{2} \hat{n}_{k\sigma} (\hat{n}_{k\sigma} - 1) \\ & + \sum_{\sigma} (c_{i\sigma}^\dagger c_{j\sigma} + \text{H.c.}) (2 - \hat{n}_i - \hat{n}_j) + \frac{1}{2} \end{aligned} \quad (\text{A.12})$$

where $\hat{\mathbf{S}}_i$ is a spin- $\frac{1}{2}$ operator for site i , and $\hat{\mathbf{I}}_i$ is an isospin operator (with components $\hat{I}_i^z = \frac{1}{2}(\hat{n}_i - 1)$ and $\hat{I}_i^+ = c_{i\uparrow}^\dagger c_{i\downarrow}^\dagger$ and $\hat{I}_i^- = (\hat{I}_i^+)^\dagger$). It can then be shown that $\hat{P}_{i,j}$ commutes with the operators for the combined spin of sites i and j , $\hat{\mathbf{S}}_{ij}$ and the combined isospin $\hat{\mathbf{I}}_{ij}$ (as well as total $\hat{S}_{ij}^z$ and charge $\hat{Q}_{ij}$), but *not* the individual site operators $\hat{\mathbf{S}}_i$, $\hat{\mathbf{I}}_i$, $\hat{S}_i^z$ or $\hat{Q}_i$.

Eq. A.12 generalizes the result of Ref. [150], where an operator which permutes two spins was first derived. In the spin-only limit (where the sites are strictly singly-occupied: $\hat{n}_i = \hat{n}_j = 1$), the parity operator can be expressed concisely as [150] $\hat{P}_{i,j} = (1 - \hat{\mathbf{S}}_{13}^2)$, with $\hat{\mathbf{S}}_{13} = (\hat{\mathbf{S}}_1 + \hat{\mathbf{S}}_3)$ the combined spin of the two dots to be permuted.

If a Hamiltonian is invariant to the permutation $i \leftrightarrow j$, then $[H, \hat{P}_{i,j}] = 0$, parity is conserved and all states can thus be classified according to it. For example, in the (mirror symmetric) single-spin 2CK model (Eq. 2.24), the overall $L \leftrightarrow R$ symmetry of the model implies that the relevant permutation operator exchanges L and R labels of the leads:

$$\hat{P}_{L,R} = \prod_{\mathbf{k}} \hat{P}_{L\mathbf{k},R\mathbf{k}} \quad (\text{A.13})$$

which clearly yields the result $[H_{2CK}, \hat{P}_{L,R}] = 0$. All states of H_{2CK} can thus be labelled by their parity under L/R exchange. Indeed, as the parity operator $\hat{P}_{L,R}$ commutes with the operator $\hat{S}^z$ (which describes the total z -component of the spin; see Eq. A.12), we can write $\hat{P}_{L,R}|\gamma; S^z, r\rangle = \gamma|\gamma; S^z, r\rangle$, with $\gamma = \pm 1$ the parity of the state.

APPENDIX B

Effective models for frustrated systems

In this Appendix, we describe the transformations which cast the effective Hamiltonian for odd rings in terms of spin- $\frac{1}{2}$ operators for real spin $\hat{\mathbf{S}}$ and pseudospin $\hat{\mathcal{T}}$ for the local ring Hilbert space.

For the $N_c = 3$ TQD case, the simple form of the ring states means that straightforward (if extremely lengthy) algebra yields directly the desired result, Eq. B.13 below. However, it is in fact not necessary to know the explicit form of the states (which can only be obtained by numerical diagonalization for larger rings): manipulations can still be performed on a generalized effective Hamiltonian by exploiting the mirror symmetry and $SU(2)$ spin symmetry of the problem.

In Sec. 7.1.1 we showed that for any (odd) N_c , the lowest states of an isolated ring are a pair of doublets, which have different parity under $\hat{P}_{\text{ring}}^{N_c}$ (see Eq. 7.3). As this structure is common to all rings, in the following we will drop the index “ N_c ” for notational convenience.

Our starting point is Eq. 7.15 (which is equivalent to Eq. 6.10 for the TQD studied in Chapter 6):

$$\begin{aligned}
 H_{\text{eff}}^{\text{trans}} = \sum_{\gamma=\pm} \frac{1}{2} J_K [& \hat{1}_{\gamma} (\hat{\mathbf{S}}_1 + \hat{\mathbf{S}}_{N_c}) \hat{1}_{\gamma} \cdot (\hat{\mathbf{s}}_{L0} + \hat{\mathbf{s}}_{R0}) \\
 & + \hat{1}_{\gamma} (\hat{\mathbf{S}}_1 - \hat{\mathbf{S}}_{N_c}) \hat{1}_{-\gamma} \cdot (\hat{\mathbf{s}}_{L0} - \hat{\mathbf{s}}_{R0})] \\
 & + \hat{1}_{\gamma} E_{\gamma},
 \end{aligned} \tag{B.1}$$

where $\hat{1}_{\gamma} = \sum_{S^z} |\gamma; S^z\rangle \langle \gamma; S^z|$ is the unity operator for the appropriate doublet $\gamma = +/ -$. We now wish to cast Eq. B.1 in terms of spin and pseudospin operators

with the following components:

$$\hat{S}^z = \sum_{\gamma=\pm, S^z} |\gamma; S^z\rangle S^z \langle \gamma; S^z|, \quad (\text{B.2a})$$

$$\hat{T}^z = \sum_{\gamma=\pm, S^z} |\gamma; S^z\rangle \frac{1}{2} \gamma \langle \gamma; S^z|, \quad (\text{B.2b})$$

and

$$\hat{S}^\pm = \sum_{\gamma} |\gamma; \pm \frac{1}{2}\rangle \langle \gamma; \mp \frac{1}{2}|, \quad (\text{B.3a})$$

$$\hat{T}^\pm = \sum_{S^z} |\pm; S^z\rangle \langle \mp; S^z|. \quad (\text{B.3b})$$

The lowest ring states $|\gamma; S^z\rangle$ are each eigenstates of $\hat{S}^z$ and $\hat{T}^z$; in particular, the eigenvalues of $\hat{T}^z \equiv \frac{1}{2}(\hat{1}_+ - \hat{1}_-)$ correspond simply to (half) the parity of the appropriate doublet. By contrast, the doublets are interconverted by $\hat{T}^\pm$ (Eq. B.3b), such that $\hat{T}^\pm |\mp; S^z\rangle = |\pm; S^z\rangle$ acts to switch the parity of the lowest ring states, but $\hat{T}^\pm |\pm; S^z\rangle = 0$.

The last term of Eq. B.1 is the simplest to deal with. We note that

$$\begin{aligned} \hat{1}_+ E_+ + \hat{1}_- E_- &\equiv \frac{1}{2}(\hat{1}_+ - \hat{1}_-)(E_+ - E_-) + \frac{1}{2}(\hat{1}_+ + \hat{1}_-)(E_+ + E_-) \\ &= E_\Delta \hat{T}^z + \frac{1}{2} \hat{1}(E_+ + E_-). \end{aligned} \quad (\text{B.4})$$

This term is thus equivalent to a magnetic field acting on the pseudospin (and we can neglect the term $\hat{1}(E_+ + E_-)$, which is constant for a given J and J').

To cast the first line of Eq. B.1 in terms of $\hat{\mathbf{S}}$ and $\hat{\mathbf{T}}$ operators however, it is necessary to show that $\hat{1}_\gamma \hat{\mathbf{S}}_i \hat{1}_\gamma \propto \hat{\mathbf{S}}_\gamma$. To that end, we consider first the z -component:

$$\hat{1}_\gamma (\hat{S}_i^z) \hat{1}_\gamma = \sum_{S^z} |\gamma; S^z\rangle \langle \gamma; S^z| \hat{S}_i^z |\gamma; S^z\rangle \langle \gamma; S^z|. \quad (\text{B.5})$$

Now, Eq. B.5 is proportional to the operator $\hat{S}_\gamma^z = \sum_{S^z} |\gamma; S^z\rangle S^z \langle \gamma; S^z|$ only if $\langle \gamma; S^z | \hat{S}_i^z | \gamma; S^z \rangle \propto S^z$.

The same issue arises in recasting the second line of Eq. B.1 in terms of spin and pseudospin operators. Again considering the z -components, terms of the following type arise:

$$\sum_{S^z} |\gamma; S^z\rangle \langle \gamma; S^z| \hat{S}_i^z |-\gamma; S^z\rangle \langle -\gamma; S^z| \equiv \sum_{S^z} (\hat{T}^+ + \hat{T}^-) |-\gamma; S^z\rangle \langle \gamma; S^z| \hat{S}_i^z |-\gamma; S^z\rangle \langle -\gamma; S^z|. \quad (\text{B.6})$$

Again, the right hand side is proportional to $(\hat{T}^+ + \hat{T}^-) \hat{S}_\gamma^z$ only if the matrix element $\langle \gamma; S^z | \hat{S}_i^z | -\gamma; S^z \rangle \propto S^z$. We thus consider the generalized case of $\langle \gamma; S^z | \hat{S}_i^z | \gamma'; S^z \rangle$

In fact, such elements are *always* proportional to S^z due to the $SU(2)$ spin symmetry of the model. This can be most easily shown by expressing the states $|\gamma; S^z\rangle$ in terms of Clebsch-Gordon coefficients [153].

We shall take here a concrete example of the $N_c = 3$ TQD, but note that the following is straightforwardly extensible for any N_c . We consider the vector-coupling of the spin on dot 2 to the combined spin of dots 1 and 3, viz:

$$|S_{13}; S, S^z\rangle = \sum_{S_1^z, S_2^z, S_3^z} C_{\frac{1}{2}, S_2^z, S_{13}, \mu}^{S, S^z} C_{\frac{1}{2}, S_1^z, \frac{1}{2}, S_3^z}^{S_{13}, \mu} |S_1^z, S_2^z, S_3^z\rangle, \quad (\text{B.7})$$

where $C_{j_1, m_1, j_2, m_2}^{J, M} \equiv \langle j_1, j_2, m_1, m_2 | J, M \rangle$ are the standard Clebsch-Gordon coefficients, and for the lowest TQD doublets (so $S = \frac{1}{2}$), $S_{13} = 0$ corresponds to the $\gamma = +$ state while $S_{13} = 1$ corresponds to $\gamma = -$ (see Sec. 6.1.1 and Eq. 6.2).

Thus the elements we wish to consider may be written as

$$\begin{aligned} \langle S'_{13}; S^z | \hat{S}_i^z | S_{13}; S^z \rangle &= \sum_{\substack{S_1^z, S_2^z, S_3^z \\ \mu, \mu'}} (\hat{S}_i^z) C_{\frac{1}{2}, S_2^z, S'_{13}, \mu'}^{\frac{1}{2}, S^z} C_{\frac{1}{2}, S_1^z, \frac{1}{2}, S_3^z}^{S'_{13}, \mu'} C_{\frac{1}{2}, S_2^z, S_{13}, \mu}^{\frac{1}{2}, S^z} C_{\frac{1}{2}, S_1^z, \frac{1}{2}, S_3^z}^{S_{13}, \mu} \\ &= \sum_{\substack{S_1^z, S_2^z, S_3^z \\ \mu, \mu'}} (\hat{S}_i^z) C_{\frac{1}{2}, -S_2^z, S'_{13}, -\mu'}^{\frac{1}{2}, -S^z} C_{\frac{1}{2}, -S_1^z, \frac{1}{2}, -S_3^z}^{S'_{13}, -\mu'} C_{\frac{1}{2}, -S_2^z, S_{13}, -\mu}^{\frac{1}{2}, -S^z} C_{\frac{1}{2}, -S_1^z, \frac{1}{2}, -S_3^z}^{S_{13}, -\mu} \\ &= \sum_{\substack{S_1^z, S_2^z, S_3^z \\ \mu, \mu'}} (-\hat{S}_i^z) C_{\frac{1}{2}, S_2^z, S'_{13}, \mu'}^{\frac{1}{2}, -S^z} C_{\frac{1}{2}, S_1^z, \frac{1}{2}, S_3^z}^{S'_{13}, \mu'} C_{\frac{1}{2}, S_2^z, S_{13}, \mu}^{\frac{1}{2}, -S^z} C_{\frac{1}{2}, S_1^z, \frac{1}{2}, S_3^z}^{S_{13}, \mu} \\ &= -\langle S'_{13}; -S^z | \hat{S}_i^z | S_{13}; -S^z \rangle, \end{aligned} \quad (\text{B.8})$$

where we have used the general property of the Clebsch-Gordon coefficients [153] that $C_{j_1, m_1, j_2, m_2}^{J, M} = (-1)^{j_1+j_2-J} C_{j_1, -m_1, j_2, -m_2}^{J, -M}$ and note that the phase factors cancel in Eq. B.8 when each dot is a spin- $\frac{1}{2}$ object.

While Eq. B.8 has been derived for $N_c = 3$, the result holds for any N_c , and so the arguments below are quite general.

As the lowest state of a ring, $|\gamma; S^z\rangle$, is always a *doublet* state, Eq. B.8 implies that $\langle \gamma; S^z | \gamma \hat{S}_1^z + \gamma' \hat{S}_{N_c}^z | \gamma'; S^z \rangle \propto S^z$. Indeed, in the absence of a magnetic field, the z -direction of the spin is completely arbitrary, and so it follows [153] that

$$\begin{aligned} \hat{1}_\gamma (\hat{\mathbf{S}}_1 + \hat{\mathbf{S}}_{N_c}) \hat{1}_\gamma &= \sum_{S^z, S^{z'}} |\gamma; S^z\rangle \langle \gamma; S^z | \hat{\mathbf{S}}_1 + \hat{\mathbf{S}}_{N_c} | \gamma; S^{z'} \rangle \langle \gamma; S^{z'} | \\ &= 2 \langle \gamma; \frac{1}{2} | \hat{S}_1^z + \hat{S}_{N_c}^z | \gamma; \frac{1}{2} \rangle \hat{\mathbf{S}}_\gamma, \end{aligned} \quad (\text{B.9})$$

and

$$\begin{aligned}\hat{1}_\gamma(\hat{\mathbf{S}}_1 - \hat{\mathbf{S}}_{N_c})\hat{1}_{-\gamma} &= \sum_{S^z, S^{z'}} (\hat{T}^+ + \hat{T}^-)|-\gamma; S^z\rangle\langle\gamma; S^z|\hat{\mathbf{S}}_1 - \hat{\mathbf{S}}_{N_c}|-\gamma; S^{z'}\rangle\langle-\gamma; S^{z'}| \\ &= 2\langle\gamma; \tfrac{1}{2}|\hat{S}_1^z - \hat{S}_{N_c}^z|-\gamma; \tfrac{1}{2}\rangle(\hat{T}^+ + \hat{T}^-)\hat{\mathbf{S}}_{-\gamma}.\end{aligned}\quad (\text{B.10})$$

Using Eqs. B.9 and B.10 together with Eq. B.4 in the effective Hamiltonian Eq. B.1, we now obtain

$$\begin{aligned}H_{\text{eff}}^{\text{trans}} &= \sum_{\gamma=\pm} J_K [\langle\gamma; \tfrac{1}{2}|\hat{S}_1^z + \hat{S}_{N_c}^z|\gamma; \tfrac{1}{2}\rangle\hat{\mathbf{S}}_\gamma \cdot (\hat{\mathbf{s}}_{L0} + \hat{\mathbf{s}}_{R0}) \\ &\quad + \langle\gamma; \tfrac{1}{2}|\hat{S}_1^z - \hat{S}_{N_c}^z|-\gamma; \tfrac{1}{2}\rangle(\hat{T}^+ + \hat{T}^-)\hat{\mathbf{S}}_{-\gamma} \cdot (\hat{\mathbf{s}}_{L0} - \hat{\mathbf{s}}_{R0})] \\ &\quad + \hat{T}^z E_\Delta.\end{aligned}\quad (\text{B.11})$$

We define the effective couplings (to first order) as

$$J_{K\gamma} = \langle\gamma; \tfrac{1}{2}|\hat{S}_1^z + \hat{S}_{N_c}^z|\gamma; \tfrac{1}{2}\rangle J_K \quad (\text{B.12a})$$

$$J_{\text{mix}} = \langle\gamma; \tfrac{1}{2}|\hat{S}_1^z - \hat{S}_{N_c}^z|-\gamma; \tfrac{1}{2}\rangle J_K \equiv \langle-\gamma; \tfrac{1}{2}|\hat{S}_1^z - \hat{S}_{N_c}^z|\gamma; \tfrac{1}{2}\rangle J_K, \quad (\text{B.12b})$$

and note that $\sum_{\gamma=\pm} J_{K\gamma}\hat{\mathbf{S}}_\gamma = \sum_{\gamma=\pm} \left[\tfrac{1}{2}(J_{K+} + J_{K-}) + (J_{K+} - J_{K-})\hat{T}^z \right] \hat{\mathbf{S}}_\gamma$.

Finally we use $\hat{\mathbf{S}} = \sum_\gamma \hat{\mathbf{S}}_\gamma$ (which follows from the definition of real spin in Eq. B.2 and B.3) to write the effective Hamiltonian in the vicinity of the transition purely in terms of spin and pseudospin operators,

$$\begin{aligned}H_{\text{eff}}^{\text{trans}} &= (\tfrac{1}{2}J_A + J_B\hat{T}^z)\hat{\mathbf{S}} \cdot (\hat{\mathbf{s}}_{L0} + \hat{\mathbf{s}}_{R0}) \\ &\quad + J_{\text{mix}}(\hat{T}^+ + \hat{T}^-)\hat{\mathbf{S}} \cdot (\hat{\mathbf{s}}_{L0} - \hat{\mathbf{s}}_{R0}) \\ &\quad + E_\Delta\hat{T}^z,\end{aligned}\quad (\text{B.13})$$

with

$$J_A = (J_{K+} + J_{K-}) \quad J_B = (J_{K+} - J_{K-}) \quad (\text{B.14})$$

which is precisely Eq. 6.13 in Chapter 6 or Eq. 7.18 in Chapter 7.

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