

# Engineering quantum states of fermionic many-body systems



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# Abstract

Controlling and stabilising collective phases of many-body quantum systems is a problem of deep fundamental and technological interest. In this thesis, we perform a theoretical investigation on how useful quantum phases may be engineered in strongly correlated fermionic lattice systems, especially through periodic driving.

We first compute the phase diagram of the one-dimensional  $t$ - $J$  model with the addition of non-standard pair hopping terms. We show that at dilute fillings these terms enhance superconductivity while, counter-intuitively, suppressing it at large fillings. We argue that this is due to dynamical constraints originating from the fact that local pairs cannot overlap. We conjecture that these constraints may play a more significant role in the physics of two-dimensional systems where the  $t$ - $J$  model is studied as a candidate model of high- $T_c$  superconductivity. We begin to investigate these dynamical constraints on a ladder geometry.

We then study the fermionic Hubbard model under periodic driving. We show that the driving induces a strong and robust singlet-pairing effect consistent with a superconducting state. This could provide a new mechanism for light-induced superconductivity in some classes of strongly correlated materials. We show using Floquet theory that the dynamics of the driven Hubbard model are described precisely by the  $t$ - $J$  model studied in the previous section. As the driven Hubbard model is also implementable with ultracold fermions in an optical lattice, our results could lead to their use as a quantum simulator for a broad class of candidate models for high- $T_c$  superconductivity.

# Contents

|          |                                                                   |           |
|----------|-------------------------------------------------------------------|-----------|
| <b>1</b> | <b>Introduction</b>                                               | <b>1</b>  |
| 1.1      | Structure of the thesis . . . . .                                 | 4         |
| 1.2      | Publications . . . . .                                            | 5         |
| <b>2</b> | <b>Model fermionic Hamiltonians</b>                               | <b>6</b>  |
| 2.1      | Non-interacting particles . . . . .                               | 6         |
| 2.1.1    | Wannier states . . . . .                                          | 8         |
| 2.2      | The Hubbard model . . . . .                                       | 9         |
| 2.2.1    | As a description of quantum materials . . . . .                   | 10        |
| 2.2.2    | As a description of ultracold atoms in optical lattices . . . . . | 12        |
| 2.2.3    | Discussion . . . . .                                              | 13        |
| 2.3      | Large $U$ limit and the $t$ - $J$ model . . . . .                 | 14        |
| 2.4      | Conclusions . . . . .                                             | 20        |
| <b>3</b> | <b>Tensor Network Theory</b>                                      | <b>21</b> |
| 3.1      | Introduction . . . . .                                            | 21        |
| 3.2      | Tensor algebra notation . . . . .                                 | 23        |
| 3.3      | The Schmidt decomposition . . . . .                               | 25        |
| 3.4      | Matrix Product States . . . . .                                   | 27        |
| 3.4.1    | Canonical forms . . . . .                                         | 29        |
| 3.5      | Expectation values . . . . .                                      | 31        |
| 3.6      | Matrix Product Operators . . . . .                                | 34        |
| 3.6.1    | Applying an MPO to an MPS . . . . .                               | 36        |
| 3.6.2    | Expectation values . . . . .                                      | 37        |
| 3.6.3    | Constructing MPOs . . . . .                                       | 38        |
| 3.6.4    | Addition and compression of MPOs . . . . .                        | 44        |
| 3.7      | Ground state calculations with MPS . . . . .                      | 46        |
| 3.8      | Time evolving block decimation . . . . .                          | 50        |

|          |                                                                                      |            |
|----------|--------------------------------------------------------------------------------------|------------|
| 3.9      | Infinite TEBD . . . . .                                                              | 53         |
| 3.9.1    | Computing ground states with iTEBD . . . . .                                         | 55         |
| 3.9.2    | Canonical Form for iMPS . . . . .                                                    | 56         |
| 3.10     | $U(1)$ symmetry and charge conservation . . . . .                                    | 59         |
| 3.11     | Mixed state evolution with MPOs . . . . .                                            | 61         |
| 3.11.1   | Time evolution of density operators . . . . .                                        | 62         |
| 3.12     | Conclusions . . . . .                                                                | 63         |
| <b>4</b> | <b>The phase diagram of the <math>t</math>-<math>J</math> model in one dimension</b> | <b>66</b>  |
| 4.1      | The $t$ - $J$ model . . . . .                                                        | 68         |
| 4.2      | Phase diagram . . . . .                                                              | 69         |
| 4.2.1    | Phase-separated region . . . . .                                                     | 72         |
| 4.2.2    | Superconducting region . . . . .                                                     | 74         |
| 4.2.3    | Spin-gapped region . . . . .                                                         | 75         |
| 4.2.4    | Magnetic Correlations . . . . .                                                      | 76         |
| 4.3      | Effective Bosonic Model . . . . .                                                    | 78         |
| 4.4      | Discussion . . . . .                                                                 | 83         |
| 4.5      | $t$ - $J$ - $\alpha$ Ladder systems . . . . .                                        | 84         |
| 4.5.1    | Ladder Hamiltonians . . . . .                                                        | 85         |
| 4.5.2    | Results . . . . .                                                                    | 87         |
| 4.6      | Conclusions and outlook . . . . .                                                    | 91         |
| <b>5</b> | <b>Periodically driven systems and Floquet theory</b>                                | <b>93</b>  |
| 5.1      | Floquet theory for the Schrödinger equation . . . . .                                | 95         |
| 5.1.1    | Analogy with Bloch's theorem . . . . .                                               | 96         |
| 5.1.2    | Example: Driven two-level atom . . . . .                                             | 98         |
| 5.2      | Effective Hamiltonians . . . . .                                                     | 101        |
| 5.2.1    | Example: Driven single-band model . . . . .                                          | 104        |
| 5.3      | Floquet Heating . . . . .                                                            | 107        |
| 5.4      | Conclusions . . . . .                                                                | 110        |
| <b>6</b> | <b>Enhanced superexchange pairing in the periodically driven Hubbard model</b>       | <b>112</b> |
| 6.1      | The driven Hubbard model . . . . .                                                   | 115        |
| 6.1.1    | Quasienergy spectrum . . . . .                                                       | 116        |
| 6.2      | Driving enhanced fermion pairing . . . . .                                           | 118        |
| 6.2.1    | Zero temperature . . . . .                                                           | 118        |

|          |                                                                                                              |            |
|----------|--------------------------------------------------------------------------------------------------------------|------------|
| 6.2.2    | Finite temperature . . . . .                                                                                 | 123        |
| 6.3      | Effective $t$ - $J$ model . . . . .                                                                          | 125        |
| 6.3.1    | Floquet analysis . . . . .                                                                                   | 126        |
| 6.3.2    | Comparison to the $t$ - $J$ - $\alpha$ model . . . . .                                                       | 132        |
| 6.3.3    | Floquet heating . . . . .                                                                                    | 133        |
| 6.4      | Conclusions . . . . .                                                                                        | 136        |
| <b>7</b> | <b>Conclusions and outlook</b>                                                                               | <b>137</b> |
| <b>A</b> | <b>Jordan–Wigner transformation</b>                                                                          | <b>140</b> |
| <b>B</b> | <b>Automatic construction of MPOs</b>                                                                        | <b>142</b> |
| <b>C</b> | <b>Details of DMRG Calculations in Chapter 4</b>                                                             | <b>146</b> |
| <b>D</b> | <b>Additional details and calculations for Chapter 6</b>                                                     | <b>149</b> |
| D.1      | Calculation of the quasienergy matrix for general sublattice driving .                                       | 149        |
| D.2      | Details of numerical calculations . . . . .                                                                  | 152        |
| <b>E</b> | <b>Floquet engineering the <math>t</math>-<math>J</math>-<math>\alpha</math> model in an optical lattice</b> | <b>155</b> |
| E.1      | The driving term . . . . .                                                                                   | 155        |
| E.2      | Engineering the $t$ - $J$ - $\alpha$ model . . . . .                                                         | 156        |
|          | <b>Bibliography</b>                                                                                          | <b>161</b> |

# Chapter 1

## Introduction

The ability to control, switch and stabilise states of physical systems underpins almost all modern technology. At the time of writing, the CPU in an iPhone contains  $\sim 4.8$  billion transistors, whose state must switch  $\sim 2.4$  billion times per second to perform computations [1]. Similarly, for these devices to practically store data, the physical state of their internal flash memory must be stable over many years [2]. In the near future, quantum technologies will require quantum states of systems comprised of large numbers of interacting subsystems to be controlled, switched and stabilised on similarly rapid timescales.

Within this extremely broad goal, the ability to dynamically modify the quantum phases of such many-body systems is attracting significant interest. At low temperatures, the collective macroscopic properties of many-body quantum systems, such as their conductivity or magnetic susceptibility, often depends delicately on the microscopic details the Hamiltonian [3]. Dynamically modifying these microscopic details through external driving, and studying the ensuing changes in the macroscopic properties of the system is thus of great technological, as well as fundamental interest. The overarching goal of this thesis is to theoretically explore how one can dynamically control and switch the phases of fermionic many-body systems by external driving.

Striking examples of this have been discovered in the domain of so-called strongly correlated materials, that is, solid state systems where quantum effects and strong electron-electron interactions are important. In this setting, THz laser pulses are emerging as a promising tool to control and probe phases of matter. In experiments, a single low-energy degree of freedom is targeted with a femtosecond THz laser pulse. Rather than heating the system, a drastic change in the material's properties can result. These include insulator to metal transitions [4], or magnetic ordering [5], but

perhaps most excitingly, can result superconducting-like states out of equilibrium, at temperatures well above the material's equilibrium critical temperature [6, 7, 8, 9].

Since the discovery of high temperature superconductors in 1986 [10], there has been intense effort to discover a material which superconducts at room temperature. These attempts have, so far, proven unsuccessful. This failure is in-part due to the lack of an agreed-upon theory which both explains the phenomenon, and has predictive power which can inform materials engineering efforts. The ultimate goal would be a microscopic Hamiltonian which can be shown to have the phase diagram of high- $T_c$  superconductors, including the superconducting, antiferromagnetic insulator, metallic and pseudogap phases [11]. These problems carry over to light-induced superconductivity, although by now, many theories have been proposed to explain this effect, for example in Refs. [12, 13, 14, 15, 16].

The lack of a complete theory high- $T_c$  superconductivity is partly due to a fact that the candidate many-body Hamiltonians which are conjectured to explain it are extremely difficult to solve [17], as well as the fact that experimentally accessible signatures of superconductivity are often difficult to calculate, and vice-versa. High- $T_c$  superconductors often have the structure of two-dimensional sheets which are weakly coupled together, and so the relevant geometry for a microscopic model is two-dimensional [18]. This presents a formidable theoretical problem, since this dimensionality is too low to fully justify mean-field theory [19], while the most powerful numerical methods are most effective in one dimension [20].

A promising tool to assist in tackling these problems is quantum simulation [21]. The core idea of quantum simulation is as follows. We have a physical system we would like to understand (i.e. a high- $T_c$  superconductor), whose microscopic Hamiltonian is unknown to us. We also have some candidate Hamiltonians which are conjectured to explain the properties of this system, but we are unable to theoretically predict relevant experimental properties from these. One solution is to take a different physical system, over which you have a large degree of control, and can verifiably implement a desired Hamiltonian to a good approximation. Then, one can make measurements on this physical system and extract relevant properties of the Hamiltonian. Finally, by comparing to the original physical system of interest, one sees how well the simulated Hamiltonian describes the actual system [22]. Ultracold atoms in optical lattices, owing to their strong isolation from the environment and highly tuneable system parameters, are by now one of the most developed platforms for performing quantum simulations of strongly-correlated lattice models [23, 24].

One such lattice model is the Hubbard model [25, 26, 27], a single-band model of fermions with a nearest-neighbour tunneling  $t$  and an on-site repulsion  $U$ . We will demonstrate in Chapter 2 that in the strongly correlated limit  $t \ll U$ , this model reduces to the  $t$ - $J$  model, which is one of the aforementioned candidate models of high- $T_c$  superconductivity. We shall see that the  $t$ - $J$  model captures the physics of a single-particle tunnelling  $t$ , and a local singlet-pairing interaction  $J = t^2/U \ll t$ .

In this thesis we make theoretical contributions on two fronts. The first front is related to light-induced superconductivity in solid state systems. We show in the latter part of this thesis that applying strong periodic driving to a minimal model of a strongly correlated material with a metallic ground state leads to a strong enhancement of singlet pairing, consistent with a superconducting state. We furthermore demonstrate that this effect is resistant to heating and robust to a changes in several experimentally relevant parameters. This constitutes a new mechanism by which light-induced superconductivity may be realised in some classes of strongly correlated materials. Specifically, we study a periodically driven Fermi-Hubbard model and show that this pairing enhancement is explained by the fact that the driven model's dynamics are approximately described by precisely the  $t$ - $J$  Hamiltonian. In particular, driving allows us to break the usual perturbative relation between  $t$  and  $J$  and enter the regime  $J \gtrsim t$ .

In anticipation of this result, in the first part of this thesis we explore the ground-state phase diagram of the  $t$ - $J$  model in one dimension including the parameter regime  $J \gtrsim t$ . Additionally, we include pair-hopping terms which are usually ignored, but are crucial for accurately describing the driven Hubbard model. We show that the pair-hopping imposes constraints which, in one dimension, counterintuitively inhibits superconductivity at large fillings. We conjecture that these constraints might play a more significant role in two dimensions, i.e. the relevant geometry for high- $T_c$  superconductivity. We take some first steps to exploring the role of these constraints in higher dimensions with a study of two-leg ladder systems, finding that weakly coupled chains favour superconducting pair correlations, while strongly coupled chains suppress them.

The second front is related to quantum simulation of high- $T_c$  superconductivity. Specifically, as the driven Hubbard model we study is equally applicable to ultracold fermions in a shaken optical lattice, this means that one can directly implement the  $t$ - $J$  model and control its parameters in this setting. We also show that the pair-hopping can be controlled depending on how the driving is implemented. This allows a large degree of control of the Hamiltonian's parameters, and therefore opens a path

to studying a wider class of candidate models for high- $T_c$  superconductivity in an optical lattice-based quantum simulator.

## 1.1 Structure of the thesis

In Chapter 2, we introduce the microscopic models which we study in this thesis. In particular, we motivate the Hubbard model as a model of both strongly correlated electron systems, and of ultracold fermions in an optical lattice. We then demonstrate that it reduces to the  $t$ - $J$  model in the limit of strong interactions.

In Chapter 3, we introduce numerical methods based on tensor network theory, which are the backbone of the calculations contained within this thesis. We will see that although exact classical simulation of arbitrary quantum systems is indeed exponentially hard, for a wide class of quantum states of interest, we can perform classical simulations of them with only polynomial resources. While this is important for understanding how the numerical results in Chapters 4 and 6 are obtained, this is not crucial for the discussion of the physics, and may be skipped on a first reading.

In Chapter 4, we use the tensor network methods introduced in the previous chapter to compute the phase diagram of the  $t$ - $J$  model including the pair-hopping terms which are usually neglected. We explore in detail the new physics induced by these terms, and begin to investigate their role in higher dimensions by studying ladder systems.

In Chapter 5, we provide background on Floquet theory, specifically Floquet engineering of many-body quantum systems. We explain how periodically driven Hamiltonians may be described by effective static Hamiltonians, whose properties are drastically different from the equilibrium Hamiltonians. We also discuss, in general terms, the heating that occurs in many-body interacting systems.

In Chapter 6, we study the Hubbard model under in-gap periodic driving. We show that this periodic driving leads to a large increase in pairing in the system consistent with a superconducting state, and use Floquet theory to show that the driven system is described by the  $t$ - $J$  model studied in Chapter 4, where now the driving amplitude can be used to control the ratio  $J/t$ , and thus explore the phase diagram we obtained there.

Finally, in Chapter 7, we summarise again our results and suggest possibilities for future avenues of research.

## 1.2 Publications

Some of the results presented in this thesis were published as

1. J.R. Coulthard, S.R. Clark, S. Al-Assam, A. Cavalleri and D. Jaksch. Enhancement of superexchange pairing in the periodically driven Hubbard model. *Phys. Rev. B* **96**, 085104 (2017).
2. J.R. Coulthard, S.R. Clark and D. Jaksch. Ground-state phase diagram of the one-dimensional  $t$ - $J$  model with pair hopping terms. *Phys. Rev. B* **98**, 035116 (2018).

Additionally, the author contributed to the manuscript

3. M. Kiffner, J.R. Coulthard, F. Schlawin, A. Ardavan and D. Jaksch. Manipulating quantum materials with quantum light. arXiv:1806.06752 (2018).

# Chapter 2

## Model fermionic Hamiltonians

In this chapter, we discuss the main concepts in many-body physics which are important for the rest of the thesis, and introduce the important microscopic models studied in later chapters. We begin by reviewing band structures of noninteracting particles in Sec. 2.1. In Sec. 2.2, we introduce the Hubbard model as a key model both as a description of quantum materials and of ultracold fermionic atoms in optical lattices. We then go on to consider the strongly repulsive limit of the Hubbard model and derive the  $t$ - $J$  model in Sec. 2.3, which will play a central role in Chapters 4 and 6.

### 2.1 Non-interacting particles

Here we review an important basic concept from solid-state theory, namely, band structures of noninteracting particles. This forms the basis for the microscopic models which we will discuss in the rest of the chapter. In this section we shall consider noninteracting particles of mass  $m$ , in a potential  $V(x)$  confined to one spatial dimension, though it is simple to extend our discussion to higher dimensions. The time-independent Schrödinger equation (TISE) for a single particle is

$$\left[ \frac{\hat{p}^2}{2m} + V(x) \right] \phi(x) = E\phi(x), \quad (2.1)$$

Where  $\hat{p} = -i\frac{\partial}{\partial x}$  in units where  $\hbar = 1$ , which we shall adopt throughout this thesis. For a periodic potential with lattice constant  $a$ , such that  $V(x+a) = V(x)$ , Bloch's theorem [28] gives that solutions to this TISE are

$$\phi_q(x) = e^{iqx} u_q(x), \quad \text{where} \quad u_q(x+a) = u_q(x). \quad (2.2)$$

The addition of a periodic  $V(x)$  has broken the continuous translational symmetry of the Hamiltonian to a discrete symmetry. As a consequence, the particle's momentum

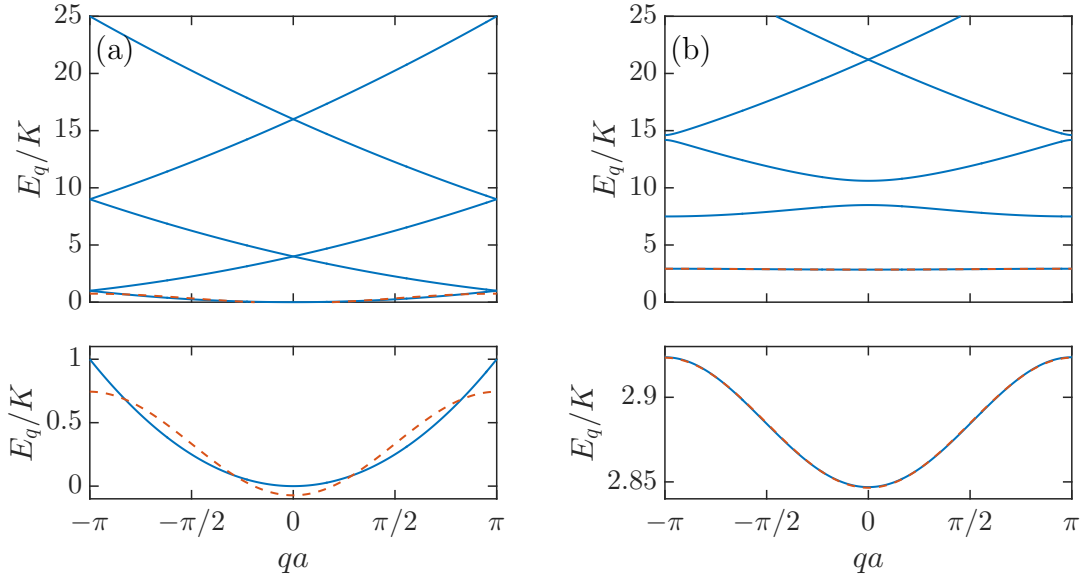


Figure 2.1: The band structure computed using Eq. (2.7) for a potential  $V_0 \sin^2(kx)$  with (a)  $V_0 = 0$ , and (b)  $V_0 = 10K$ . In the lower panels we show the lowest Bloch band, along with the tight-binding approximation, shown as the red dashed line, computed by taking only the two dominant components of  $E_q$ .

is no longer conserved. Instead, the conserved quantity which we use to label the eigenstates is the quasimomentum  $q$ , sometimes called the crystal momentum. Due to the periodicity,  $q$  is only uniquely defined up to  $q \rightarrow q + 2\pi/a$ , and as such we need only consider  $-\pi/a \leq q < \pi/a$ , called the “first Brillouin zone”. In addition, if we consider a finite lattice consisting of  $L$  sites, with periodic boundary conditions  $\phi_q(x + aL) = \phi_q(x)$ , then substituting this into the definition of  $\phi_q(x)$  results in the further constraint that  $qaL = 2n\pi$  for integer  $n$ . That is,  $q$  can only take  $L$  distinct discrete values. Substituting  $\phi_q(x)$  into Eq. (2.1), we obtain

$$\left[ \frac{(\hat{p} + q)^2}{2m} + V(x) \right] u_q(x) = E_q u_q(x). \quad (2.3)$$

To solve this equation, we exploit the periodicity of  $V(x)$  and  $u_q(x)$  and write them as Fourier series,

$$V(x) = \sum_{k=-\infty}^{\infty} v_k e^{i2\pi kx/a}, \quad \text{and} \quad u_q(x) = \sum_{k=-\infty}^{\infty} b_{q,k} e^{i2\pi kx/a}. \quad (2.4)$$

Substituting these into Eq. (2.3) gives

$$\sum_{k=-\infty}^{\infty} \frac{(2\pi k/a + q)^2}{2m} b_{q,k} e^{i2\pi kx/a} + \sum_{l=-\infty}^{\infty} \sum_{k=-\infty}^{\infty} b_{q,k} v_l e^{i2\pi(k+l)x/a} = E_q \sum_{k=-\infty}^{\infty} b_{q,k} e^{i2\pi kx/a}. \quad (2.5)$$

Then, since the  $e^{ikq}$  are all linearly independent, the equality must hold for all groups of terms with the same exponent, in other words,

$$\frac{(2\pi k/a + q)^2}{2m} b_{q,k} + \sum_{p=-\infty}^{\infty} v_{k-p} b_{q,p} = E_q b_{q,k}, \quad (2.6)$$

or, in matrix form

$$\mathbf{H}_q \vec{b}_q = E_q \vec{b}_q, \quad (2.7)$$

where  $\vec{b}_q$  is a column vector of Fourier coefficients of the Bloch wavefunctions  $u_q(x)$ , and

$$(\mathbf{H}_q)_{i,j} = K(2j + qa/\pi)^2 \delta_{i,j} + v_{i-j}, \quad \text{and} \quad K = \left(\frac{\pi}{a}\right)^2 \frac{1}{2m}. \quad (2.8)$$

We compute the band structure by choosing the set of discrete points  $q_n = 2\pi n/La$ , with  $-L/2 < n \leq L/2$  inside the first Brillouin zone. Then for each of these points, we solve the eigenvalue equation by truncating the number of Fourier coefficients kept in Eq. (2.7). For the purposes of illustration, we show the band structure for a potential  $V(x) = V_0 \sin^2(\pi x/a)$  in Fig. 2.1 for various values of the potential depth  $V_0$ . This potential is felt, for example, by ultracold atoms trapped in a light field established by two counter-propagating laser beams [24]. In this case,  $K$  corresponds to the energy gained by a stationary atom absorbing a photon of wavelength  $2a$  from the light field, called the “recoil energy”. As we will touch upon in Sec. 2.2.1, in a condensed matter setting,  $V(x)$  is the (screened) Coulomb potential set up by a lattice of positive nuclei and felt by the electrons.

We see that in Fig. 2.1, in the absence of the trapping potential,  $V_0 = 0$ , we obtain a quadratic free-particle dispersion, which is folded into the first Brillouin zone. For finite  $V_0$  then, roughly speaking, bands with  $E_q < V_0$  acquire a gap to the higher bands, and thus correspond to bound states of the potential, while those with  $E_q > V_0$  remain gapless and form a continuum of unbound states. In the following we will, for the most part, neglect the existence of these higher excited bands. However, when we discuss periodically-driven systems in Chapter 5, it will become clear that these states can play a role in undesired heating processes.

### 2.1.1 Wannier states

The Bloch wavefunctions, which we discussed in Sec. 2.1, form a complete set of orthogonal single-particle states on our Hilbert space. However, as these states are typically delocalised over the entire lattice, they are not well suited for working with

systems where local interactions are important. We may instead define an alternative set of states  $\{w_n\}$  known as Wannier states by

$$\phi_n^{(q)}(x) = \sum_j w_n(x - X_j) e^{iq \cdot X_j}, \quad (2.9)$$

i.e. we have written the Bloch wavefunction as a superposition of wavefunctions which are centered about a lattice site positioned at  $X_j$ . We can then extract the Wannier state by taking the Fourier transform

$$w_n(x - X_j) = \frac{1}{\nu_0} \int_{\text{BZ}} dq \phi_n^{(q)}(x) e^{-iq \cdot X_j}, \quad (2.10)$$

where the integral is taken over the first Brillouin zone  $-\pi/a \leq q < \pi/a$  of the reciprocal lattice, which has a volume  $\nu_0 = 2\pi/a$ . It is simple to check that these Wannier functions form a complete orthonormal basis for single-particle states. It is important to note that the  $\{w_n\}$  are not unique, and the choice of Wannier states is not arbitrary and will in general affect the final interacting many-body Hamiltonian we derive. Specifically, if we transform the Bloch states as

$$u_n^{(q)}(x) \rightarrow e^{i\theta_n(q)} u_n^{(x)}(x), \quad (2.11)$$

where the phase  $\theta_n(q)$  depends on the quasimomentum, then one obtains another valid set of Wannier functions centered about the same point  $X_j$ . However, this transformation will change how localised the states are about this  $X_j$ . For describing fermions with local interactions, we seek a Wannier basis which minimises the spread<sup>1</sup>  $\langle (x - X_j)^2 \rangle$ . There exist algorithms for numerically computing such spread-minimising Wannier functions [31, 32], which we shall not discuss here.

## 2.2 The Hubbard model

Realistic quantum materials are typically extremely complicated to describe, with multiple electronic bands crossing the Fermi level, in addition to orbital, spin and lattice (phonon) degrees of freedom [33]. To gain insight into the properties of quantum materials, one usually resorts to simplified model Hamiltonians, where it is easier to understand the physics. While solutions to these simplified Hamiltonians will not

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<sup>1</sup>The Wannier functions which minimize this spread are sometimes called “maximally localised”. There is also a related notion of “maximally localised” which refers to a set of Wannier states which have exponential tails. As discussed in Ref. [29], it was a long standing problem to determine whether the spread-minimising Wannier functions are also exponentially localised, which was finally shown in [30].

quantitatively reproduce the properties of real systems, if chosen correctly they can still share their qualitative features and provide important physical insights. Perhaps the most important of these these simplified models is the Hubbard model [25, 26, 27], which is the central model discussed in this thesis. Here we will motivate the Hubbard model as a simplified model of quantum materials, and as an accurate model of ultracold fermions trapped in an optical lattice.

### 2.2.1 As a description of quantum materials

Generally, materials consist of a regular lattice of ionic cores, and electrons which move throughout this lattice. The (first-quantised) Hamiltonian describing such a system is [33]

$$\hat{H} = \sum_{i=1}^N \left( \frac{\hat{p}_i^2}{2m} + V_l(x_i) \right) + \sum_{i<j} V_c(x_i - x_j). \quad (2.12)$$

The first term is just the single-particle Hamiltonian from Eq. (2.1), where  $V_l$  is the lattice potential set up by electrostatic interaction with the ions. The second term is the Coulomb interaction between electrons,

$$V_c(x_i - x_j) = \frac{e^2}{|x_i - x_j|}, \quad (2.13)$$

in units where  $4\pi\epsilon_0 = 1$ . Note that Eq. (2.12) already makes the severe approximation that the lattice is completely static, with the ions forming a fixed background in which the electrons move. Even within this approximation, Eq. (2.12) is difficult, if not impossible to solve, due to the strong (and highly nonlocal) electron-electron interactions. However, in some circumstances, this can be simplified somewhat. Namely, the potential a given electron feels from far away electrons will be “screened” by the positive ions. Likewise, the lattice potential felt by an electron will be screened by the presence of other electrons. In this case, it is justified to replace  $V_l$  by a weaker effective lattice potential  $V(x)$ , and replace  $V_c$  by a weaker, more local electron-electron interaction  $U(x_i, x_j)$ , i.e.

$$\hat{H} \approx \sum_{i=1}^N \left( \frac{\hat{p}_i^2}{2m} + V(x_i) \right) + \sum_{i<j} U(x_i, x_j). \quad (2.14)$$

Writing this Hamiltonian in second-quantised form, we have

$$\hat{H} = \hat{H}_0 + \hat{H}_1, \quad (2.15)$$

where

$$\begin{aligned}\hat{H}_0 &= \sum_{\sigma} \int dx \hat{\Psi}_{\sigma}^{\dagger}(x) \left[ -\frac{\nabla^2}{2m} + V(x) \right] \hat{\Psi}_{\sigma}(x), \\ \hat{H}_1 &= \sum_{\sigma, \sigma'} \int dx \int dx' \hat{\Psi}_{\sigma}^{\dagger}(x) \hat{\Psi}_{\sigma'}^{\dagger}(x') U(x, x') \hat{\Psi}_{\sigma'}(x') \hat{\Psi}_{\sigma}(x).\end{aligned}\quad (2.16)$$

Here  $\hat{\Psi}_{\sigma}^{(\dagger)}(x)$  are field operators which annihilate (create) a spin- $\sigma$  fermion at position  $x$ . We then expand the field operators in the Wannier basis,

$$\hat{\Psi}_{\sigma}(x) = \sum_{n,j} w_n(x - X_j) \hat{c}_{n,j,\sigma}, \quad (2.17)$$

where  $\hat{c}_{\sigma,j}$  annihilates a spin- $\sigma$  fermion in the Wannier state localised about site  $j$  associated with Bloch band  $n$ . Substituting this into Eq. (2.15), we obtain

$$\hat{H} = - \sum_n \sum_{i,j,\sigma} t_{i,j\sigma}^{(n)} \hat{c}_{n,i,\sigma}^{\dagger} \hat{c}_{n,j,\sigma} + \sum_{\alpha\beta\gamma\delta} \sum_{\sigma\sigma'} \sum_{ijkl} U_{ijkl}^{\alpha\beta\gamma\delta} \hat{c}_{\alpha,i,\sigma}^{\dagger} \hat{c}_{\beta,j,\sigma'}^{\dagger} \hat{c}_{\gamma,k,\sigma'} \hat{c}_{\delta,l,\sigma}, \quad (2.18)$$

where

$$t_{i,j}^n = \frac{1}{\nu_0} \int_{\text{BZ}} dq E_n^{(q)} e^{iq \cdot (X_i - X_j)}, \quad (2.19)$$

is just the Fourier transform of the  $n$ th Bloch band, and

$$U_{ijkl}^{\alpha\beta\gamma\delta} = \int dx \int dx' w_{\alpha}^{*}(x - X_i) w_{\beta}^{*}(x - X_j) U(x, x') w_{\gamma}(x' - X_k) w_{\delta}(x' - X_l). \quad (2.20)$$

We now make some simplifying assumptions about our quantum material.

1. We assume that only one band crosses the Fermi level, and all higher bands are sufficiently far separated in energy that they do not contribute to the physics. We therefore project the Hamiltonian in Eq. (2.18) onto a single Bloch band.
2. We assume that the hopping matrix elements  $t_{i,j}$  are dominated by nearest-neighbour processes, i.e.  $t_{i,i\pm 1} \gg t_{i,i\pm r}$  where  $r > 1$ . We see from Eq. (2.19) and Fig. 2.1 that this is the case if the electrons are tightly bound, resulting in a nearly cosinusoidal band structure.
3. We assume that the electron-electron interactions are strongly screened, and that the Wannier basis is sufficiently well localised that  $U_{iiii} \gg U_{ijkl}$  with  $j, k, l \neq i$ .

With these approximations, Eq. (2.18) becomes the famed Hubbard model,

$$\hat{H}_{\text{Hub}} = U \sum_j \hat{n}_{j,\uparrow} \hat{n}_{j,\downarrow} - t \sum_{\langle ij \rangle, \sigma} \left( \hat{c}_{i,\sigma}^{\dagger} \hat{c}_{j,\sigma} + \text{H.c.} \right). \quad (2.21)$$

We note again that  $\hat{c}_{j,\sigma}$  annihilates a spin- $\sigma$  electron in the Wannier function  $W_0(x - X_j)$ . Note that the sum  $\langle ij \rangle$  is a sum over *unique* nearest-neighbour lattice sites  $i$  and  $j$ .

### 2.2.2 As a description of ultracold atoms in optical lattices

In the context of electrons in a solid, approximations 1–3 above are rather crude, and are unlikely to be fully justified in most cases. Thus, while it may qualitatively capture the relevant physics in some specific materials, the Hubbard model cannot be expected to be quantitatively accurate. One system where the model *is* a quantitatively accurate description, however, is in the case of ultracold atoms trapped in optical lattices [34, 32], as we will outline here.

Ultracold fermions trapped in an optical lattice obey the same basic second-quantised Hamiltonian Eq. (2.15) which leads to Eq. (2.18) [34]. However, in this case, one is able to control the system parameters so as to implement the Hubbard model to an excellent approximation [23, 24]. Firstly, by increasing the intensity of the optical lattice, we can increase the potential depth  $V_0$ . As we saw in Fig. 2.1, doing this leads to well-separated Bloch bands, and a nearly cosinusoidal band structure. Therefore, approximations 1 and 2 in the previous section can be made extremely accurate in this setting.

Now we consider the interaction term. As the ultracold atoms are electrically neutral, there is no long-range Coulomb interaction as in the case of electrons. Instead, they only interact at very short ranges. Specifically, when the atoms are sufficiently cold and dilute, we may approximate their interactions as purely two-body  $s$ -wave scattering [23]. One then can then treat the two-body scattering process using a “zero-range pseudopotential” [35]. When the corresponding  $s$ -wave scattering length  $a_s$  and particle momentum  $k$  satisfy  $ka_s \ll 1$ , this pseudopotential reduces to a simple contact interaction within the Born approximation<sup>2</sup>, given by

$$\hat{H}_1 = g \int dx \int dx' \hat{\Psi}_\uparrow^\dagger(x) \hat{\Psi}_\downarrow^\dagger(x') \delta(x - x') \hat{\Psi}_\downarrow(x') \hat{\Psi}_\uparrow(x). \quad (2.22)$$

In three dimensions,  $g = 4\pi a_s/m$ . Note that  $a_s$ , and hence  $g$  is adjustable by tuning an external magnetic field close to a Feshbach resonance [23]. Substituting the expansion of  $\hat{\Psi}$  in terms of Wannier states in Eq. (2.17), we again obtain

$$\hat{H}_1 = \sum_{ijkl} U_{ijkl} \hat{c}_{i,\uparrow}^\dagger \hat{c}_{j,\downarrow}^\dagger \hat{c}_{k,\downarrow} \hat{c}_{l,\uparrow}, \quad (2.23)$$

where

$$U_{ijkl} = g \int dx w_0^*(x - X_i) w_0^*(x - X_j) w_0(x - X_k) w_0(x - X_l) \quad (2.24)$$

---

<sup>2</sup>When this does not hold (for example, near a Feshbach resonance where the scattering length diverges) then the full pseudopotential is required, specifically  $V(r) = g\delta(r) \left(\frac{\partial}{\partial r}\right) r$ . The role of the  $\left(\frac{\partial}{\partial r}\right) r$  is to remove any divergences in the two-body wavefunction as the relative separation  $r \rightarrow 0$ .

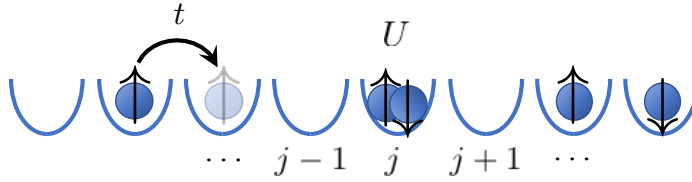


Figure 2.2: Schematic of the one-dimensional Hubbard model. Lattice sites may be occupied by spin “up” or “down” fermions. These fermions can tunnel to nearest-neighbour lattice sites with an amplitude  $t$ . If two Fermions of opposite spin occupy the same lattice site, they pay an energy penalty  $U$ .

Note that we have already projected the Hamiltonian into the lowest Bloch band. Because of the  $\delta(x - x')$  form of the interaction,  $U_{ijkl}$  has acquired the form of an overlap integral between the Wannier states. In a deep lattice, the spread-minimising Wannier states will have negligible overlap for states on different lattice sites. Therefore only the overlap integral  $U_{iiii}$  contributes. The Hamiltonian therefore again reduces to the Hubbard model

$$\hat{H}_{\text{Hub}} = U \sum_j \hat{n}_{j,\uparrow} \hat{n}_{j,\downarrow} - t \sum_{\langle ij \rangle, \sigma} \left( \hat{c}_{i,\sigma}^\dagger \hat{c}_{j,\sigma} + \text{H.c.} \right). \quad (2.25)$$

### 2.2.3 Discussion

The Hubbard model, Eq. (2.25) encapsulates the interplay between kinetic energy and local interactions which is at the heart of many physical phenomena. These include the metal-insulator transition [36], ferromagnetism [37] and antiferromagnetism [38]. The Hubbard model in two dimensions is also conjectured to capture the essential physics of high- $T_c$  superconductivity [39]. Furthermore, despite its simplified nature, it has been shown to provide a quantitatively accurate description of some materials, such as organic salts [4, 40], and forms the basis of more complex models accounting for e.g. multiple orbitals [14, 41].

There are only two processes in the Hubbard model; a nearest-neighbour hopping  $t$  and an on-site repulsion  $U$ , which we sketch in Fig. 2.2. Despite its apparent simplicity, the Hubbard model has so far resisted exact solution, except in one dimension, via the Bethe ansatz [42], and in infinite dimensions via dynamical mean-field theory [43]. For this reason, one often resorts to simulating the Hubbard model in order to extract information about its properties. These simulations broadly fall into two categories, classical simulation and quantum simulation. Classical simulation involves numerically solving the Hamiltonian to find, for example, its ground state, and then

compute some desired property of this ground state. In its simplest form, this is done by constructing a matrix representation of the desired Hamiltonian in some basis and numerically diagonalising it. A more sophisticated classical simulation method based on tensor networks is the subject of Chapter 3.

Quantum simulation, by contrast, involves constructing a well-controlled physical system which is known to implement the desired Hamiltonian to a good approximation [22]. Then, one can directly perform experiments to measure its properties. As noted in Sec. 2.2.2, the properties of ultracold fermions in optical lattices make them an ideal platform for performing quantum simulations of the Hubbard model [44, 24].

## 2.3 Large $U$ limit and the $t$ – $J$ model

The physics at the heart of the Hubbard model is the competition between delocalisation driven by the kinetic energy  $t$  and localisation driven by the interaction  $U$ . Let us consider a half-filled system (i.e. an average number of fermions per site  $n = 1$ ). When  $t \neq 0$ ,  $U = 0$ , the half-filled Hubbard model reduces to a noninteracting tight-binding model, whose eigenstates are delocalised Bloch waves, as we discussed in Sec. 2.1. The ground state in this limit is therefore metallic. In the opposite limit  $t = 0$ ,  $U \neq 0$ , the eigenstates are product states with one fermion on each site. The particles are then completely localised. Therefore, it is argued that as a ratio of  $U/t$ , there is a phase transition between delocalisation due to the hopping, and localisation due to the interaction [33]. This is the famous Mott Transition, and the insulating phase is known as the Mott insulator [45]. The Mott insulator is insulating at half-filling and does not correspond to a filled Bloch band. Excitations of the Mott insulator are pairs of holes (often called “holons” in this context), and double-occupations (often called “doublons”).

Throughout this thesis we will be particularly interested in the limit of the Hubbard model in which  $U \gg t$ , the so-called strongly interacting limit, and *away* from half-filling. In this limit, processes which change the number of doublons are strongly suppressed, since they cannot conserve energy. In particular, if  $n \leq 1$ , the fraction of doublons in the ground state should be strongly suppressed. However, the hopping term will still induce second-order processes which virtually create and destroy doublons. We will see that this gives rise to a weak nearest-neighbour antiferromagnetic pairing interaction, which is described by the so-called  $t$ – $J$  model. Later, in Chapter 6, we will demonstrate that the weak antiferromagnetic pairing can be made dominant by periodically driving the system.

We present here a standard way of deriving the  $t$ - $J$  model based on a very general method of degenerate perturbation theory [38]. We break up the Hubbard Hamiltonian into  $\hat{H}_{\text{Hub}} = U\hat{D} - t\hat{T}$ , where

$$\hat{D} = \sum_j \hat{n}_{j,\uparrow}\hat{n}_{j,\downarrow}, \quad \text{and} \quad \hat{T} = \sum_{[ij],\sigma} \hat{c}_{j,\sigma}^\dagger \hat{c}_{i,\sigma} \quad (2.26)$$

Where the second sum over  $[ij]$  denotes the sum over all neighbouring pairs of sites  $i$  and  $j$  (including double-counting).

Let us first consider the limit  $t = 0$ . The Hamiltonian is trivially diagonalised by configuration states  $|\{n_{i,\sigma}\}\rangle$ , where

$$\begin{aligned} |\{n_{j,\sigma}\}\rangle &= |n_{1,\uparrow}, n_{1,\downarrow}, n_{2,\uparrow}, n_{2,\downarrow} \cdots n_{L,\uparrow}, n_{L,\downarrow}\rangle \\ &= \prod_{j=1}^L \prod_{\sigma=\uparrow,\downarrow} (\hat{c}_{j,\sigma}^\dagger)^{n_{j,\sigma}} |0\rangle. \end{aligned} \quad (2.27)$$

These configuration states have eigenvalues  $mU$ , where  $m$  is the number of doubly-occupied sites in the configuration. As the energy depends only on the number of doublons and not where they are located in the lattice, these eigenstates are highly degenerate. When we apply the perturbation  $t\hat{T}$ , these degenerate manifolds are then weakly coupled together, which breaks the degeneracy, as we show in Fig. 2.3. Provided the coupling is sufficiently weak, a system beginning with a well-defined number of doublons will not leave this sector (i.e. the number of doublons will be quasi-conserved). Our task is to find an effective Hamiltonian which governs the dynamics within one of these manifolds (namely the ground state manifold containing zero doublons). This is a very general procedure which we will employ multiple times in this thesis in order to study the effect of weak couplings between sectors which have large energy separations. In particular, we shall employ this in Chapter 5 and Chapter 6 to derive effective static Hamiltonians for periodically driven systems.

We first define  $\mathbb{P}_n$  to be the projectors which project onto the manifold containing  $n$  doublons, such that  $\sum_n \mathbb{P}_n = \mathbb{1}$ . In general, the effective Hamiltonian within a degenerate manifold  $\mathbb{P}_n$  of a Hamiltonian  $\hat{H}_0 |n\rangle = E_n |n\rangle$ , split by a perturbation  $\lambda \hat{H}_1$  which couples the manifolds is given by [38]

$$\hat{H}_{\text{eff}} = E_n \mathbb{P}_n + \lambda \mathbb{P}_n \hat{H}_1 \mathbb{P}_n + \lambda^2 \sum_{m \neq n} \frac{\mathbb{P}_n \hat{H}_1 \mathbb{P}_m \hat{H}_1 \mathbb{P}_n}{E_n - E_m}. \quad (2.28)$$

We restrict ourselves to the zero doublon manifold of the Hubbard model, so we take  $n = 0$ ,  $\lambda = -t$ , and  $\hat{H}_1 = \hat{T}$ . We therefore have

$$\hat{H}_{\text{eff}} = -t \mathbb{P}_0 \hat{T} \mathbb{P}_0 - \frac{t^2}{U} \sum_{m>0} \frac{\mathbb{P}_0 \hat{T} \mathbb{P}_m \hat{T} \mathbb{P}_0}{m}. \quad (2.29)$$

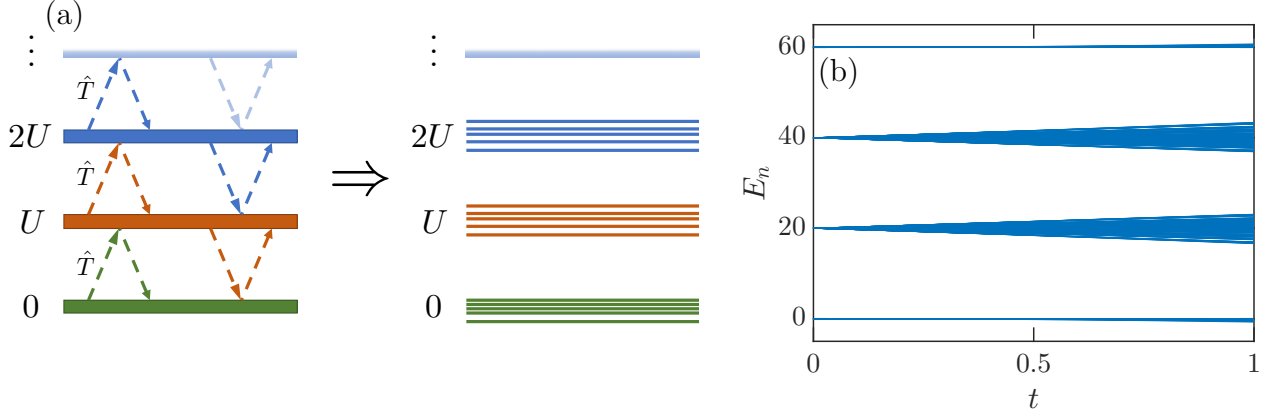


Figure 2.3: In (a) we show a schematic energy level diagram illustrating the degenerate perturbation theory. On the left, we show the degenerate Hubbard bands. To second order, the kinetic energy perturbation induces virtual transitions to adjacent Hubbard bands and back again, causing splitting of these degenerate levels. In (b) we show the spectrum for a one-dimensional, half-filled, 6-site Hubbard model with  $U = 20t_0$ , as a function of hopping  $t/t_0$ , computed with exact diagonalisation. We see that the initially degenerate bands are split by the kinetic energy perturbation.

As expected, the first order term simply causes fermions to hop without changing the doublon number, while the second order term induces virtual transitions to and from other doublon sectors. To simplify this second term further, we consider the product

$$\mathbb{P}_m \hat{T} \mathbb{P}_0 = \sum_{[ij], \sigma} \mathbb{P}_m \hat{c}_{j, \sigma}^\dagger \hat{c}_{i, \sigma} \mathbb{P}_0. \quad (2.30)$$

Reading from right to left, we see that this is a sum of processes which each take a state containing zero doublons, and moves a single fermion from site  $i$  to site  $j$ . Moving a single fermion can either not create a doublon, in which case  $\mathbb{P}_{m \neq 0}$  kills the state, or it can create a doublon on site  $j$ , in which case only  $\mathbb{P}_1$  results in a nonzero contribution. Furthermore, since we know the doublon must have been created on site  $j$ , we can write this term as

$$\sum_{[ij], \sigma} \mathbb{P}_m \hat{c}_{i, \sigma}^\dagger \hat{c}_{j, \sigma} \mathbb{P}_0 = \sum_{[ij], \sigma} \hat{n}_{j, \uparrow} \hat{n}_{j, \downarrow} \hat{c}_{j, \sigma}^\dagger \hat{c}_{i, \sigma} \mathbb{P}_0. \quad (2.31)$$

Substituting this, and  $\hat{T}$  into the second term of Eq. (2.29), we find

$$\hat{H}_{\text{eff}} = -t \mathbb{P}_0 \hat{T} \mathbb{P}_0 - \frac{t^2}{U} \mathbb{P}_0 \sum_{[lk], b} \sum_{[ij], a} \hat{c}_{l, b}^\dagger \hat{c}_{k, b} \hat{n}_{j, \uparrow} \hat{n}_{j, \downarrow} \hat{c}_{j, a}^\dagger \hat{c}_{i, a} \mathbb{P}_0. \quad (2.32)$$

if  $j \neq l \neq k$ , then  $\hat{n}_{j, \uparrow} \hat{n}_{j, \uparrow}$  commutes through the hopping term on the left. Then, since  $\hat{n}_{j, \uparrow} \hat{n}_{j, \uparrow} \mathbb{P}_0 = \hat{n}_{j, \uparrow} \hat{n}_{j, \uparrow} \mathbb{P}_0 = 0$ , these terms vanish. Similarly, if  $j = l \neq k$ , then

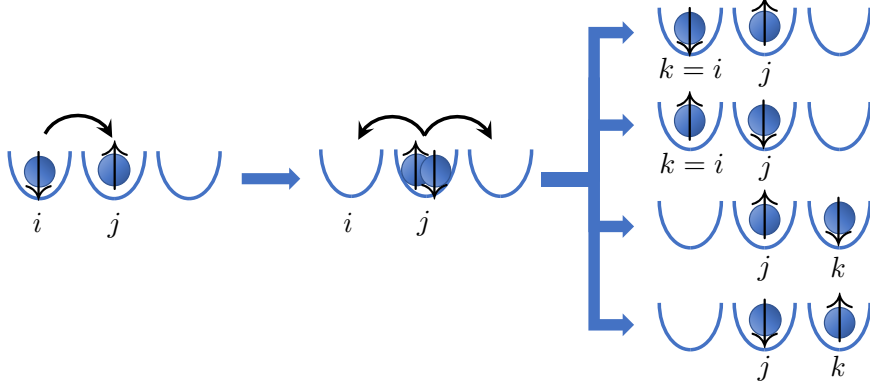


Figure 2.4: Schematic of some of the virtual hopping processes in the strongly-repulsive Hubbard model. A fermion on site  $i$  hops to a site occupied by an opposite-spin fermion on site  $j$ . There are then four possible hopping processes which destroy the doublon and move a fermion onto site  $k$ , which may be the same as site  $i$ .

$\hat{n}_{l,\uparrow}\hat{n}_{l,\uparrow}$  commutes through the  $\hat{c}_k$ , where it is killed by the  $\hat{c}_l^\dagger$ . We find that the only nonzero contribution is  $k = j$ . Physically, this is simply because the first hopping process creates a doublon on site  $j$ , and in order to take us back to the zero-doublon manifold, the second hopping process must remove a fermion from site  $j$ . In full, the effective Hamiltonian in the zero-doublon manifold is given by

$$\hat{H}_{\text{eff}} = \mathbb{P}_0 \left[ -t\hat{T} - \frac{t^2}{U} \sum_{[ijk]} \sum_{a,b} \hat{c}_{k,b}^\dagger \hat{c}_{j,b} \hat{n}_{j,\uparrow} \hat{n}_{j,\downarrow} \hat{c}_{j,a}^\dagger \hat{c}_{i,a} \right] \mathbb{P}_0, \quad (2.33)$$

where the sum over  $[ijk]$  is a sum over all combinations of all next-nearest-neighbour combinations, again including double-counting, and furthermore including  $i = k$ . A schematic of some of these processes is shown in Fig. 2.4.

We can rewrite this in a more insightful way by noticing the following. The intermediate state in the second-order process contains a doublon, which consists of two opposite-spin fermions in the same spatial Wannier wavefunction. Hence, the overall antisymmetry of the wavefunction requires that they are in a spin-singlet state. Since  $\hat{T}$  does not couple to the spin degree of freedom, they must always have been in a spin-singlet, which just gets redistributed by the second-order process. Therefore we can write the effective Hamiltonian as

$$\begin{aligned} \hat{H}_{\text{eff}} = \mathbb{P}_0 \left[ -t \sum_{\langle ij \rangle \sigma} (\hat{c}_{i,\sigma}^\dagger \hat{c}_{j,\sigma} + \text{H.c.}) - J \sum_{\langle ij \rangle} \hat{b}_{ij}^\dagger \hat{b}_{ij} \right. \\ \left. - \frac{J}{2} \sum_{\langle ijk \rangle} (\hat{b}_{ij}^\dagger \hat{b}_{jk} + \text{H.c.}) \right] \mathbb{P}_0. \end{aligned} \quad (2.34)$$

Here we have defined  $\hat{b}_{ij} = (\hat{c}_{j,\downarrow} \hat{c}_{i,\uparrow} - \hat{c}_{j,\uparrow} \hat{c}_{i,\downarrow})/\sqrt{2}$  to be the annihilation operator for a spin-singlet on sites  $i$  and  $j$ , and  $J = 4t^2/U$  is the so-called superexchange energy. Note that we have also changed the sums over  $[\dots] \rightarrow \langle \dots \rangle$ , which now do *not* double-count neighboring pairs and, correspondingly, we have explicitly included the Hermitian conjugate terms.

The first term is a single-particle hopping term from the Hubbard model, with the additional constraint that it cannot create doublons. The second term reduces the energy of the system by  $J$  for each bond which contains a nearest-neighbour singlet pair. The final term is a hopping term which moves a nearest-neighbour singlet pair from one bond to a neighbouring bond. Before continuing, for completeness, we rewrite the superexchange term in its more common form. To do this, we first expand the singlet operators as

$$\begin{aligned} 2\hat{b}_{ij}^\dagger \hat{b}_{ij} = & \hat{c}_{i,\uparrow}^\dagger \hat{c}_{j,\downarrow}^\dagger \hat{c}_{j,\downarrow} \hat{c}_{i,\uparrow} - \hat{c}_{i,\downarrow}^\dagger \hat{c}_{j,\uparrow}^\dagger \hat{c}_{j,\uparrow} \hat{c}_{i,\downarrow} \\ & - \hat{c}_{i,\uparrow}^\dagger \hat{c}_{j,\downarrow}^\dagger \hat{c}_{j,\uparrow} \hat{c}_{i,\downarrow} + \hat{c}_{i,\downarrow}^\dagger \hat{c}_{j,\uparrow}^\dagger \hat{c}_{j,\downarrow} \hat{c}_{i,\uparrow}. \end{aligned} \quad (2.35)$$

Then, using  $\hat{n}_{j,\sigma} = \hat{c}_{j,\sigma}^\dagger \hat{c}_{j,\sigma}$ , defining the spin-flip operators  $\hat{S}_j^+ = \hat{c}_{j,\uparrow}^\dagger \hat{c}_{j,\downarrow}$ , and  $\hat{S}_j^- = \hat{c}_{j,\downarrow}^\dagger \hat{c}_{j,\uparrow}$ , and anticommuting some fermionic operators, we can write this as

$$2\hat{b}_{ij}^\dagger \hat{b}_{ij} = \hat{n}_{i,\uparrow} \hat{n}_{j,\downarrow} - \hat{S}_i^- \hat{S}_j^+ - \hat{S}_i^+ \hat{S}_j^- + \hat{n}_{i,\downarrow} \hat{n}_{j,\uparrow}. \quad (2.36)$$

Finally, using  $\hat{S}^\pm = \hat{S}^x \pm i\hat{S}^y$ , and that  $(\hat{n}_{i,\uparrow} \hat{n}_{j,\downarrow} + \hat{n}_{i,\downarrow} \hat{n}_{j,\uparrow}) = (\hat{n}_i \hat{n}_j - 4\hat{S}_i^z \hat{S}_j^z)/2$ , where  $\hat{S}_j^z = (\hat{n}_{j,\uparrow} - \hat{n}_{j,\downarrow})/2$ , we obtain the antiferromagnetic Heisenberg-like coupling

$$-J \sum_{\langle ij \rangle} \hat{b}_{ij}^\dagger \hat{b}_{ij} = J \sum_{\langle ij \rangle} \left( \hat{S}_i^x \hat{S}_j^x + \hat{S}_i^y \hat{S}_j^y + \hat{S}_i^z \hat{S}_j^z - \frac{\hat{n}_i \hat{n}_j}{4} \right). \quad (2.37)$$

In fact, at exactly half-filling, we see that there is no way to perform a single particle hop or a pair-hop without creating a doublon and taking us out of the  $\mathbb{P}_0$  manifold. Therefore, the first and last terms drop out of Eq. (2.34), and the low-energy physics is determined solely by this Heisenberg coupling. The half-filled Hubbard model therefore has an antiferromagnetic ground state in the limit of strong interactions.

We pause briefly to make some general comments on the Hamiltonian in Eq. (2.34). Note that nowhere in our derivation did we make use of any lattice geometry, merely that we have some sites which are connected in some way by hopping matrix elements. This effective model thus applies for any any geometry, and in particular, any dimension.

This Hamiltonian has a long and rich history [11]. Often, it is argued that close to half-filling, pair-hopping processes are rare, and these terms are therefore neglected [38]. When the pair-hopping term is neglected, Eq. (2.34) is known as the  $t$ - $J$  model. However, as these terms appeared at the same order in the perturbation as the superexchange, there is no a priori reason to neglect them. Moreover, we will see in Chapter 4 that the presence of the pair hopping radically changes the phase diagram of the model, even close to half-filling.

We already noted in the previous section that the Hubbard model has an exact solution in one dimension via the Bethe ansatz. However, as the projection breaks the  $SO(4)$  symmetry of the Hubbard model, the  $t$ - $J$  model does not have this exact solution, except for the specific choice of parameters  $J = 2t$  [38, 46]. One might then wonder what the usefulness of this Hamiltonian is. Since we have projected out double-occupations, the local Hilbert space dimension of each site is  $d = 3$  rather than  $d = 4$ , and so the Hilbert space dimension of an  $L$ -site lattice is  $3^L$ . This growth is still exponential, but it makes numerical solutions for small systems more tractable than the Hubbard model, particularly for exact diagonalisations<sup>3</sup>. Furthermore, while the Bethe ansatz may offer an exact solution in one dimension, experimentally accessible observables are often still rather difficult to obtain from it, and so numerical simulation is often preferable.

The main advantage of this Hamiltonian, however, is a conceptual one. Projecting into the zero-doublon sector of the system has provided additional physical insights into the behaviour of the strongly repulsive Hubbard model at low energies. Surprisingly, although we began with a model with purely repulsive on-site interactions, the interplay between these strong interactions and the hopping resulted in an effective model which explicitly contains a nearest-neighbour interaction which favours the formation of singlet pairs, and thus could lead to superconductivity. However, as  $t \ll J$  in this derivation, in equilibrium the pairing is necessarily washed out by the single-particle kinetic energy.

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<sup>3</sup>For example, if one can exactly solve an  $L = 14$  site Hubbard model with  $d^L = 268435456$  states, then one can solve a  $t$ - $J$  model with  $14 \log(4) / \log(3) \approx 18$  sites.

## 2.4 Conclusions

In this chapter, we have introduced the microscopic fermionic models which we will focus on in this thesis. Specifically, we have motivated the Hubbard model as a qualitative description of certain types of quantum materials, and as a good approximation to ultracold fermions trapped in optical lattices. We further demonstrated that low-energy properties of the Hubbard model are described by the  $t$ - $J$  model with  $J \ll t$ , which reveals a weak nearest-neighbour singlet pairing effect. In Chapter 4, we shall assume that this perturbative connection  $J = 4t^2/U \ll t$  can be broken, and explore the phase diagram of the  $t$ - $J$  model with  $J \gtrsim t$ . Furthermore, we will analyse the influence of the pair-hopping which is usually discarded. Then, in Chapter 6, we will show how periodically driving the Hubbard model can suppress single-particle tunneling  $t$  while sustaining the superexchange  $J$  and pair-hopping. This will effectively allow us to traverse the phase diagram of Chapter 4, opening up the possibility of engineering, e.g. superconducting states out of equilibrium.

# Chapter 3

## Tensor Network Theory

### 3.1 Introduction

As we discussed in the previous chapter, in this thesis we are primarily interested in many-body quantum systems defined on a lattice of  $L$  sites. Each lattice site has a local Hilbert space  $\mathcal{H}_j$  spanned by  $d$  basis states  $\{|s_j\rangle\}$ . Although fermions lack such a local structure, as we outline in Appendix A, in some cases we can use the Jordan-Wigner transformation [3] to map the fermionic problem onto a spin system which *does* have this local structure. In all numerical fermionic calculations in this thesis, we implicitly perform the Jordan-Wigner transformation and do the calculation in the spin picture. The total Hilbert space,  $\mathcal{H}$ , of the full many-body system is then

$$\dim\{\mathcal{H}\} = \dim\{\mathcal{H}_1 \otimes \mathcal{H}_2 \otimes \cdots \otimes \mathcal{H}_L\} = d^L,$$

increasing exponentially with the number of lattice sites. It therefore very quickly becomes computationally infeasible to numerically diagonalise these systems for more than a modest number of lattice sites<sup>1</sup>.

In order to make progress, we are therefore required to make some assumptions which allow us to reduce the size of the space of states we consider. Fortunately, usual physical states (ground states, thermal states, and low-lying excited states) of many-body quantum systems with short-ranged interactions will generally not correspond to arbitrary vectors in  $\mathcal{H}$ . Rather, these states will belong to a subset of  $\mathcal{H}$  in which entanglement is limited. To be more precise, we show an example in Fig. 3.1(a), a two-dimensional system which is bipartitioned by the blue boundary. For typical

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<sup>1</sup>We have performed exact diagonalisation calculations on the Hubbard model for up to 14 sites, with 14 fermions, while we have performed tensor network calculations for the same model with  $L = 60$  sites. To perform this with exact diagonalisation would require storing  $\sim 4^{60}$  complex numbers. Storing each of these as double-precision floating point numbers would require  $\sim 10^{28}$  gigabytes of RAM to store, or roughly  $10^{26}$  of our cluster nodes.

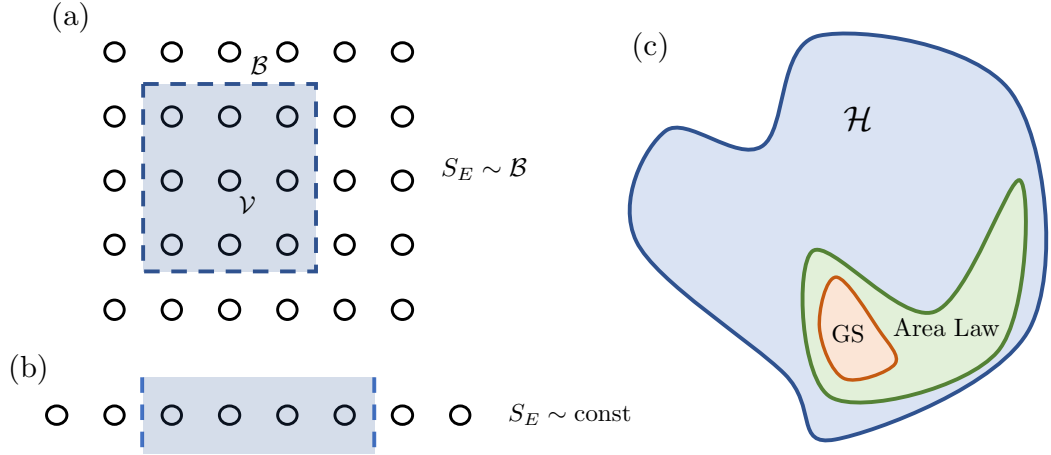


Figure 3.1: In (a) we schematically show a two-dimensional quantum system, with a subsystem of volume  $\mathcal{V}$  and boundary  $\mathcal{B}$  enclosed in blue. For states of interest, the entanglement entropy between the enclosed subsystem and the rest of the system grows as the size of the boundary  $\mathcal{B}$ . In (b) we see that in one dimension, the area, and thus entanglement, does not grow with system size. In (c) we illustrate that states which the area law occupy a small piece of the full Hilbert space  $\mathcal{H}$  which contains the ground states and low-lying excited states of interest. This is the basis for the effectiveness of TNT.

states of interest, the entanglement entropy  $S_E$  grows not as the volume  $\mathcal{V}$  of the subsystem enclosed by the boundary, but the size of the boundary  $\mathcal{B}$  [47, 48]. The area law is most powerful for one dimensional systems, as shown in Fig. 3.1(b). If we make a cut to bipartition the system, the “area” of the boundary is independent of the system size, and so the entanglement entropy  $S_E$  is independent of the system size, provided the Hamiltonian in question is local, and there is a gap between the ground state and the first excited state<sup>2</sup> [49]. The cartoon in Fig. 3.1(c) illustrates the usefulness of this idea. The states which obey the Area law occupy a small corner of the full Hilbert space, which contains the states we are interested in. Thus, by efficiently parametrising these area law states, we can greatly reduce the size of the space we need to consider, and greatly increase the efficiency of calculations.

In this chapter we will introduce the main numerical methods used for calculations within this thesis, based on tensor network theory (TNT). We will see that it is simple to construct states, parametrised as a network of tensors, which automatically obey the area law, and as a result have vastly fewer parameters than the full Hilbert space dimension  $d^L$ . By using such a tensor network as an ansatz for the state of our

<sup>2</sup>Even in systems where this gap does not exist, local interactions are often sufficient for an approximate area law to hold, for example in 1D critical systems.

many-body system, we will explain how to compute ground states and perform time evolution for many-body quantum states, obtaining an exponential speedup compared with using an exact representation.

The structure of the chapter is as follows. We first provide a brief introduction to tensor algebra, introducing the standard diagrammatic language for describing tensor network algorithms. We then make the connection between this tensor algebra and many-body quantum states, showing how to construct matrix product states, a class of tensor networks well-suited for describing one-dimensional systems. We then discuss the density matrix renormalisation group, and time evolving block decimation, algorithms for finding tensor network representations of ground states of quantum systems, and their time evolution, respectively. We then describe how to extend the time evolution algorithm to translationally-invariant infinite systems, and to the computation of thermal mixed states and their unitary evolution. We also describe how to exploit  $U(1)$  symmetry in these algorithms to further increase their efficiency.

## 3.2 Tensor algebra notation

Here we introduce the concept of a tensor and the diagrammatic language for manipulating them. We will introduce the concepts and notation necessary for understanding the algorithms employed in this thesis. See e.g. Ref. [50] for a more comprehensive review.

A tensor is defined as a multidimensional array of complex numbers  $A_{ijk\dots}$ . The number of indices which a tensor has is called its rank. We will see that it is very useful to use a diagrammatic representation of these tensors. As a concrete example, consider the four-dimensional tensors  $A_{ijkl}$  and  $B_{efdg}$ , which we show in Fig. 3.2(a). A rank  $N$  tensor is represented by a node with  $N$  legs, one for each index. As such, we will use the words “leg”, and “index” interchangeably. For example, a rank 2 tensor,  $M_{ij}$ , is a matrix, and a rank 1 tensor,  $v_i$ , is a vector.

If two tensor legs have the same dimension, we may perform a contraction over them, for example

$$C_{jkldeg} = \sum_{\alpha} A_{\alpha jkl} B_{de\alpha g}, \quad (3.1)$$

that is, we make one index in each tensor the same, and sum over it. This operation is depicted graphically in Fig. 3.2(b), where the leg connecting the two nodes represents the index to be summed over. The resulting tensor has all of the uncontracted legs of  $A$  and  $B$ . We note that a contraction between two rank 2 tensors is equivalent to a

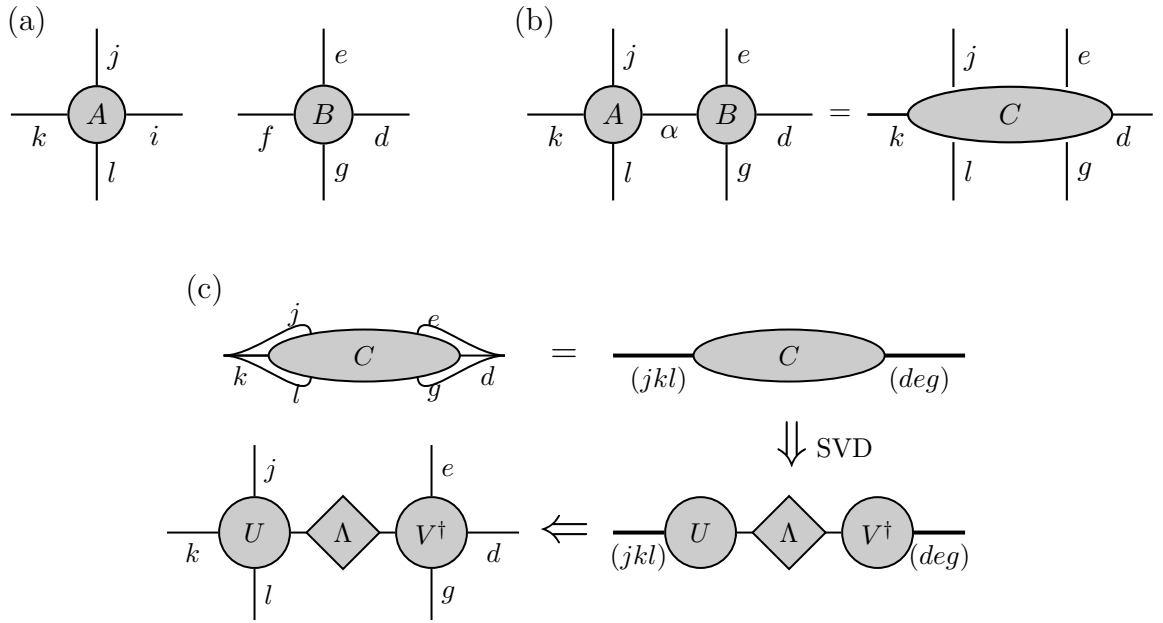


Figure 3.2: A demonstration of the diagrammatic representation of tensors. In (a) we show a pair of tensors  $A$  and  $B$ , each with four indices (legs). If legs  $i$  and  $j$  are connected we can contract over this index to produce the tensor  $C$ , shown in (b). In (c) we show a very common method of factorising tensors. First we reshape  $C$  into a matrix by merging legs  $j$ ,  $k$  and  $l$  on one side and  $d$ ,  $e$  and  $g$  on the other. We then factorise the matrix via a singular value decomposition, before reshaping the resulting matrices back into tensors by splitting the legs.

matrix-matrix multiplication, and a contraction between a rank 2 tensor and a rank 1 tensor is equivalent to a matrix-vector multiplication.

In many circumstances, we will want to merge multiple legs of a tensor into one larger leg, thus reducing the tensor rank. For example, in Fig. 3.2(c), we reshape the 6-leg tensor into a 2-leg matrix. Note that the dimension of each new, larger, leg (often called a “fat leg”) is the product of the dimensions of the legs which were merged. Once in this two-leg form, we can then apply a range of numerical linear algebra techniques developed for matrices to the tensor. The most important example is matrix the factorisation known as the singular value decomposition (SVD), which will be used extensively in the algorithms described in this chapter. The SVD takes an arbitrary matrix  $m \times n$  matrix  $M$ , and factorises it into  $M = U\Lambda V^\dagger$ .  $U$  is an  $m \times m$  matrix, while  $\Lambda$  and  $V^\dagger$  are  $n \times n$  matrices. Furthermore, these matrices satisfy  $U^\dagger U = \mathbb{1}$  and  $V^\dagger V = \mathbb{1}$ . Finally, the matrix  $\Lambda$  is diagonal with real and non-negative  $\lambda_i = \Lambda_{ii}$  [51]. Without loss of generality we will always assume  $\lambda_1 \geq \lambda_2 \geq \dots \geq \lambda_n$ . The computational cost of performing the SVD, if  $m < n$  is  $\mathcal{O}(mn^2)$  [51].

### 3.3 The Schmidt decomposition

Here we will make the link between the rather abstract notion of tensor manipulations introduced in the previous section, and physical states of quantum systems. We will introduce the concept of the Schmidt decomposition and show how it naturally leads to the representation of the state of a many-body system as a tensor network.

We consider a bipartite quantum system with halves  $A$  and  $B$ . The local Hilbert space dimension of each subsystem is  $d_A$  and  $d_B$ . The local Hilbert spaces are spanned by the basis states  $|i_A\rangle, |i_B\rangle$ , with  $i_A = 1, 2, \dots, d_A$ , and  $i_B = 1, 2, \dots, d_B$  respectively. The combined state of the system can be written as

$$|\psi_{AB}\rangle = \sum_{i_A, i_B} C_{i_A, i_B} |i_A\rangle |i_B\rangle. \quad (3.2)$$

We can consider the coefficients  $C_{i_A, i_B}$  as a  $d_A \times d_B$  matrix of complex numbers representing the state of the system. We then factorise the matrix  $C$  using the SVD described in the previous section,

$$C = U\Lambda V^\dagger \Rightarrow C_{i_A, i_B} = \sum_{\alpha, \beta} U_{i_A, \alpha} \Lambda_{\alpha, \beta} (V^\dagger)_{\beta, i_B}, \quad (3.3)$$

where the number of singular values is equal to the smaller of the dimensions  $d_A$  and  $d_B$ . Inserting this into Eq. (3.2), and reordering the sums, we obtain

$$|\psi_{AB}\rangle = \sum_{\alpha,\beta} \Lambda_{\alpha,\beta} \sum_{i_A} U_{i_A,\alpha} |i_A\rangle \sum_{i_B} (V^\dagger)_{\beta,i_B} |i_B\rangle, \quad (3.4)$$

$$= \sum_{\alpha=1}^R \lambda_\alpha |U_\alpha\rangle |V_\alpha\rangle, \quad (3.5)$$

where in the last line we have used the unitarity of  $U$  and  $V$  to define a new set of orthonormal basis vectors  $\{|U_\alpha\rangle\}$  and  $\{|V_\alpha\rangle\}$  on the  $A$  and  $B$  subsystems, known as the Schmidt basis. We have also used that  $\Lambda$  is diagonal to eliminate the sum over  $\beta$ , and we have used the ordering of the elements  $\lambda_\alpha$  to restrict the sum to the nonzero terms  $1 \leq \alpha \leq R$ . The number of nonzero terms  $R$  is called the Schmidt rank of the state.

The Schmidt decomposition can be interpreted physically as follows. Suppose we do a projective measurement of  $A$  in the Schmidt basis, obtaining the result  $|U_j\rangle$ . The resulting state of  $B$  is then *guaranteed* to be the corresponding  $|V_j\rangle$ . Moreover, since the  $\{|V_j\rangle\}$  are orthogonal, these different outcomes are distinguishable by local measurements on the  $B$  subsystem. The Schmidt decomposition of the state  $|\psi\rangle$  can therefore be interpreted as the decomposition which best reveals the quantum correlations between the two subsystems.

This can be made more concrete by considering the distribution of Schmidt coefficients  $s_\alpha$  in Eq. (3.5). If only one coefficient is nonzero, then the state of the system is a product state, and so  $A$  and  $B$  are uncorrelated. Conversely, the more uniform the Schmidt coefficients are, the more complex the correlations between them. We can quantify this observation by calculating the entanglement entropy between the two subsystems. Tracing out the  $B$  subsystem in Eq. (3.2), one obtains the reduced density matrix of the  $A$  subsystem  $\rho^A$  as

$$\rho^A = \sum_{\alpha} \lambda_\alpha^2 |U_\alpha\rangle \langle U_\alpha|. \quad (3.6)$$

In other words,  $\Lambda^2$  is precisely the reduced density matrix of one of the subsystems written in the Schmidt basis. Then, computing the Von Neumann entropy [52] of  $\rho^A$ ,

$$S_E = -\text{Tr}(\rho^A \log_2 \rho^A) = -\sum_{\alpha} \lambda_\alpha^2 \log_2 \lambda_\alpha^2. \quad (3.7)$$

Therefore, the closer the Schmidt coefficients are to uniform, the more entangled the two subsystems are. Moreover, since  $\lambda_\alpha$  are real and positive, they assign an

“importance” to each term in the state. If some  $\lambda_\alpha$  are much smaller than others, then we can approximate the state  $|\psi\rangle$  by a state with a lower Schmidt rank  $|\tilde{\psi}\rangle$  by throwing away the smaller terms,

$$|\psi\rangle \approx |\tilde{\psi}\rangle = \sum_{\alpha=1}^{\chi} \lambda_\alpha |U_\alpha\rangle |V_\alpha\rangle, \quad (3.8)$$

where the error in the approximation is

$$|||\tilde{\psi}\rangle - |\psi\rangle||^2 = 1 - \sum_{\alpha=1}^{\chi} \lambda_\alpha^2 = \sum_{\alpha=\chi+1}^R \lambda_\alpha^2, \quad (3.9)$$

i.e., the sum of the discarded weights in the reduced density matrix. We will see in the following section that making this approximation will allow us to construct a very efficient representation of many-body states.

### 3.4 Matrix Product States

We have seen that for a two-body system, the Schmidt decomposition allows us to approximate a weakly-entangled state by a state with a lower rank. Here we will see how we can generalise this to many-body systems and obtain a tensor network representation of any quantum state, and which is only efficient for weakly-entangled states. Suppose we have a many-body system defined on a lattice of  $L$  sites. For simplicity, we assume each lattice site has the same physical dimension  $d$ . The local Hilbert space of lattice site  $j$  is spanned by the basis vectors  $\{|s_j\rangle\}$ . A quantum state on the full many-body Hilbert space can then be expanded as

$$|\psi\rangle = \sum_{\{s_j\}} \Psi_{s_1, \dots, s_L} |s_1, s_2, \dots, s_L\rangle, \quad (3.10)$$

where the sum is performed over all configurations, i.e., all choices of the physical indices  $\{s_j\}$ . Here, the expansion coefficients  $\Psi_{s_1, \dots, s_L}$  can be considered as a tensor with  $L$  legs, as shown in top row of Fig. 3.3(a).

Now we choose a bipartition of the system between the first lattice site  $s_1$  and the rest of the system  $[s_2, \dots, s_L]$ . We then perform a Schmidt decomposition (i.e., SVD  $C$ ), and contract the resulting  $\Lambda$  matrix onto the right hand side of the system, factorising the initial tensor into two. We can then choose another bipartition between the first two sites  $[s_1, s_2]$  and the rest of the system  $[s_3, \dots, s_L]$ . Repeating this for

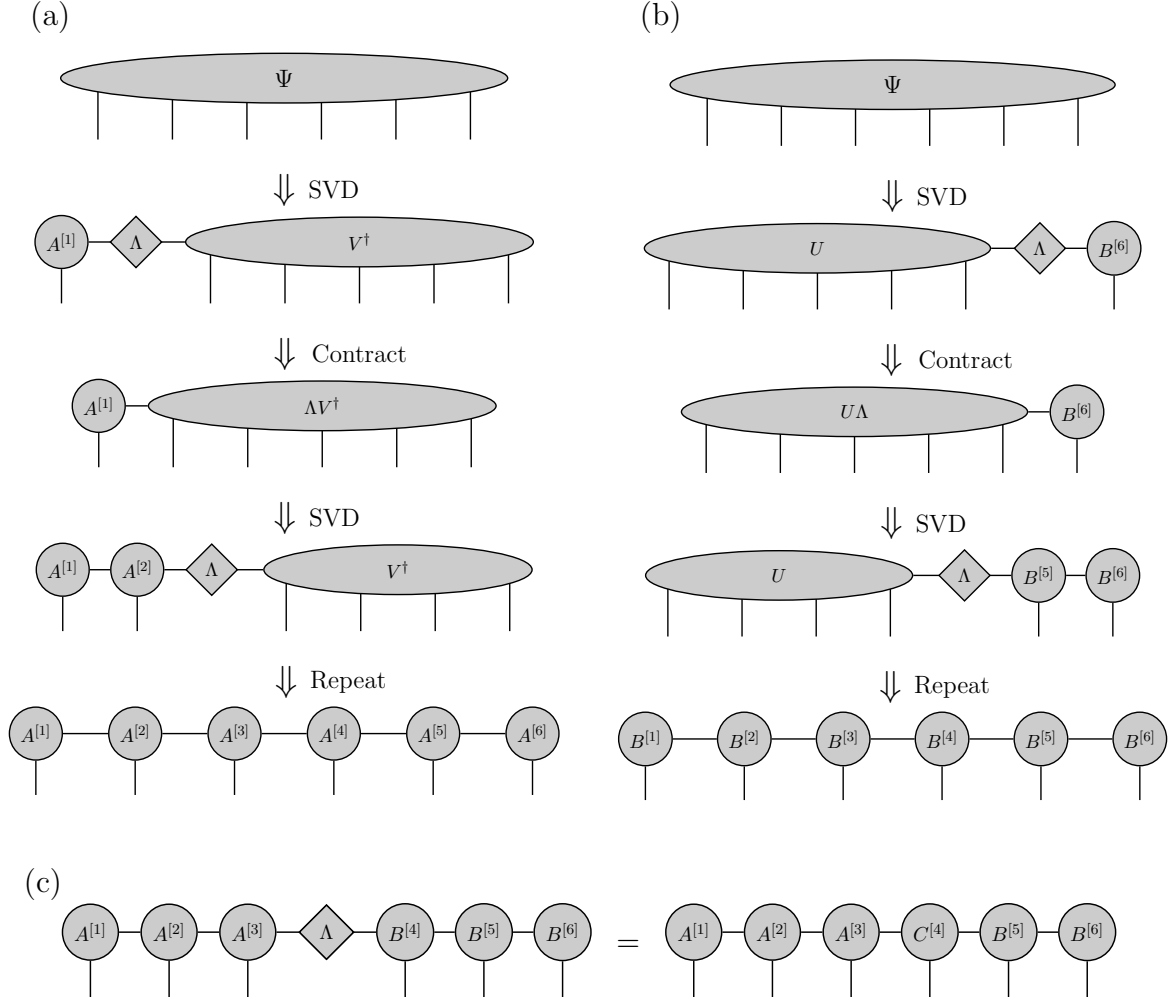


Figure 3.3: We show graphically the construction of an MPS from a full state vector  $|\psi\rangle$  (represented by a dense tensor  $\Psi$ ), via repeated SVDs and contractions. In (a) we start on the left site of the system, performing a series of SVDs and contractions until we obtain an MPS consisting of left-canonical  $A$  tensors which satisfy Eq. (3.12). If we begin instead with the rightmost tensor as in (b), we obtain an MPS of right-canonical  $B$  tensors satisfying Eq. (3.13). We can combine these two, performing SVDs from both the left and the right. Contracting the  $\Lambda$  matrix onto one of the nodes, as shown in (c), then yields a mixed-canonical MPS with a tensor  $C$  called the orthogonality centre.

all contiguous bipartitions of the system results in the tensor network at the bottom, which we write as

$$|\psi\rangle = \sum_{s_1, \dots, s_L} A^{[1]s_1} A^{[2]s_2} \dots A^{[L]s_L} |s_1, s_2, \dots, s_L\rangle. \quad (3.11)$$

Here we have suppressed the internal indices of the tensors, so  $A^{[j]s_j}$  for a given value of  $s_j$  is a matrix. The expansion coefficient for a given configuration  $\{s_j\}$  is then given by a product of matrices, and so this type of tensor network is called a matrix product state (MPS).

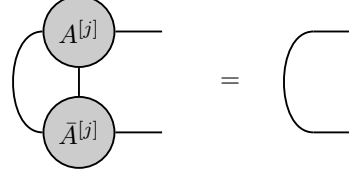
We have so far not made reference to any special properties of the state  $|\psi\rangle$ , or even to the geometry of the system in question, and so clearly this process of constructing an MPS can be carried out for any many-body state. In general, the maximum number of nonzero singular values at a bond will be  $d^{L/2}$  (at the central bond), and so the MPS would be no more efficient than the full vector representation. However, if at each bipartition we are able to truncate the number of singular values kept, then the number of coefficients needed to represent the state can be greatly reduced. In particular, if we consider MPS which have a fixed maximum bond dimension  $\chi \ll d^{L/2}$ , independent of  $L$ , then we see that the entanglement entropy for any contiguous bipartition is bounded by  $\log_2 \chi$  (for  $\chi$  uniform Schmidt coefficients), independent of the size of the system. In other words, the MPS with fixed bond dimension automatically satisfy the area law discussed in the introduction. We can therefore expect MPS to accurately capture ground states and low-lying excited states of gapped, local Hamiltonians, with a number of parameters  $\mathcal{O}(\chi^2 L)$ .

One can think of the process of constructing an MPS as a form of data compression. Broadly speaking, data compression works by making assumptions about the structure of the data being considered, and using this to construct a representation with a much smaller number of parameters compared to the uncompressed data. This is precisely what is done with an MPS, i.e., we make the assumption that our state is weakly entangled. MPS compression has been applied to systems outside the context of quantum mechanics, including image compression [53], and for efficiently finding solutions to partial differential equations [54, 55]. In these contexts, MPS are sometimes called tensor trains [56].

### 3.4.1 Canonical forms

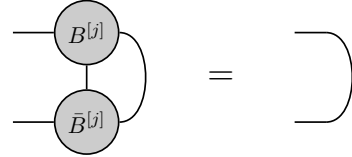
MPS representations of states are not unique, which can easily be seen by inserting a resolution of the identity  $X^{-1}X$  in between two tensors in the chain. This gauge

freedom leads to so-called “canonical forms”, which simplify many MPS algorithms. In fact, following the left-to-right SVD sweep in Fig. 3.3(a), we find that since all of the  $A$  tensors except for the final one are formed from the  $U$  matrices of the SVD, they inherit its unitarity and thus obey the orthogonality relation



$$\sum_{\alpha, s_j} A^{[j]s_j} (A^{[j]s_j})^\dagger = \mathbf{1}. \quad (3.12)$$

Instead choosing our first bipartition to be between the last two sites, and sweeping from right to left as shown in Fig. 3.3(b) yields an MPS where the tensors obey the different orthogonality relation

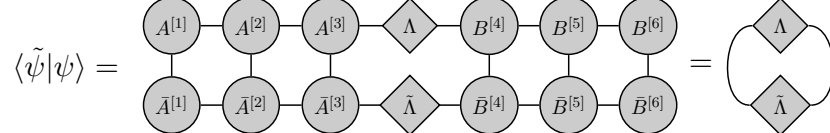


$$\sum_{\beta, s} B^{[j]s_j} (B^{[j]s_j})^\dagger = \mathbf{1}. \quad (3.13)$$

Finally, instead of sweeping in one direction, one can perform SVDs from both the left and the right, resulting in the form given in Fig. 3.3. The tensors to the left of the  $\Lambda$  matrix obey Eq. (3.12), while the tensors to the right obey Eq. (3.13). We therefore can see that this form is equivalent to the Schmidt decomposition of the system across this bond, with  $\Lambda$  being the Schmidt coefficients. The  $\Lambda$  matrix is sometimes contracted onto one of the neighbouring tensors resulting in the tensor  $C$  which is called the orthogonality centre, and obeys neither orthogonality relation. This is known as the mixed-canonical form, and is key to the efficiency, simplicity and stability in many MPS algorithms [20].

As an example of the usefulness of the mixed-canonical form, we discuss how to approximate an MPS by another MPS with a smaller bond dimension. In general, when one performs operations on an MPS, either variational minimisation or time evolution, the bond dimension of the MPS increases. In many circumstances this bond dimension growth can be exponential, and therefore it is essential for us to be able to reduce it again. Computationally, the cheapest way to do this is by performing a sequence of local truncations while exploiting the mixed-canonical form. Suppose

that  $|\psi\rangle$  is an MPS in mixed-canonical form. We choose a  $|\tilde{\psi}\rangle$  which is identical to  $|\psi\rangle$  except that we keep only the  $\tilde{\chi}$  largest singular values and set the rest to 0. The orthogonality conditions greatly simplify this inner product, and so the overlap between the two states is given by



$$\langle \tilde{\psi} | \psi \rangle = \sum_{i=1}^{\tilde{\chi}} \Lambda_i^2 < 1. \quad (3.14)$$

The fidelity error in approximating  $|\psi\rangle$  by  $|\tilde{\psi}\rangle$  is therefore given by the sum of the squares of the discarded singular values. Furthermore, having set the smallest singular values in  $\tilde{\Lambda}$  to 0, we can also throw away the parts of the tensors to the left and right of  $\tilde{\Lambda}$  which would be multiplied by these 0 values, thus reducing the number of parameters in our representation. Note that this is only possible due to the mixed-canonical form. If we did not have this, then the error would not be bounded by the discarded singular values, and the approximation would not be well-controlled. By performing contractions and SVDs to shift the orthogonality centre along the MPS, we can truncate each bond like this, obtaining a smaller MPS representation<sup>3</sup>. This is sometimes referred to as a “compression sweep”. Note that this amounts to transforming the MPS such that the decomposition as the bond to be truncated is the Schmidt decomposition. The truncation at that bond is then locally optimal.

### 3.5 Expectation values

Having a representation of a many-body state which uses only a small number of parameters is not, by itself, very useful. In order to be a useful parameterisation, we must also be able to efficiently extract physical properties of interest for the system (for example, local particle density, spin, and pair densities). Fortunately, MPSs provide a way to efficiently compute expectation values of operators. Consider, for example, the expectation value of a local operator which acts on a single site,

<sup>3</sup>Although this is cheap, it is not optimal. This is because although the truncations at each bond are optimal, the state at each truncation has already accumulated errors from all of the previous truncations. We are therefore compounding a sequence of local approximation which is not guaranteed to be globally optimal. To get the optimal approximation, we must perform the full variational minimisation of  $\| |\tilde{\psi}\rangle - |\psi\rangle \|^2$ , which can be done in a DMRG-style manner [57].

$$\langle \psi | \hat{O}_3 | \psi \rangle =$$

If the site on which the operator is applied is also the orthogonality centre of the MPS, then, using Eq. (3.12) and Eq. (3.13), the full expectation value calculation collapses to a contraction involving only three tensors, allowing efficient and simple computation.

As we will see in later chapters, the phases of many-body systems are often characterised by the long-range behaviour of correlation functions of the form  $\langle \hat{O}_j \hat{P}_{j+r} \rangle$ , where  $r \gg 1$ . We assume that the orthogonality centre is between sites  $j$  and  $j+r$ , so the tensors outside of this range once again collapse to identities. The expectation value contraction is given by

$$\langle \psi | \hat{O}_j \hat{P}_{j+r} | \psi \rangle =$$

We can then sequentially contract all of the legs from leftmost to rightmost in order to efficiently evaluate the expectation value.

Considering expectation values of this type can also provide further insight into the properties of MPSs. Let us assume that our state is translationally invariant<sup>4</sup> (as is common for many systems of interest, for example in condensed matter), so that all of the tensors in the MPS can be identical (up to a gauge transformation) and have a bond dimension  $\chi$ . We further assume that the MPS is in mixed canonical form with the orthogonality centre  $C$  on site  $j$ . All of the tensors to the right of this are therefore  $B^{[i]} = B$ . In this case, we can form the expectation value by defining the left boundary vector,

$$L_{a,b} = \sum_{\sigma, \sigma', \alpha} C_{\alpha,a}^{\sigma} O^{\sigma, \sigma'} \bar{C}_{\alpha,b}^{\sigma}, \quad (3.15)$$

the right boundary “vector”,

$$R_{a,b} = \sum_{\sigma, \sigma', \alpha} B_{a,\alpha}^{\sigma} P^{\sigma, \sigma'} \bar{B}_{b,\alpha}^{\sigma}, \quad (3.16)$$

<sup>4</sup>We will exploit this in Sec. 3.9 to efficiently compute the time evolution of an infinite system.

and the transfer operator,

$$E_{a,b,c,d} = \sum_{\sigma} B_{a,b}^{\sigma} \bar{B}_{c,d}^{\sigma}. \quad (3.17)$$

The transfer operator is closely analogous to the transfer matrix in statistical mechanics [58]. Following this analogy, we can construct the expectation value for the correlation function as

$$\langle \hat{O}_j \hat{P}_{j+r} \rangle = L E^{r-1} R, \quad (3.18)$$

where we have formed  $L$  into a row vector by merging the indices  $a$  and  $b$  in Eq. (3.15), and similarly formed  $R$  into a column vector. We have formed  $E$  into a  $\chi^2 \times \chi^2$  matrix by combining indices  $a, c$  on the left, and  $b, d$  on the right. We can expand the right boundary vector  $R$  in the right eigenvectors of  $E$ ,

$$R = \sum_i a_i X_i, \quad (3.19)$$

where  $X_i$  is the right eigenvector corresponding to the eigenvalue  $e_i$ . The correlator is then

$$\langle \hat{O}_j \hat{P}_{j+r} \rangle = L E^{r-1} R = \sum_i a_i e_i^{r-1} (L^\dagger X_i). \quad (3.20)$$

It can be shown rigorously that for a completely left- or right-orthonormalised MPS,  $e_i \leq 1$  [20]. However, on physical grounds one can argue that for systems with local interactions, correlators should not grow exponentially. Long range correlators therefore always take the form of a sum of exponential decays. At first glance, this would present a problem for many physical systems<sup>5</sup>, including those we will study in later chapters, whose correlators decay as a power law  $r^{-\alpha}$ . However, provided we have enough terms (i.e., our bond dimension is large enough), the sum-of-exponentials in Eq. (3.20) can approximate a power-law decay over a large number of sites.

### Example: The Ising model

As an example of this, we consider the ground state of the spin-1/2 transverse-field Ising model [3],

$$\hat{H}_{\text{Ising}} = -J \sum_j \left( \hat{S}_j^z \hat{S}_{j+1}^z + g \hat{S}_j^x \right). \quad (3.21)$$

where  $\hat{S}_j^{(x,z)}$  are operators acting on the local spin-1/2 degree of freedom on site  $j$ .  $J$  is the strength of the (ferromagnetic) coupling between adjacent spins, and  $g$  is the

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<sup>5</sup>An exception to this is  $\alpha = 0$ , which may result when, for example,  $\hat{O}$  and  $\hat{P}$  have nonzero expectation values and are not correlated

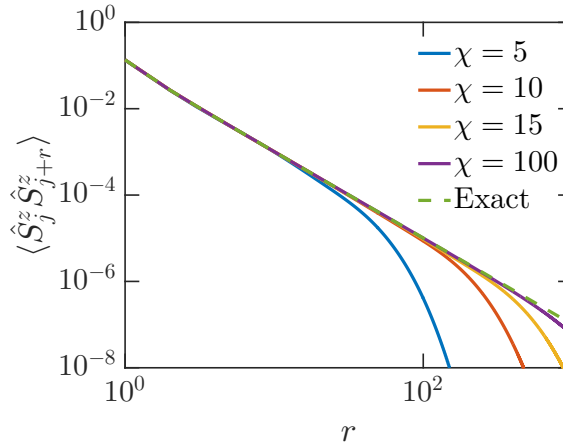


Figure 3.4: We illustrate how a power law decay can be approximated by an MPS. We show the correlator  $\langle S_j^z S_{j+r}^z \rangle$  for the critical Ising model for various bond dimensions  $\chi$ . The MPS naturally approximates the power-law decay by a sum of exponentials, and so an exponential tail develops after a correlation length governed by the smallest exponent  $e_i$  in Eq. (3.20). The larger the  $\chi$ , the more exponentials are included in the sum, and so the correlations are accurately approximated over a longer range. We computed these results with the iTEBD algorithm which we describe in Sec. 3.9.

relative strength of the applied transverse magnetic field. At  $g = 1$ , it is known that the two-point correlator is [59]

$$\langle \hat{S}_j^z \hat{S}_{j+r}^z \rangle = \frac{1}{\pi^2(4r^2 - 1)}. \quad (3.22)$$

We plot this in Fig. 3.4, along with the correlator computed from the MPS approximations of the ground state of the model, which we obtained by the infinite time evolving block decimation algorithm (see Sec. 3.9). We see that initially the MPS follows the analytical solution over a range of a few hundred sites, before it picks up an exponential tail due to the finite  $\chi$ . The larger we make the bond dimension, the more exponentials are used in the sum approximating the algebraic decay, and so the more accurate the approximation.

## 3.6 Matrix Product Operators

As well as local operators, we would also like to be able to work with larger operators which are defined across the entire  $L$ -site Hilbert space, for example, momentum space operators, or indeed the many-body Hamiltonian itself. Although these operators are typically sparse when written as matrices in the configuration basis, the size of the

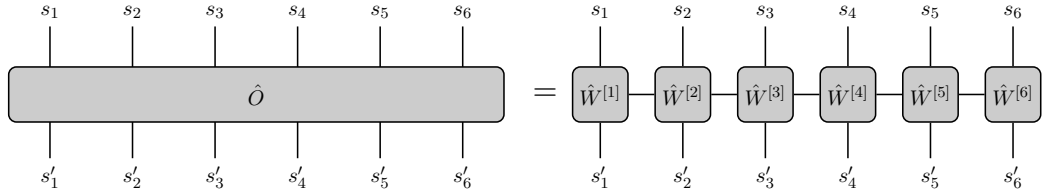


Figure 3.5: Graphical representation of a full operator on the left hand side, with its MPO form on the right.

operator will in general still grow exponentially just as the vectors did. Fortunately, by exploiting the same tensor network structure as the MPS, we can obtain a similarly efficient representation of many operators.

We can write any operator on our many-body Hilbert space as

$$\hat{O} = \sum_{\{s_j\}, \{s'_j\}} O_{s_1, s_2, \dots, s_L, s'_1, s'_2, \dots, s'_L} |s_1, \dots, s_L\rangle \langle s'_1, \dots, s'_L|, \quad (3.23)$$

where

$$O_{s_1, s_2, \dots, s_L, s'_1, s'_2, \dots, s'_L} = \langle s_1, s_2, \dots, s_L | \hat{O} | s'_1, s'_2, \dots, s'_L \rangle \quad (3.24)$$

are the matrix elements of the operator in the configuration basis, of which there are generally a number  $\mathcal{O}(d^{2L})$ .

Completely analogously to MPS, we can construct a tensor network representation for operators on our many-body Hilbert space, called matrix product operators (MPOs). One of the most important examples for us will be MPOs representing the Hamiltonians of our system, which will allow us to efficiently compute ground states of the Hamiltonian, as we discuss in Sec. 3.7. A second important example will be MPOs which represent the density operator, allowing us to carry out computations with mixed states on our Hilbert space, as explained in Sec. 3.11. Generically, using the same sequence of SVDs and contractions which yielded the MPS representation, we can obtain a representation of  $\hat{O}$  as an MPO,

$$\hat{O} = \sum_{\{s_j\}, \{s'_j\}} W^{s_1, s'_1} W^{s_2, s'_2} \dots W^{s_L, s'_L} |s_1, \dots, s_L\rangle \langle s'_1, \dots, s'_L|, \quad (3.25)$$

We have factorised the full operator into a contraction of  $L - 2$  rank-4 tensors, with one rank-3 tensor at each end to ensure that the resulting operator matrix elements are scalars. We show this decomposition graphically in Fig. 3.5. As with MPSs, if the maximum bond dimension of the MPO is bounded by  $D \ll d^L$ , then the MPO contains a number of parameters which scales only polynomially with the system size,

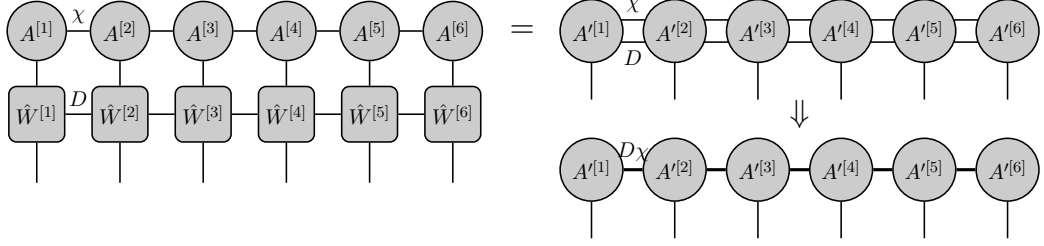


Figure 3.6: Graphical representation of an MPO with bond dimension  $D$  applied to an MPS with bond dimension  $\chi$ . By sequentially contracting the  $W$  tensors with the  $A$  tensors we obtain the  $A'$  tensors on the right hand side, with two internal legs per bond. By merging these two internal legs, we obtain the new MPS representation below with bond dimension  $D\chi$ .

$\mathcal{O}(LD^2d^2)$ . For this reason, we never want to construct the full operator representation, but instead construct and work with the MPO representation directly, which we discuss in Sec. 3.6.3.

### 3.6.1 Applying an MPO to an MPS

One commonly wants to compute the action of an operator onto a state. With the full representation, this would constitute the multiplication of a  $d^L$  element vector by a  $d^L \times d^L$  (potentially sparse) matrix. However, in the MPO representation, shown graphically in Fig. 3.6, we can perform the multiplication one site at a time. The total cost of this application is then  $\mathcal{O}(D^2d^2\chi^2L)$ , again exponentially faster than the full representation provided  $D$  is small<sup>6</sup>. By performing the contraction and then merging the resulting legs, we see that if the initial MPS has bond dimension  $\chi$ , and the MPO has bond dimension  $D$ , then the resulting MPS has bond dimension  $D\chi$ . As  $D$  can be fairly large, ranging from 1 – 100 depending on the operator, this can result in a rapid growth in bond dimension if we are required to compute a sequence of MPO multiplications (for instance, during a time evolution algorithm [60]). Fortunately, this new bond dimension is often (though not always) much larger than necessary to accurately represent the new MPS, and so one can perform a compression sweep to reduce the bond dimension while incurring only a small error. There are more efficient algorithms for computing these approximations without explicitly computing  $\hat{O}|\psi\rangle$  exactly, either by variationally minimising  $\| |\tilde{\psi}\rangle - \hat{O}|\psi\rangle \|$  [61], or by performing truncated SVDs after the application of each node [62].

<sup>6</sup>The naive cost of multiplying an  $m \times n$  matrix onto an  $n \times p$  matrix is  $\mathcal{O}(nmp)$

The observation that applying an MPO to an MPS grows the bond dimension by a factor  $D$  also provides a nice physical interpretation of the MPO bond dimension. Since the bond dimension  $\chi$  of an MPS is directly related to the amount of entanglement which can be captured by the ansatz, and applying an MPO grows this bond dimension by a factor  $D$ , the bond dimension of the MPO therefore corresponds to the maximum amount of entanglement which can be generated by the operator. The limiting case is an operator which is a tensor product of single-site operators. Such an operator has a bond dimension  $D = 1$  and does not increase the MPS bond dimension. More generally, we expect MPOs which represent Hamiltonians containing only local interactions should have a small bond dimension  $D$ , an observation which we will make more precise in Sec. 3.6.3.

### 3.6.2 Expectation values

One frequently uses MPOs to represent nonlocal observables (such as those in momentum space) in the system, and we would like to compute the expectation values of these operators with respect to some MPS. Such an expectation value is given by

$$\langle \psi | \hat{O} | \psi \rangle =$$

Since the network has no free legs, it represents a scalar value. It is important to note that the order in which we contract the tensors together is critical. If we first contract horizontally along the virtual legs of the MPS and MPO, and then the physical legs, then we end up reconstructing the full state vector, and so computing the expectation value would cost  $\mathcal{O}(d^L)$  operations. If we instead contract the physical legs of each column before contracting the virtual indices and moving on to the next column, then the cost of the contraction remains polynomial in both time and memory.

Even within this vertical contraction order we have some choice over which tensor to contract first, as we illustrate in Fig. 3.7. If we contract  $W$  first, then the total cost in time for the contraction is  $\mathcal{O}(\chi^2 D^2 d^2 + \chi^3 d^2 D)$ , while if we contract  $A$  first, the total time for the contraction is  $\mathcal{O}(\chi^2 D^2 d^2 + \chi^3 d D)$  (faster by a factor  $d$  in the second term). In general, the optimal contraction order is the one which minimises the product of the dimensions of the open legs throughout the contraction, though determining this order for a general tensor network is NP-hard [63, 64].

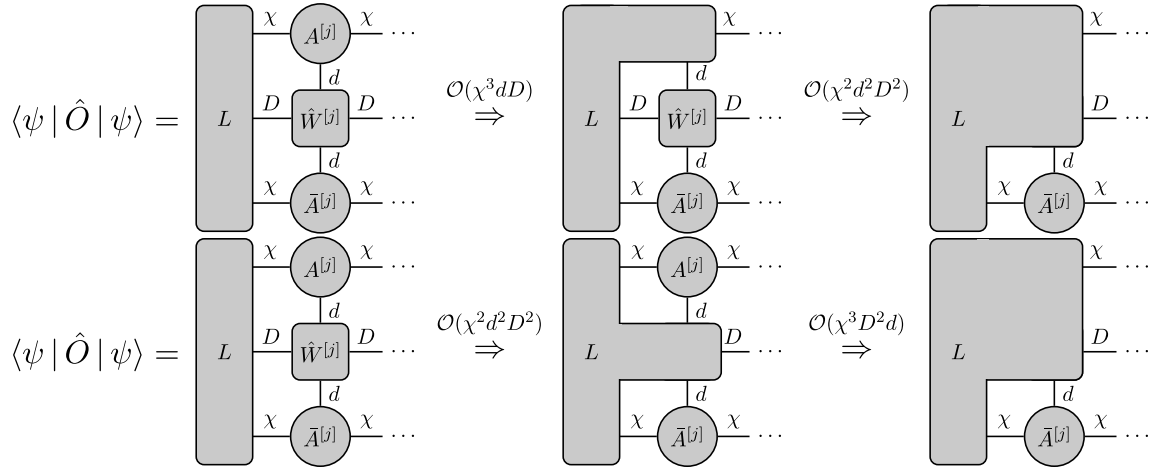


Figure 3.7: Graphical representation of an expectation value of an MPO. We note that the upper and lower contraction orders have different computational costs,  $\mathcal{O}(\chi^3 d D + \chi^2 d^2 D^2)$  compared with  $\mathcal{O}(\chi^3 d^2 D + \chi^2 d^2 D^2)$ , so the upper contraction order is faster by a factor  $d$  in the first term.

We conclude by pointing out that the property of MPS that expectation values are contractible in polynomial time is not a general feature of all tensor networks. For example, expectation values with respect to projected entangled pair states (PEPS), which are the generalisation of MPS to higher dimensions, are not contractible in polynomial time [65]. The calculation of expectation values must therefore be done approximately. Other tensor network states, like correlator product states [66], or neural network states [67, 68] are also not exactly contractible. However, individual matrix elements can be extracted in polynomial time, thus making them amenable to Monte Carlo sampling.

### 3.6.3 Constructing MPOs

We now turn our attention to how to construct MPO representations of operators. As outlined previously, one can always construct an MPO representation from the full matrix representation of the operator by sequential SVDs. However, this has an exponential cost, and so we need to be able to construct operators in their MPO form directly. To demonstrate how to explicitly construct MPOs, we draw a connection to finite state machines. Consider the MPO whose matrices are

$$\hat{W}^{[j]} = \hat{W} = \begin{pmatrix} \hat{A} & \hat{B} \\ 0 & \hat{C} \end{pmatrix}, \quad (3.26)$$

were we have formed the matrix on the right hand side by using the internal indices as the column and row indices of the matrix, with the physical indices of the operators folded into the matrix elements. Furthermore, we contract the left index of the first node, and the right index of the last node with the boundary vectors

$$\hat{L} = \begin{pmatrix} 1 & 0 \end{pmatrix} \quad \text{and} \quad \hat{R} = \begin{pmatrix} 0 \\ 1 \end{pmatrix}, \quad (3.27)$$

respectively, to ensure that the resulting operator has the correct dimensions. Multiplying out this MPO, we see that the resulting operator is

$$\begin{aligned} \hat{O} = & \hat{B} \otimes \hat{C} \otimes \cdots \otimes \hat{C} + \hat{A} \otimes \hat{B} \otimes \cdots \otimes \hat{C} + \cdots + \\ & \hat{A} \otimes \cdots \otimes \hat{A} \otimes \hat{B} \otimes \hat{C} + \hat{A} \otimes \cdots \otimes \hat{A} \otimes \hat{B}, \end{aligned} \quad (3.28)$$

i.e., the sum of all terms with a string of any number of  $\hat{A}$  operators, followed by a single  $\hat{B}$  operator, followed by a string of any number of  $\hat{C}$  operators. We can express this as a finite state machine (FSM):

```
state 1:
    Insert A and stay in state 1
    OR Insert B and move to state 2
state 2:
    Insert C and stay in state 2.
```

This may be concisely represented as the graph in Fig. 3.8(a), which consists of numbered vertices (representing the states) connected by directed edges (representing the allowed transitions between states)<sup>7</sup>. Each edge has an associated operator (which may be site specific). The full operator is constructed from the FSM as follows. Beginning at vertex 1, we follow the directed edges, appending the associated operator to the operator string. Whenever there are multiple edges leaving a vertex, we take the sum over the different possibilities.

We can then convert an FSM to an MPO representation in the following way. We first enumerate the graph vertices  $1, 2, \dots, N$ . Then, if two vertices  $i$  and  $j$  are connected by an edge then we simply insert the operator at element  $i, j$  in the MPO node. We can already see from this that the bond dimension  $D$  of the MPO is given by the number of vertices (or states) in the FSM.

FSMs are an important construct in the field of language processing. Languages which can be parsed by a FSM are so-called “regular languages”. Even when a language is not regular, a FSM is often used to perform lexical analysis on a stream

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<sup>7</sup>To avoid confusion, in tensor network diagrams we refer to nodes and legs, while in FSMs we refer to vertices and edges.

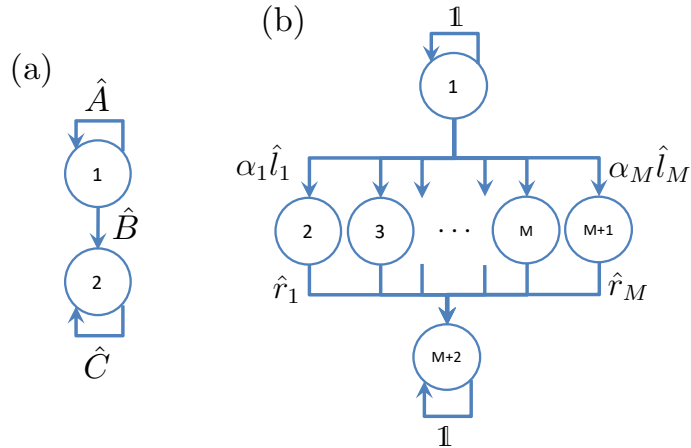


Figure 3.8: (a) The graph representation of a simple FSM corresponding to the MPO in Eq. (3.26). (b) The graph representation of the FSM corresponding to a sum of nearest-neighbour interactions Eq. (3.33).

of characters, converting it into a stream of “tokens”, after which more complicated relationships between the tokens are expressed. For the uninitiated reader, we provide a brief introduction to FSMs and language processing in Appendix A. This connection between regular languages, FSMs and MPOs provides a convenient and powerful insight into MPO representations of operators. Namely, if an operator is “simple” to write down (in the precise sense that it can be expressed as a regular expression), then it can be expressed in the form of a FSM and hence an MPO. The relationship is summarised by

$$\text{Regular Hamiltonian} \leftrightarrow \text{Finite state machine} \leftrightarrow \text{Matrix product operator.} \quad (3.29)$$

In the following examples, we will see that even when we know in principle how to construct the FSM of an operator, it can still be cumbersome to find a compact representation, as well as assign quantum numbers (see Sec. 3.10), and perform the Jordan-Wigner transformation for fermionic systems. We have therefore used the connection to language processing to implement a flexible and powerful interface for use in MATLAB with the TNT library [69]. This interface allows for the creation of MPOs and initiation of DMRG calculations simply by writing out the Hamiltonian in a  $\text{\LaTeX}$ -like script. We give a brief overview of this interface in Appendix B.

### Example: Sum of on-site operators

One of the simplest MPOS we can construct is a specific case of Eq. (3.26), namely a sum of on-site operators, e.g.

$$\hat{O} = \sum_j \alpha_j \hat{o}_j. \quad (3.30)$$

This is obtained by setting  $\hat{A} = \hat{B} = \mathbb{1}$ , and  $\hat{C} = \alpha_j \hat{o}_j$ , i.e.,

$$\hat{W}^{[j]} = \begin{pmatrix} \mathbb{1} & \alpha_j \hat{o}_j \\ 0 & \mathbb{1} \end{pmatrix}. \quad (3.31)$$

The trick of setting  $\hat{A} = \hat{B} = \mathbb{1}$  gives us all translations of the operator  $\alpha_j \hat{o}_j$  and is used very commonly in constructing MPOs.

### Example: Sum of nearest-neighbour operators

Models with only nearest-neighbour interactions, despite their simplicity, cover a wide range of Hamiltonians of interest, including the Ising model [3], (extended) Hubbard models for both bosons [34] and fermions [25], and the  $t$ - $J$  model [70]. In Fig. 3.8(b), we show the FSM for a sum of  $M$  nearest-neighbour interactions,

$$\hat{O} = \sum_j \sum_{k=1}^M \alpha_k \hat{l}_{j,k} \hat{r}_{j+1,k}, \quad (3.32)$$

where  $j$  is a site index, and  $k$  indexes the operators in the sum. For simplicity, here and in the following examples, we assume that the operator is translationally invariant, i.e.,  $\hat{l}_{j,k} = \hat{l}_k$ , but this need not be the case in general. Note that the fact that an operator  $\hat{l}_k$  *must* be followed by an operator  $\hat{r}_k$  is encoded in the structure of the FSM by the insertion of an additional vertex for each term in the sum. Translating the FSM to MPO form, we obtain

$$\hat{W}^{[j]} = \begin{pmatrix} \mathbb{1} & \alpha_1 \hat{l}_1 & \cdots & \alpha_M \hat{l}_M & 0 \\ 0 & 0 & \cdots & 0 & \hat{r}_1 \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & \cdots & 0 & \hat{r}_M \\ 0 & 0 & \cdots & 0 & \mathbb{1} \end{pmatrix}. \quad (3.33)$$

The bond dimension of this MPO is simply  $M + 2$ .

### Example: Sum of operator strings

We can generalise this further to strings of operators, i.e.,

$$\hat{O} = \sum_j \sum_{k=1}^M \alpha_k \hat{o}_{j,k} \hat{p}_{j+1,k} \cdots \hat{y}_{j+R(k)-1,k} \hat{z}_{j+R(k),k}, \quad (3.34)$$

where again  $j$  is a site index, and  $k$  indexes different terms.  $R(k)$  is the length of the operator string in term  $k$  (i.e., the range of the interaction in that term). Again, the FSM shown in Fig. 3.9(a) reflects the fact that if an operator  $\hat{o}_{j,k}$  appears in the string, then it must be followed by the rest of the  $k$ th string in sequence. The corresponding MPO nodes are

$$\hat{W}^{[j]} = \left( \begin{array}{c|cccc|c|cccc|c} \mathbb{1} & \alpha_1 \hat{o}_1 & 0 & \cdots & 0 & \cdots & \alpha_M \hat{o}_M & 0 & \cdots & 0 & 0 \\ \hline 0 & 0 & \hat{p}_1 & \cdots & 0 & \cdots & 0 & \cdots & \cdots & 0 & 0 \\ \vdots & \vdots & \ddots & \ddots & \vdots & \cdots & \vdots & \ddots & \ddots & \vdots & \vdots \\ \vdots & \vdots & \vdots & 0 & \hat{y}_1 & \cdots & \vdots & \ddots & \ddots & \vdots & 0 \\ \hline 0 & 0 & \cdots & \cdots & 0 & \cdots & 0 & \cdots & \cdots & 0 & \hat{z}_1 \\ \hline \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \vdots & \vdots \\ \hline 0 & 0 & \cdots & \cdots & 0 & \cdots & 0 & \hat{p}_M & \cdots & 0 & 0 \\ \vdots & \vdots & \ddots & \ddots & \vdots & \cdots & \vdots & \ddots & \ddots & \vdots & \vdots \\ \hline 0 & \vdots & \ddots & \ddots & \vdots & \cdots & \vdots & \cdots & 0 & \hat{y}_M & 0 \\ \hline 0 & 0 & \cdots & \cdots & 0 & \cdots & 0 & \cdots & \cdots & 0 & \hat{z}_M \\ \hline 0 & 0 & \cdots & \cdots & \cdots & \cdots & 0 & \cdots & \cdots & 0 & \mathbb{1} \end{array} \right). \quad (3.35)$$

The resulting MPO has a bond dimension  $2 + \sum_k R(k)$ . However, as we will see in the next subsection, if multiple terms share the same operators, then this construction can create some redundancy, which we can eliminate to obtain a more efficient representation. We can use such an MPO to create interactions with a finite range, or to implement Hamiltonians for ladder systems, as we discuss in more detail in the latter part of Chapter 4.

### Example: Approximating long-range interactions

Many physical interactions are not nearest-neighbour, or even have a finite range, as in the previous examples. Coulomb interactions [71], dipole-dipole interactions [72], and Rydberg interactions [73] all have power-law decay which can extend over many hundreds of sites. We have already seen in Sec. 3.5 that MPS cannot encode power-law-decaying correlators, but can approximate them by a sum of exponential decays.

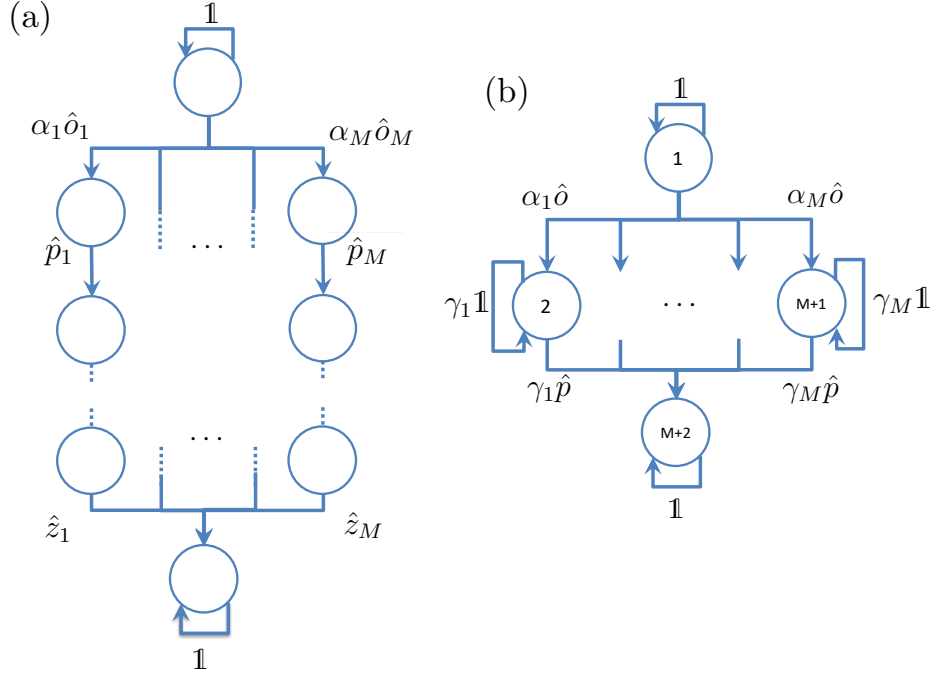


Figure 3.9: (a) The FSM graph representation of a sum of strings of operators. (b) The FSM graph representing a sum of exponentially decaying interaction terms.

Analogously, there is no exact MPO representation of a power-law decay, but we can easily represent a sum of (potentially complex) exponential decays, i.e.,

$$\hat{O} = \sum_{j=1}^L \sum_{k,r} \alpha_k (\gamma_k)^r \hat{o}_j \hat{p}_{j+r}. \quad (3.36)$$

We can see this from the FSM picture in Fig. 3.9(b), by considering vertices which are connected to themselves via an identity operator. If the coefficient in front of the identity operator is  $\gamma_k < 1$ , then each time we take that edge and thus move one site along in the term, the accumulated coefficient will be smaller by a factor  $\gamma_k$ . Thus after taking the edge  $r$  times, the term will have accumulated a coefficient  $(\gamma_k)^r$ . Translating from the FSM representation of this in Fig. 3.9(b), we see that the MPO nodes are

$$\hat{W}^{[j]} = \begin{pmatrix} \mathbb{1} & \alpha_1 \hat{o} & \alpha_2 \hat{o} & \cdots & \alpha_M \hat{o} & 0 \\ 0 & \gamma_1 \mathbb{1} & 0 & \cdots & 0 & \gamma_1 \hat{p} \\ \vdots & 0 & \gamma_2 \mathbb{1} & \ddots & \vdots & \gamma_2 \hat{p} \\ 0 & \vdots & 0 & \ddots & 0 & \vdots \\ 0 & 0 & \vdots & \ddots & \gamma_M \mathbb{1} & \gamma_M \hat{p} \\ 0 & 0 & 0 & \cdots & 0 & \mathbb{1} \end{pmatrix}, \quad (3.37)$$

and that the bond dimension of this MPO is  $D = M + 2$ . Now, suppose we want to approximate interaction

$$\hat{H} = \sum_j \sum_r J(r) \hat{o}_j \hat{p}_{j+r}. \quad (3.38)$$

To determine the values of the coefficients  $\alpha_p$  and exponents  $\gamma_p$  which best approximates this, we must solve the optimisation problem

$$\min_{\{\lambda_p, \alpha_p\}} \sum_{p=1}^M \sum_r^{r_{\text{cutoff}}} |\alpha_p (\gamma_p)^r - J(r)|^2. \quad (3.39)$$

Although this problem is nonlinear, the specific form of the exponential decay allows an efficient solution to be obtained using standard linear algebra methods [60]. In fact, this method can be used to approximate a wide class of functions. For example, since the exponents can be complex, Fourier series expansions are contained within this class of MPOs, and so any sufficiently smooth (in the sense that it is well approximated by a low-order Fourier series) interaction term can be efficiently represented by an MPO.

### 3.6.4 Addition and compression of MPOs

These FSMs allow us to construct efficient MPO representations for a wide range of Hamiltonians. However, two final ingredients are necessary in order to utilise these to their full potential. The first is the ability to add together two MPOs, the second is to reduce the dimension of a given MPO.

Recall from our definition of an FSM that if there is a branch at a vertex, then we take the sum the terms resulting from traversing the different paths. From this it is clear that to take the sum of two FSMs, we simply need to merge the first and last nodes. We show an example of this in Fig. 3.10, for the operators

$$\sum_j \hat{A}_j \hat{B}_{j+1} \hat{C}_{j+2} + \sum_j \hat{A}_j \hat{D}_{j+1} \hat{E}_{j+2} \hat{C}_{j+3}. \quad (3.40)$$

The first term has an  $D = 4$  MPO representation, and the second term has a  $D = 5$  MPO representation. Summing the two FSMs yields an FSM with two separate branches and an MPO with a bond dimension  $D = 7$ . In general, the sum of two FSMs with a number of vertices  $D_1$  and  $D_2$  will be  $D_1 + D_2 - 2$ . We now see that the FSMs in Fig. 3.9(a) have exactly the structure of single operator strings added together in this way.

However, this procedure often has the effect of introducing some redundancy in the FSM. In other words, the bond dimension of the corresponding MPO may be

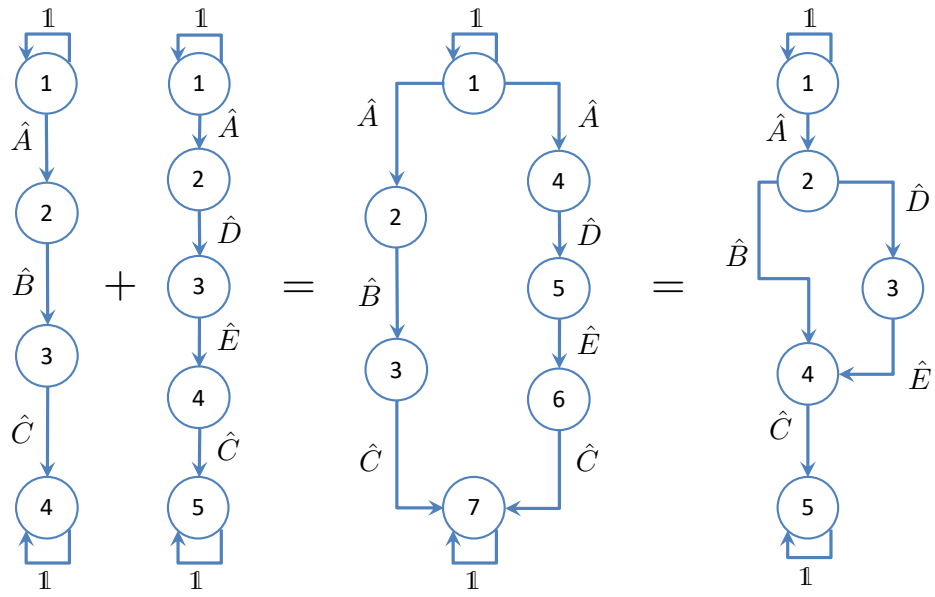


Figure 3.10: An example of the sum of two FSMs representing translations of operator strings. We take the sum by merging the first and last nodes of the FSMs to obtain the FSM in the centre. Then, because vertices 2 and 4 have identical *incoming* edges, we can merge them. Similarly, since vertices 3 and 6 have the same *outgoing* edges, we can also merge these. This results in the more efficient FSM representation on the right.

larger than necessary. As we discuss in Sec. 3.7, this can substantially impact the efficiency of calculations involving MPOs. Fortunately, in the FSM picture, it is simple to identify and eliminate such redundancies, as we illustrate with the example in Fig. 3.10. Because the two outgoing edges connected to the first vertex share the same operator ( $\hat{A}$ ), we can merge the two vertices these edges lead to without altering the FSM, thus reducing the number of vertices (and hence the MPO bond dimension  $D$ ) by one. Similarly, the two edges which connect to the last vertex both carry  $\hat{C}$  operators, and so we can merge the two vertices these edges come from. This gives the FSM on the right of Fig. 3.10, which has a number of vertices (and hence an MPO bond dimension) of 5.

MPO compression performed this way is essentially exact, i.e., there is no numerical imprecision coming from merging nodes. We conclude this section by noting that in some circumstances, calculations are not substantially affected by not having such an exact representation, and so it suffices to use a lower- $D$  MPO which merely approximates the original. This can be obtained by merging the physical legs of the MPO to form an MPS, and using the variational MPS compression given in [61].

### 3.7 Ground state calculations with MPS

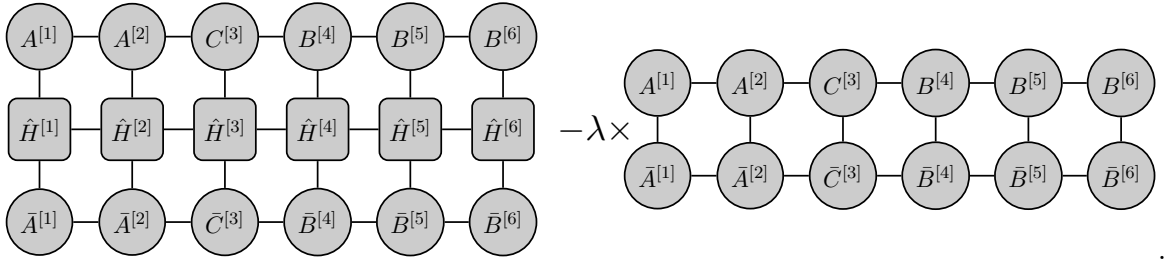
Having explained how to represent states and operators as one-dimensional tensor networks and extract useful quantities from these, we now discuss how to use these to compute properties many-body quantum systems.

The first algorithm we discuss is for computing ground states of many-body Hamiltonians. It has its origins in the density matrix renormalisation group (DMRG) algorithm by S. White [74]. It was later that the ground states produced by DMRG are MPSs [75]. It was since shown that variationally minimising the energy of an MPS leads to the same answer as DMRG [20]. As such, DMRG is sometimes used to refer to both the original White algorithm, and the variational approach. While DMRG and its variational successors are not guaranteed to converge to an (even approximate) ground state, it turns out that for local Hamiltonians, they usually converge to the ground state in polynomial time [20]. These algorithms have since developed into one of the leading methods for computing the ground states and low-lying excited states of one dimensional chains [76], ladder systems [77, 78], which we will discuss further in Chapter 4, and even two-dimensional systems [79], and quantum chemistry systems [80], which have an intrinsically nonlocal structure.

In the MPS approach, one simply takes an MPS  $|\psi\rangle$  as a variational ansatz for the ground state of a many-body Hamiltonian, and attempts to find the MPS which minimises the energy expectation value  $\langle\psi|\hat{H}|\psi\rangle$ . However, trying to simultaneously optimise all  $\mathcal{O}(d\chi^2L)$  parameters for the ansatz would still present a formidable computational task. Therefore, one typically resorts to updating only one or two tensors at each step [20].

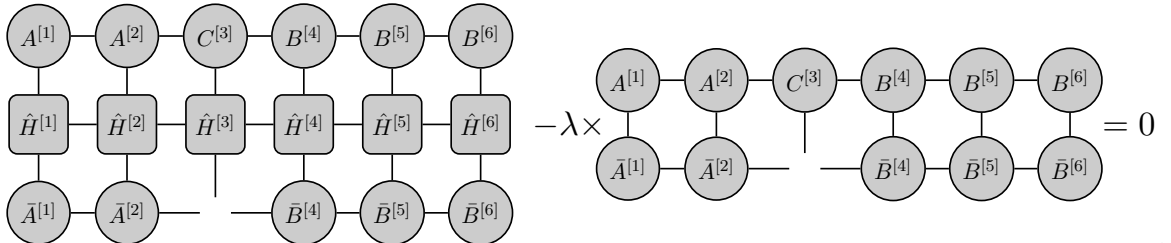
In the following we present the algorithm diagrammatically. For reasons that will become apparent shortly, we begin with an MPS  $|\psi\rangle$  which is in mixed canonical form with the orthogonality center  $C^{[j]}$  on site  $j$ , which we refer to as the “active site”. We begin by considering the expectation value  $\langle\psi|\hat{H}|\psi\rangle$ . We wish to optimise this with respect to the single tensor  $C^{[j]}$  while constraining the norm of the state  $\langle\psi|\psi\rangle = 1$ . We therefore introduce the Lagrange multiplier  $\lambda$ , and seek a minimum of the expression

$$\langle\psi|\hat{H}|\psi\rangle - \lambda\langle\psi|\psi\rangle, \quad (3.41)$$



To find the minimum, we then look for zeroes of the partial derivative with respect to the single tensor  $\bar{C}^{[j]}$ .

$$\frac{\partial}{\partial \bar{C}^{[j]}} \left( \langle\psi|\hat{H}|\psi\rangle - \lambda\langle\psi|\psi\rangle \right) = 0. \quad (3.42)$$



It is then clear from the graphical representation that this is, in fact, a generalised eigenvalue equation for the tensor  $C^{[j]}$ . To be explicit, we define  $\mathbf{H}$  to be the network in the first term with the tensor  $C^{[j]}$  and  $\bar{C}^{[j]}$  removed, and similarly  $\mathbf{M}$  is the network

in the second term with  $C^{[j]}$  and  $\bar{C}^{[j]}$  removed. Reshaping the networks  $\mathbf{H}$  and  $\mathbf{M}$  into matrices, and the tensor  $C^{[j]}$  into a vector, we obtain the generalised eigenvalue equation

$$\mathbf{H}C^{[j]} = \lambda \mathbf{M}C^{[j]}. \quad (3.43)$$

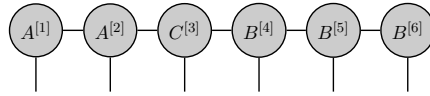
However, since we chose our MPS ansatz to be in mixed canonical form with the orthogonality center on site  $j$ , we can see that the contractions of the  $A$  tensors and the  $B$  tensors in the second term collapse to identities, i.e.,  $\mathbf{M} = \mathbf{1}$ . The equation then simplifies to a standard eigenvalue equation.

$$\mathbf{H}C^{[j]} = \lambda C^{[j]}. \quad (3.44)$$

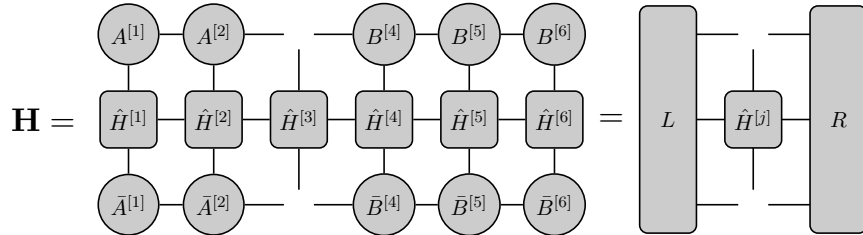
Therefore, to minimise the energy, at each step we choose  $A^{[j]}$  to be the eigenvector which corresponds to the smallest eigenvalue of the network  $\mathbf{H}$ , typically computed with the Lanczos method<sup>8</sup>[51]. This minimisation step has a nice physical interpretation. At each step, when we compute the eigenvector for the active site  $A^{[j]}$ , we are effectively asking the question ‘‘Given the state of the rest of the system (which we hope is close to the ground state), what is the effective Hamiltonian felt by site  $j$ ?’’. We then set the tensor at site  $j$  to be the ground state of this effective Hamiltonian. The new tensor then forms part of the environment for the optimisation of the next site. By iteratively sweeping back and forth, we eventually converge on an MPS approximation to the full many-body ground state.

To summarise, the basic ground-state algorithm is then given as follows:

1. Begin with an MPS with the orthogonality centre on site  $j$ .

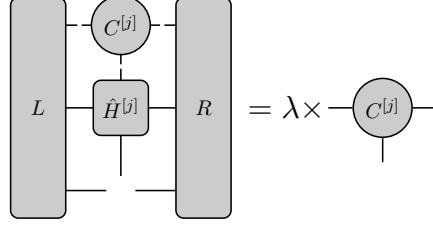


2. Construct the network  $\mathbf{H}$  by contracting the tensors to the left and right of site  $j$  with the Hamiltonian.

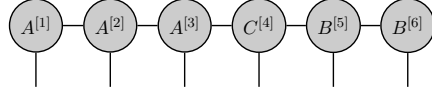


<sup>8</sup>This method is based on multiplying an initial guess for the vector by powers of  $H$ , which costs  $\mathcal{O}(\chi^3(d^2 + d)D)$  for our Eq. (3.44) [81]

3. Compute the eigenvector corresponding to the smallest eigenvalue of  $\mathbf{H}$ . This is the new tensor  $C^{[j]}$ .



4. Shift the orthogonality centre onto site  $j + 1$  by contracting together tensors  $j$  and  $j + 1$  performing an SVD, and contracting the resulting singular value matrix onto tensor  $j + 1$ .



5. Repeat from step 2, shifting the active site back and forth across the MPS until convergence is reached.

There are, however, a number of drawbacks with this single-site algorithm [81]. Firstly, there is no way to grow the Schmidt basis when performing the update, and thus we are stuck with a fixed bond dimension for the duration of the algorithm, even if the initial bond dimension is too small to accurately capture the ground state. Because of this, the algorithm is prone to getting stuck in local minima. There are two standard ways around this. First, and simplest, is to use a two-site update, where we simultaneously optimise two adjacent tensors [82, 81]. This means that Lanczos step costs  $\mathcal{O}(\chi^3(d^4 + d^2)D)$ , though this tends to be dominated by the cost of the subsequent SVD,  $\mathcal{O}(\chi^3 d^3)$ . However, this also means that each update will naturally increase the Schmidt basis, which can then be locally truncated if it is necessary to reduce the bond dimension. This also allows for the mixing of quantum numbers in  $U(1)$  symmetric problems (see Sec. 3.10). The second way is to only optimise a single site at a time, but to add a perturbation which expands the Schmidt basis, assisting the algorithm in avoiding getting stuck in local minima [83, 81].

A very simple technique for accelerating this procedure is to initially choose a small  $\chi$ , and increase it in stages. Since the number of variational parameters scales  $\sim \chi^2$ , the space of states the algorithm can search is greatly restricted, and thus it is less likely to get stuck in a local minimum. Similarly, since the time for each step scales  $\sim \chi^3$ , the algorithm finds the variational minimum,  $|\psi(\chi)\rangle$  much faster.

Even though this variational minimum is unlikely to be a good approximation to the true ground state, it is much closer in the space of MPS than a random state. Thus, increasing  $\chi \rightarrow \chi'$ , using  $|\psi(\chi)\rangle$  as an initial guess for  $|\psi(\chi')\rangle$  can result in convergence after many fewer sweeps than using a random initial MPS. This technique also has the advantage that one can compute expectation values at every step and study how they extrapolate to  $\chi \rightarrow \infty$ , approaching the “true” values of the ground state.

### 3.8 Time evolving block decimation

This variational algorithm provides an extremely powerful method for computing ground-state properties of one dimensional interacting quantum systems. However, of even greater interest to us in this thesis is how these systems behave dynamically, when driven out of equilibrium. Fortunately, the same MPS framework provides several related methods for computing time evolution for these systems. The simplest of these methods, the time evolving block decimation (TEBD) algorithm, was introduced by Vidal in 2003 [84, 85]. As the name suggests, it exploits the structure of short-range interacting Hamiltonians to compute the evolution in small, manageable “blocks”. It has since been generalised to nonunitary evolution [86, 87] and translationally-invariant infinite systems [85].

Here we explain the finite-system TEBD algorithm, before going on to discuss a variant which works directly in the thermodynamic limit, and how  $U(1)$  symmetries in the Hamiltonian can be exploited to greatly increase the efficiency of the algorithm’s fundamental steps. Finally, we discuss how to use TEBD to construct thermal states and evolve them unitarily.

Let us consider, for example, a generic Hamiltonian with nearest-neighbour interactions,

$$\hat{H} = \sum_{j=1}^{L-1} \hat{h}_{j,j+1}^{(2)} + \sum_{j=1}^L \hat{h}_j^{(1)} \quad (3.45)$$

where  $\hat{h}_{j,j+1}^{(2)}$  is an operator acting on nearest-neighbour sites  $j$  and  $j+1$ , while  $\hat{h}_j$  acts on only a single site  $j$ . In our Ising model example, Eq. (3.21),  $\hat{h}_{j,j+1}^{(2)} = -J\hat{S}_j^z\hat{S}_{j+1}^z$ , while  $\hat{h}_j^{(1)} = -Jg\hat{S}_j^x$ . We wish to compute the time evolution of a state under this Hamiltonian, i.e.,

$$|\psi(\tau)\rangle = e^{-i\hat{H}\tau} |\psi(0)\rangle. \quad (3.46)$$

However, even though  $\hat{H}$  may be sparse, or even written as an MPO, computing the operator exponential is still  $\mathcal{O}(d^L)$ . However, we can use the fact that the interactions are purely local to greatly reduce the cost of computing the evolution. For convenience, we regroup the terms of the Hamiltonian as

$$\hat{H} = \sum_{j=1}^{L-1} \hat{T}_{j,j+1}, \quad (3.47)$$

where

$$\hat{T}_{j,j+1} = \hat{h}_{j,j+1}^{(2)} + l_j \hat{h}_j^{(1)} + r_j \hat{h}_{j+1}^{(1)} \quad (3.48)$$

where  $l_j = (1 + \delta_{j,1})/2$ , and  $r_{(L-1)} = (1 + \delta_{j,(L-1)})/2$ . Let us consider the evolution for a small timestep  $\delta\tau$ . We would perhaps intuitively want to decompose the propagator for the full system as a sequence of propagators for the two-site interaction,

$$e^{-i\hat{H}\delta\tau} \approx e^{-i\hat{T}_{1,2}\delta\tau} e^{-i\hat{T}_{2,3}\delta\tau} \dots e^{-i\hat{T}_{L-2,L-1}\delta\tau} e^{-i\hat{T}_{L-1,L}\delta\tau}. \quad (3.49)$$

However, in general, we will have that  $[\hat{T}_{j,j+1}, \hat{T}_{j+1,j+2}] \neq 0$ , and so this decomposition is not exact, only becoming so in the limit  $\delta\tau \rightarrow 0$ . This is, in fact, the first-order Trotter decomposition [88] for the propagator. The task of finding a more accurate approximation boils down to finding a decomposition

$$\exp(\delta\tau(A + B)) \approx F_1(A)F_2(B)F_3(A)F_4(B) \dots F_M(A), \quad (3.50)$$

where  $F_i(A)$  is some function (typically an exponential) of only the operator  $A$ . This breaks the exponential of the sum of two non-commuting operators  $A + B$  (which is expensive to compute) into a sequence of operators which are functions of only one of the operators  $A$  and  $B$ , which are cheap to compute. The first-order Trotter decomposition is given by

$$\exp(\delta\tau(A + B)) \approx S_1(\delta\tau) = \exp(\delta\tau A) \exp(\delta\tau B), \quad (3.51)$$

where it is easily verified by Taylor expanding the exponentials on both sides that the error in this decomposition is  $\sim (\delta\tau)^2 [A, B] + \mathcal{O}((\delta\tau)^3)$ . To derive a higher order expansion we first note that  $S(-\delta\tau)S(\delta\tau) \neq \mathbf{1}$ , so our first-order decomposition has the undesirable property that evolving the system forward in time by an amount  $\delta\tau$ , then evolving it backwards in time by the same amount does *not* return us to our initial state. To rectify this we symmetrise the decomposition,

$$\exp(\delta\tau(A + B)) \approx S_2(\delta\tau) = \exp\left(\frac{\delta\tau}{2}A\right) \exp(\delta\tau B) \exp\left(\frac{\delta\tau}{2}A\right). \quad (3.52)$$

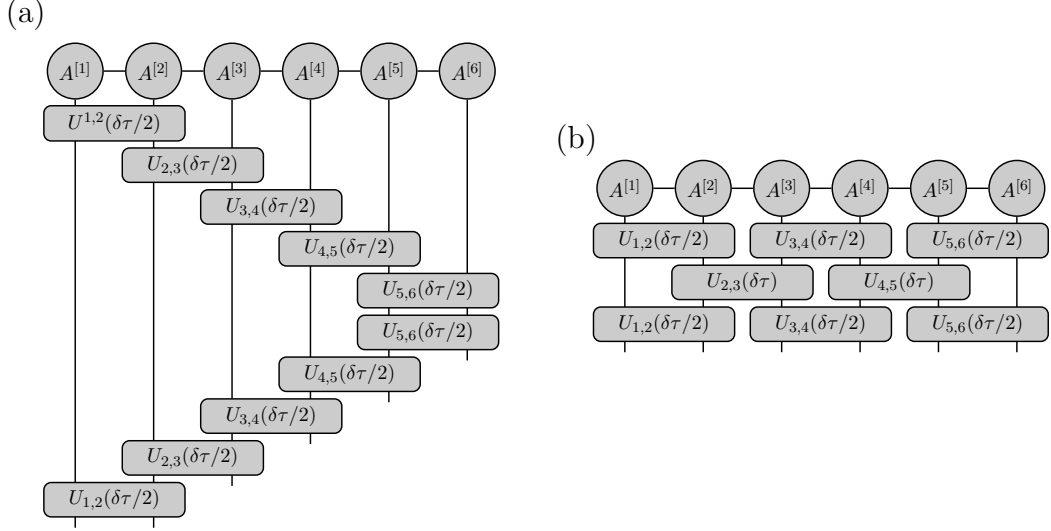


Figure 3.11: (a) The second-order Trotter decomposition of a unitary propagator as a “staircase”. (b) The second-order Trotter decomposition as a sequence of parallel, mutually-commuting gates on odd and even bonds.

We can immediately see that this decomposition *does* obey the relation  $S(-\delta\tau)S(\delta\tau) = \mathbb{1}$ . The term  $\sim (\delta\tau)^2$  then vanishes in the expression for the error.  $S_2(\delta\tau)$  is therefore a second order Trotter decomposition. By breaking up  $e^{\delta\tau(A+B)}$  into a product of more exponentials, one can derive higher order Trotter expansions. For completeness we state, but do not derive, a fourth-order Trotter expansion [88],

$$S_4(\delta\tau) = e^{\frac{s}{2}\delta\tau A} e^{s\delta\tau B} e^{\frac{1-s}{2}\delta\tau A} e^{(1-2s)\delta\tau B} e^{\frac{1-s}{2}\delta\tau A} e^{s\delta\tau B} e^{\frac{s}{2}\delta\tau A}, \quad (3.53)$$

where  $s = \frac{1}{2 - \sqrt[3]{2}}$ . Higher order decompositions are possible. However, as these involve greater numbers of contractions, it is generally not worth using when, as we outline below, the Trotter error is often small compared to the truncation error.

Returning to the many-body Hamiltonian, and armed with the second-order Suzuki-Trotter decomposition, we can now decompose the full propagator of width  $L$  into a sequence of two-site propagators. Note that we have some choice in how to do this, and two possible choices are shown in Fig. 3.11.

The “staircase” of operators shown in (a) may be obtained by successively applying the relation Eq. (3.52) repeatedly to the many-body propagator. It has the advantage that after each contraction, one can perform an SVD, and truncate while preserving the mixed-canonical form of the MPS, as we show in Fig. 3.12. We begin with an MPS in mixed-canonical form with the orthogonality centre on one of the sites connected

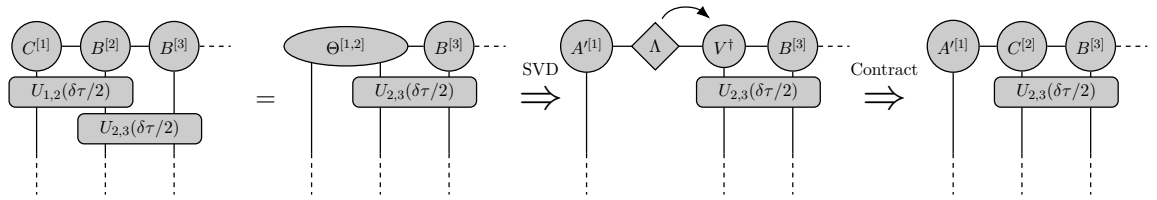


Figure 3.12: The contraction order for the staircase Trotter decomposition in TEBD. First we contract the two-site operator onto the MPS, ensuring that the orthogonality center is on one of the sites we apply the gate to. Then we SVD the two-site wide operator to re-obtain an MPS. We can then optionally truncate the bond dimension by discarding the smallest singular values in  $\Lambda$ , before shifting the orthogonality center onto the next site by contracting  $\Lambda$  onto it.

to the first two-site gate. We then contract the gate to form a two-site wide tensor  $\Theta^{[j,j+1]}$ . To restore the MPS, we SVD this node at a cost  $\mathcal{O}(\chi^3 d^3)$ . Note that the two-site gate will in general increase the entanglement between the two halves of the system. As such, in order to avoid uncontrolled growth of the bond dimension, we will need to discard the smallest singular values after the SVD. However, because we are in mixed-canonical form, from Sec. 3.4 we know that this truncation is optimal. Finally, we contract the resulting  $\Lambda$  matrix to the right, shifting the orthogonality centre ready for the next gate.

The even-odd decomposition in Fig. 3.11(b) has the advantage that many of the contractions can be done in parallel, since they do not depend on the result of other contractions on that layer. However, truncations cannot be performed in parallel without destroying the canonical form. As such, the truncations are not guaranteed to be locally optimal. Nevertheless, provided these truncations are small, the canonical form can be approximately preserved, and so with enough parallel resources, computation speed can be increased substantially.

### 3.9 Infinite TEBD

Even though finite MPS allow for an exponential improvements in terms of memory requirements and computation speed, one is often still limited to system sizes ranging from tens to hundreds of sites. However, for translationally-invariant systems, we can use MPS representations which reflect the translational invariance and hence rid ourselves from the need to store an individual tensor for every site, thus gaining a further factor  $L$  speedup.

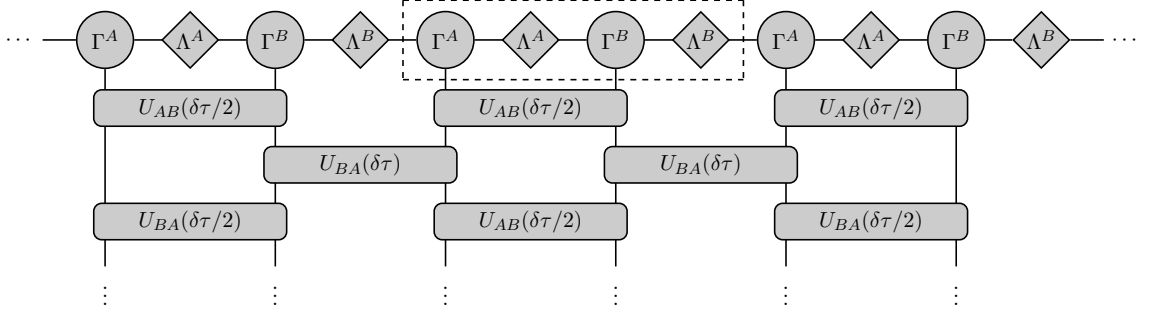


Figure 3.13: An iMPS constructed from a two-site unit cell (indicated with the dashed box). The operator  $U$ , which is Trotter-decomposed into two-site operators  $U_{AB}$  and  $U_{BA}$  is connected to the iMPS.

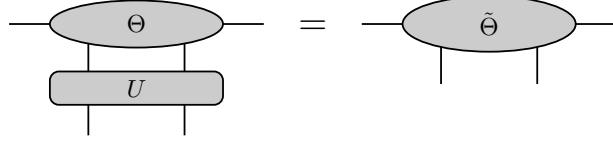
In this section we introduce the infinite TEBD (iTEBD) algorithm. We assume that our Hamiltonian is translationally-invariant with a two-site unit cell, and that therefore, in the absence of any spontaneous symmetry breaking, there exists an MPS ansatz which is also translationally invariant with a two-site unit cell consisting of site  $A$  and site  $B$ , which we use to describe the system. In order to be consistent with the literature, we keep the singular value matrices, which we denote  $\Lambda^A$  and  $\Lambda^B$ , separate from the physical tensors, which we label  $\Gamma^A$  and  $\Gamma^B$ .

A diagrammatic representation of the infinite-MPS (iMPS) is shown in Fig. 3.13, along with the second-order “odd-even” Trotter decomposition of a propagator. Because of the translational invariance, we only need to perform a contraction of one two-site gate  $U$  to evolve every even or every odd bond in the infinite state. To achieve this, we first contract together the tensors corresponding to an  $AB$  pair of sites as

$$\Theta_{s_A, s_B}^{AB} = \Lambda^B \Gamma_{s_A}^A \Lambda^A \Gamma_{s_B}^B \Lambda^B, \quad (3.54)$$

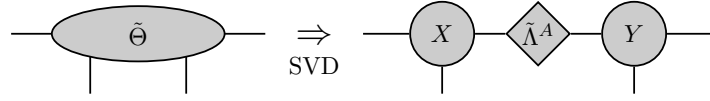
where we have suppressed the virtual indices in the  $\Lambda$  and  $\Gamma$  tensors, so that  $\Lambda^{(A/B)}$  and  $\Gamma_{s_{(A/B)}}^{(A/B)}$  are both matrices. We then apply the two-site gate  $U$  to the  $\Theta$  tensor to get the evolved tensor  $\tilde{\Theta}$ ,

$$\tilde{\Theta}_{s'_A s'_B} = \sum_{s_A, s_B=1}^d U_{s_A, s_B, s'_A, s'_B} \Theta_{s_A, s_B}. \quad (3.55)$$



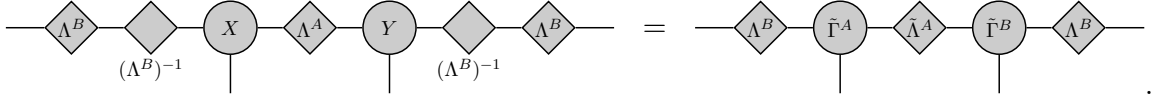
Note that here we use a tilde to denote evolved tensors. In order to get the iMPS for the evolved state, we then perform an SVD,

$$\tilde{\Theta}_{s_A s_B} = X_{s_A} \tilde{\Lambda}_A Y_{s_B}, \quad (3.56)$$



Note that since in general  $U$  will generate entanglement between the  $A$  and  $B$  sites, the bond dimension after the SVD will be larger. As such, for practical purposes, as in the finite MPS case, one truncates the bond dimension after the SVD to  $\chi$ . We discuss some technicalities of this truncation in Sec. 3.9.2. Finally, to extract the evolved  $\Gamma$  tensors, we multiply by the inverse of the  $\Lambda^B$  matrix, i.e.,

$$\tilde{\Gamma}_{s_A}^A = (\Lambda_B)^{-1} X_{s_A}, \quad \tilde{\Gamma}_{s_A}^B = Y_{s_B} (\Lambda_B)^{-1} \quad (3.57)$$



To evolve the  $BA$  bonds in the next step, we simply repeat these operations, exchanging the roles of the  $A$  and  $B$  tensors. Note that the multiplication by  $(\Lambda^B)^{-1}$  in the final step can cause numerical issues if  $\Lambda^B$  contains particularly small singular values, since a small error in the tensors  $X$  or  $Y$  resulting from the SVD will be greatly magnified. This can be avoided using a small modification proposed by Hastings [89], which stores and works exclusively with the products  $\Gamma^{A/B} \Lambda^{A/B}$ . This achieves the same result without the need to take this potentially problematic inverse.

### 3.9.1 Computing ground states with iTEBD

By setting the timestep to be the imaginary quantity  $-i\Delta\tau$ , we can also use the iTEBD algorithm to compute ground states of the infinite system [90]. The stationary state of this imaginary time evolution is given by

$$|\psi_{\text{GS}}\rangle = \lim_{\tau \rightarrow \infty} \frac{e^{-\tau \hat{H}} |\psi\rangle}{\|e^{-\tau \hat{H}} |\psi\rangle\|}, \quad (3.58)$$

where  $|\psi\rangle$  is any state which has nonzero overlap with the ground state. Every eigenstate with an energy  $\varepsilon_m > \varepsilon_0$  will decay exponentially at a rate  $\varepsilon_m - \varepsilon_0$ , and so in the limit  $\tau \rightarrow \infty$ , the component of the state which is not the ground state will have completely decayed away.

Since our Trotter decomposition of  $e^{-\tau\hat{H}}$  is not exact (as discussed in Sec. 3.8), the Hamiltonian implemented by the imaginary iTEBD is not exactly equal to the desired Hamiltonian, only becoming exact as  $\Delta\tau \rightarrow 0$ . On the other hand, the smaller we make the timestep, the more steps it takes to converge to the stationary state of Eq. (3.58). There is therefore a tradeoff between converging quickly and converging accurately to the ground state. This can be partially alleviated if we initially use a coarse timestep which allows for relatively quick convergence to a state which coarsely approximates the ground state. We then repeatedly reduce the timestep and evolve until convergence, thus reducing the Trotter error each time and gradually refining the state. This also has an added benefit in terms of the canonical form of the iMPS, which we discuss in the next subsection.

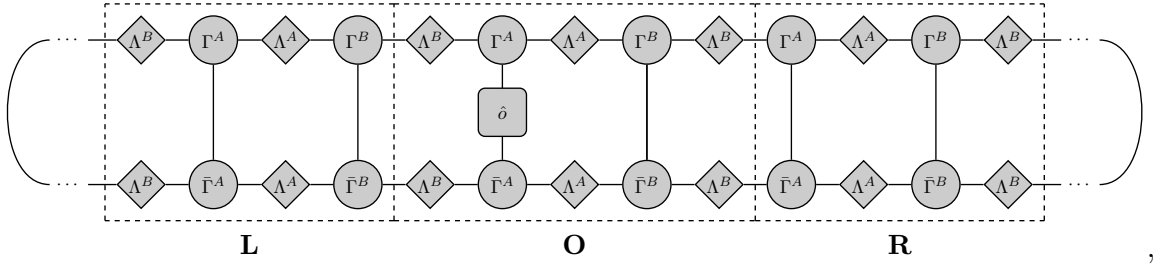
### 3.9.2 Canonical Form for iMPS

Just as with a finite MPS, we have a gauge freedom in the iMPS, as can be seen by inserting  $XX^{-1}$  pairs between each  $\Gamma$  and  $\Lambda$  tensor. Just as in the finite case, this gauge freedom implies the existence of a “canonical form” [91], which is crucial for truncations and expectation value calculations. For finite DMRG and TEBD, we saw that so long as we were careful with the order of SVDs, the convenient mixed-canonical form was automatically enforced. In the case of iMPS this is more involved. As we discussed in Sec. 3.4, a transfer operator built from left (right)-orthogonal tensors has the identity as a left (right) eigenvector with eigenvalue 1. In the case of iMPS, because the tensors are repeated infinitely, the identity must be both a left *and* right eigenvector of the transfer operator, which we show graphically in Fig. 3.14.

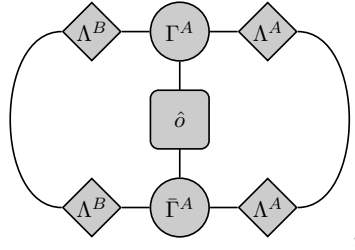
The canonical form is especially crucial for the computation of expectation values with iMPS. Suppose we wish to compute the expectation value of some local operator  $\hat{o}$ . If our iMPS were not in canonical form, then we would have to construct the network,



Figure 3.14: We show the condition for an iMPS to be in canonical form. This is the case if, at any bond, the transfer operator constructed from the  $\Gamma$  and  $\Lambda$  matrices satisfy both of these conditions (i.e., the identity is both a left and right eigenvector of the transfer operator)



where we insert the operator  $\hat{o}$  between the iMPS, and contract powers of the left and right transfer operators,  $\mathbf{L}^M$  and  $\mathbf{R}^M$  to the left and right side of this unit cell. To compute  $\langle \hat{o} \rangle$  in the thermodynamic limit, we must then take  $M \rightarrow \infty$ . This amounts to computing the dominant eigenvectors of the left and right transfer matrices, which is a rather expensive operation (especially if it is done every timestep during a real-time evolution). However, if the iMPS *is* in canonical form, when we contract identities onto the left and right of the “infinite” MPS, then the powers of  $\mathbf{L}$  and  $\mathbf{R}$  both collapse to identities, leaving us with



which is much simpler and computationally efficient.

It is simple to see that applying unitary gates without truncation (and thus evolving a state using real-time iTEBD) preserves the canonical form of the iMPS [91]. However, as the bond dimension will in general grow exponentially during the time evolution, we will eventually have to truncate, which is an inherently nonunitary operation. Fortunately, so long as the discarded singular values are small, the evo-

lution remains approximately unitary and thus the iMPS remains approximately in canonical form.

In order to take advantage of this, of course, we must begin the time evolution with a state that is already in canonical form. Product states are trivially in canonical form, but these are not very physical states. For example, we would like to be able to perform computations starting with the ground state of some Hamiltonian of interest. Unfortunately, for nonunitary processes like imaginary time evolutions, or like the simulation of the Lindblad equation for mixed states [86, 91], the canonical form is not preserved, and so the iMPS needs to be re-canonicalised before expectation values can be taken. This can be done in one of two ways. First, as described in Ref. [91], one can compute the dominant left and right eigenvectors of the appropriate transfer matrices, and use this to construct a gauge transformation which leaves the identity as the new dominant eigenvector. A simpler, but less efficient way is to repeatedly perform the iTEBD algorithm with  $U_{AB} = U_{BA} = \mathbb{1}$ , i.e., repeatedly performing SVDs on the odd and even bonds. It turns out that after every SVD the iMPS is brought closer and closer to canonical form.

Fortunately, for the specific case of imaginary time evolution, the procedure we describe in Sec. 3.9.1, where the timestep  $\delta\tau$  is systematically reduced, implements precisely this second method as a side-effect [91]. As  $\Delta\tau \rightarrow 0$ , the applied operators  $U = e^{-\hat{T}_{j,j+1}\Delta\tau} \rightarrow \mathbb{1}$ , and so provided we evolve for long enough with a very small imaginary timestep, the final MPS will be very nearly canonical form. We can thus compute expectation values of these iMPS without the costly construction of infinite left and right environments.

We conclude this section by pointing out a key advantage of infinite MPS algorithms compared to finite MPS. When studying condensed matter systems, we are interested in properties of the system in the thermodynamic limit, i.e., as  $L \rightarrow \infty$ . In any finite MPS calculation, observables will be affected by the presence of the boundary, and so it is necessary to compute them as various finite values of  $L$  and extrapolate to the thermodynamic limit [92]. Furthermore, as we saw in Sec. 3.5, a finite  $\chi$  induces a finite length scale beyond which correlations exponentially decay. It is therefore often necessary to also extrapolate to the  $\chi \rightarrow \infty$  limit. The interplay between the  $L \rightarrow \infty$  and  $\chi \rightarrow \infty$  limits must then be carefully accounted for [93]. In iMPS calculations, however, since the method works directly in the thermodynamic limit, one need only extrapolate in  $\chi$  [94].

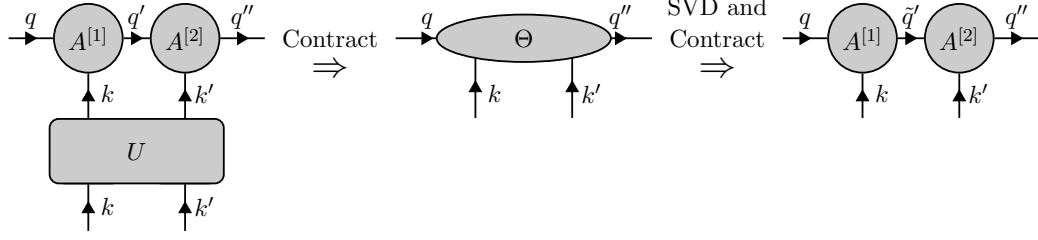


Figure 3.15: We show the application of a two site gate with  $U(1)$  symmetries. For any tensor or group of tensors, the sum of the incoming quantum numbers must be equal to the sum of the outgoing quantum numbers, leading to a block-diagonal form.

### 3.10 $U(1)$ symmetry and charge conservation

It is a broad general principle in physics that exploiting symmetries leads to a simplification of a problem, and this is equally true in the context of TNT. Here we will discuss the simplest case of this, namely the application of  $U(1)$  symmetries to MPS algorithms. If a many-body Hamiltonian has a  $U(1)$  symmetry, by Noether's theorem, there is a corresponding conserved charge [95]. Suppose we have such a charge

$$\hat{Q} = \sum_j \hat{q}_j, \quad (3.59)$$

where  $\hat{q}_j$  is the operator for some local charge at site  $j$ , such that  $[\hat{Q}, \hat{H}] = 0$ . Examples include the total  $z$  component of the spin  $\hat{S}^z = \sum_j \hat{s}_j^z$  in the Heisenberg model, or the total number of “up” and “down” fermions  $\hat{N}_\sigma = \sum_j \hat{n}_{j,\sigma}$  in the Hubbard and  $t$ - $J$  models, where  $\sigma \in \{\uparrow, \downarrow\}$ .

Since  $\hat{Q}$  commutes with the Hamiltonian, if we restrict the states we are considering to be eigenstates  $\hat{Q}|\psi\rangle = Q|\psi\rangle$  (for example, if we want to fix a fermionic model to a particular filling fraction), then the evolution under the Hamiltonian will never take us out of this subspace. As we will see shortly, this can greatly reduce the computational effort of tensor network algorithms. Here we focus specifically on the case of MPS, and for simplicity, we will assume that each site of the MPS has the same physical dimension (i.e., the many-body system consists of  $L$  copies of the same  $d$ -dimensional physical system e.g. spin-1/2 sites).

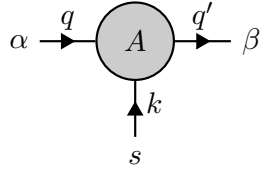
First, we require that the local physical basis states of our MPS are eigenstates of the conserved charge operators  $\hat{q}_j$ . That is,

$$|\psi\rangle = \sum_{\{s_j\}} A^{[1]s_1} A^{[2]s_2} \dots A^{[L]s_L} |s_1\rangle |s_2\rangle \dots |s_L\rangle. \quad (3.60)$$

where

$$\hat{q}_j |s_j\rangle = k_j(s_j) |s_j\rangle. \quad (3.61)$$

In other words, for each value of the physical index  $s_j$ , we can assign a corresponding (possibly non-unique) integer quantum number  $k_j$ . If the state is  $U(1)$  covariant (i.e., it has a well defined total charge  $Q$ ) then we can construct each node in the network to be  $U(1)$  invariant [82, 96]. This means that for each value of the internal indices  $\alpha, \beta$ , we assign a corresponding (again, possibly non-unique) quantum numbers  $q(\alpha)$  and  $q'(\beta)$  to the internal legs as well, i.e.,



Note that we have drawn arrows on the legs to indicate “incoming” and “outgoing” quantum numbers. Flipping the direction of an arrow flips the sign of the corresponding quantum number. Because the node is  $U(1)$  invariant, for any choice of the indices  $\alpha, \beta, s$ , we must have that  $A$  only has nonzero elements when the incoming and outgoing quantum numbers are equal [96],

$$q = q' + k. \quad (3.62)$$

As a result, if we reorder the matrix elements such that indices with the same quantum number are grouped together, then the tensor  $A$  acquires a block-diagonal form. This block-diagonal form results in much more efficient tensor operations. As an example, we take the application of a two-site gate during TEBD, shown graphically in Fig. 3.15. We require that the two-site gate is  $U(1)$  invariant, and that it therefore has the same set of physical quantum numbers  $k$  on each of its legs. When we contract this two-site gate to obtain the  $\Theta$  tensor, although it will couple different quantum number sectors, it will still be overall block-diagonal with  $q'' = q + k + k'$ . As a result, rather than performing one large contraction costing  $\mathcal{O}(\chi^2 d^2)$ , we can perform several smaller contractions at a cost  $\mathcal{O}(\sum_i \chi_i^2 d^2) < \mathcal{O}(\chi^2 d^2)$ , where  $\chi_i$  is the dimension of each matrix block.

We obtain a more significant speedup when we compute the SVD of  $\Theta$  to obtain our evolved MPS tensors, again due to the block-diagonal form of  $\Theta$ . Rather than performing an SVD costing  $\mathcal{O}(\chi^3 d^3)$ , we can perform the SVD for each block independently at a reduced cost of  $\mathcal{O}(\sum_i \chi_i^3 d^3)$ . Note that after the SVD, we will have a new set of quantum numbers on the centre bond  $\tilde{q}'$  which will in general be different

from the initial numbers  $q'$ . As a simple example, a nearest-neighbour hopping process  $(\hat{c}_j^\dagger \hat{c}_{j+1} + \text{H.c.})$  will redistribute particles on sites  $j$  and  $j + 1$ , altering the quantum numbers  $q'$ , while leaving the total number of particles on the two sites (and thus  $q$  and  $q''$ ) unchanged. Similar speedups are also obtained when finding eigenvectors and performing SVDs in the DMRG algorithm [20].

### 3.11 Mixed state evolution with MPOs

So far in this chapter we have discussed the use of matrix product methods for efficiently computing ground states, and the time evolution of pure states under unitary dynamics. However, in reality, many-body quantum systems (particularly solid-state systems) are rarely isolated from their environments, and so a mixed-state description of the state is more appropriate. In this section we therefore discuss one approach to performing mixed-state computations with tensor networks.

A density operator,  $\hat{\rho}$ , must satisfy two conditions [52]. Firstly, because its diagonal elements with respect to an arbitrary (but complete) set of orthonormal basis vectors  $|\phi_m\rangle$  represent the probabilities to measure the system in the state  $|\phi_m\rangle$ , we must have

$$\langle \phi | \hat{\rho} | \phi \rangle \geq 0, \quad (3.63)$$

for any  $|\phi\rangle$  in the Hilbert space (i.e., the operator is positive<sup>9</sup>). Secondly, because these probabilities must sum to unity, we must also have

$$\text{Tr}(\hat{\rho}) = 1. \quad (3.64)$$

Taken together, Eq. (3.63) and Eq. (3.64) imply that  $\hat{\rho}$  is Hermitian. As we discussed in Sec. 3.6, we can construct an MPO for any operator by performing successive SVDs. When the operator in question is a density operator, the resulting tensor network is called a matrix product density operator (MPDO), to distinguish it from those which do not satisfy the conditions in Eq. (3.63) and Eq. (3.64).

There is also a very physical way of constructing MPDOs which automatically satisfy Eq. (3.63) and Eq. (3.64) by introducing an auxiliary system and “purifying” the state [87]. One begins with an MPS  $|\psi\rangle$  with  $2L$  sites, where the odd sites belong to the physical system of interest, and the even sites belong to the auxiliary system (which effectively acts as a bath). If we then form the density operator of the full system  $|\psi\rangle\langle\psi|$ , and trace out the auxiliary system, then by appropriately grouping together the nodes, the resulting MPO is positive by construction.

---

<sup>9</sup>This is equivalent to the operator having all non-negative eigenvalues.

### 3.11.1 Time evolution of density operators

In Chapter 6, we will be particularly interested in the simplified special case of unitary evolution of initial mixed states under a periodically-driven Hamiltonian. Here we describe how to use a slightly modified TEBD algorithm to compute MPDO representations of thermal states and then evolve them unitarily.

The density operator for a system in thermal equilibrium at an inverse temperature  $\beta = 1/(k_B T)$ , where  $k_B$  is Boltzmann's constant and  $T$  is the temperature, is

$$\hat{\rho} = \frac{e^{-\beta \hat{H}}}{\text{Tr} \left( e^{-\beta \hat{H}} \right)}. \quad (3.65)$$

As already pointed out in Sec. 3.8, even if  $\hat{H}$  were written in MPO form, exponentiating it would present formidable task. Therefore we restrict ourselves to Hamiltonians with nearest- or next-nearest-neighbour interactions and use a modified version of the TEBD algorithm from Sec. 3.8, with an imaginary timestep  $\Delta\tau = -i\Delta\beta/2$ . We begin with an MPO representation of the identity matrix, i.e., an infinite temperature state

$$\hat{\rho}_0 = \mathbb{1}_d^{\otimes L}, \quad (3.66)$$

where  $\mathbb{1}_d$  is the  $d \times d$  density matrix, is a trivial MPO with bond dimension  $D = 1$ . We then contract each side with e.g. a second-order Trotter staircase, as we show in Fig. 3.16. We note that since each two-site gate,

$$U_{j,j+1}(\Delta\beta/2) = e^{-\hat{T}_{j,j+1}\Delta\beta/2}, \quad (3.67)$$

is the exponential of a hermitian two-site operator, the eigenvalues of  $U$  are all positive. Therefore, although due to the Trotter approximation we do not obtain the thermal MPDO of exactly the desired Hamiltonian, if we do not truncate the MPO, the resulting MPO still satisfies Eq. (3.63) and Eq. (3.64).

Once again, as applying the  $U$  gates will in general increase the correlations (both quantum and classical) in the MPDO, we will need to SVD and truncate to some maximum bond dimension  $\chi$  afterwards. We recall that it was only possible to do this truncation optimally when applying gates to an MPS because of the well-defined orthogonality centre on the bond where the gate  $U$  is applied. Since we can reshape each node of the MPO and combine the two physical legs into one, thus obtaining a vector on a larger Hilbert space, it is clear that the MPO also possesses an orthogonality centre which is preserved and shifted throughout the lattice by the TEBD

algorithm, thus assuring that the truncation after each gate  $U^{[j,j+1]}$  is optimal. Unfortunately, although this truncation is optimal in the sense it minimises the distance  $\|\hat{\rho}_{\text{Trunc}} - \hat{U}\hat{\rho}\hat{U}^\dagger\|^2$ , it can also introduce negative eigenvalues, thus leading to unphysical MPDOs if the truncation is large enough. However, we have not found this to be an issue so long as the truncation is not very large.

An alternative method that does not have this problem, which we will not discuss here in detail, is to return to the purification construction discussed above, but do not trace out the auxiliary sites, performing all time evolution with the purified system, only tracing out the auxiliary sites when computing expectation values [97]. This ensures that the final state of the system of interest is always a valid mixed state. However, the growth of entanglement between the system of interest and the auxiliary sites can limit the algorithm.

There is an additional issue with errors when computing lower temperature states (that is, larger  $\beta$ ) using imaginary time evolution. At each imaginary timestep, in order to manage entanglement growth, one must perform an SVD and truncation, which induces some noise in the state. The next imaginary timestep decays away the high energy part of the state (including the noise), but preserves the low-energy part of the noise. This can accumulate over many imaginary timesteps until very cold thermal states contain a significant amount of error, biasing the distribution towards lower energies compared to the true thermal distribution. For this reason one must take care in managing the truncation error when computing low temperature states.

Another approach to thermal state calculations is to construct an ensemble of MPS with low bond dimension called “minimally entangled typical thermal states” (METTS) [98, 62], such that the average of observables of interest over the ensemble is equal to the thermal average (up to some sampling error). The ensemble can even be evolved in real-time to compute the unitary dynamics of thermal states [99]. However, this introduces the added algorithmic complexity of managing many states in parallel.

## 3.12 Conclusions

In this chapter we have introduced very flexible and powerful tensor network algorithms for computing ground states and thermal states of one-dimensional many-body quantum systems, and the time evolution of these states. In Chapter 4, we apply the ground-state algorithm to compute the phase diagram of the one-dimensional  $t$ - $J$  model with pair-hopping, and then go on to apply DMRG to the 1.5 dimensional

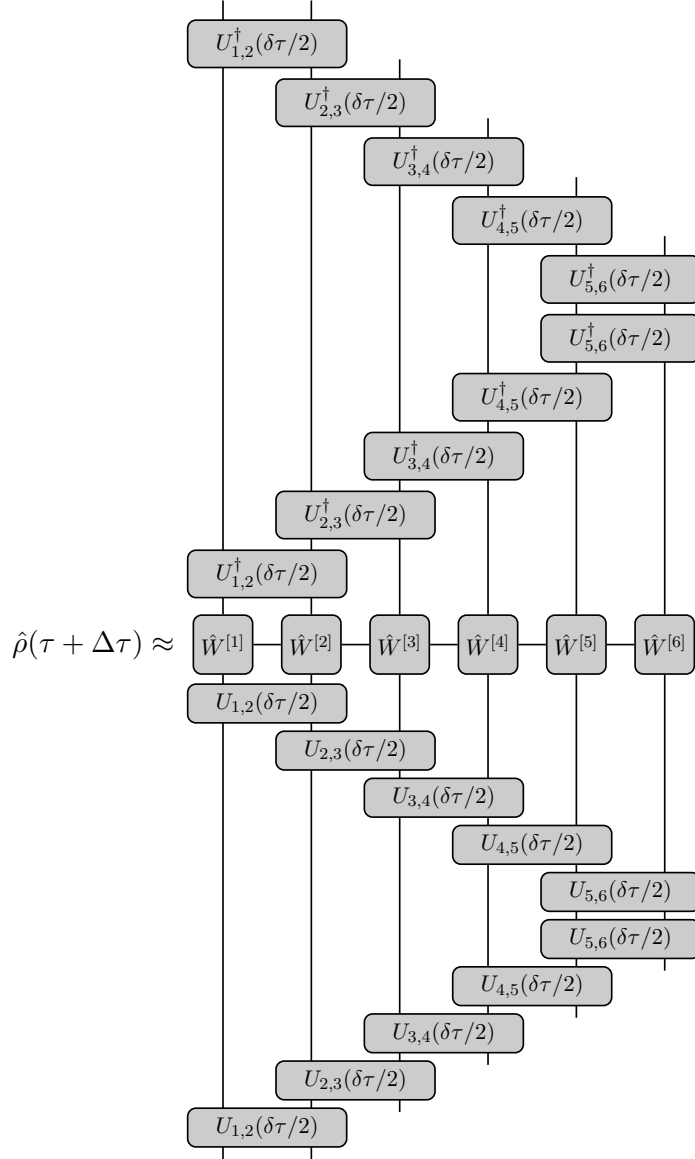


Figure 3.16: Time evolution of an MPDO using a modified TEBD. With a real timestep this implements unitary dynamics. With an imaginary timestep this constructs thermal states.

problem of this model on a ladder geometry. Later, in Chapter 6, we employ finite TEBD and iTEBD with both pure and thermal states to study the dynamics of a strongly periodically-driven Hubbard model at zero and finite temperature, and finite sizes and directly in the thermodynamic limit.

The success of tensor network theory in one dimension has led to algorithms based on generalisations of MPS to higher dimensions, known as projected entangled pair states (PEPS) for two dimensional systems [61, 100]. This ansatz is expressly designed for two dimensional systems and unlike MPS, can capture algebraically decaying correlations. Despite this, the increased computational cost of PEPS algorithms mean that DMRG remains competitive for many two-dimensional systems.

Further classes of tensor networks include tree tensor networks [101] and the multiscale entanglement renormalisation ansatz (MERA) [102], which have been developed to overcome some of the weaknesses of MPS (namely the failure to properly capture algebraically decaying correlations). Very recently, tensor network states have been unified with neural network states [67, 68]. These states, while not efficiently contractible, can capture explicitly capture states which violate the area law, unlike the tensor networks discussed here.

## Chapter 4

# The phase diagram of the $t$ – $J$ model in one dimension

The results presented in the first part of this chapter were published as J.R. Coulthard, S.R. Clark and D. Jaksch. Ground-state phase diagram of the one-dimensional  $t$ – $J$  model with pair hopping terms. *Phys. Rev. B* **98**, 035116 (2018). J.R.C. performed the calculations and wrote the majority of the manuscript.

The focus of this chapter is the  $t$ – $J$  model, which we introduced in Sec. 2.3. The model has long been a subject of significant interest as a prototypical model of strongly correlated electrons, because it encapsulates the physics of constrained hopping and magnetically induced real-space pairing (as opposed to the momentum-space pairing in BCS theory [103]). As such, the  $t$ – $J$  model has been widely studied for its relevance to high- $T_c$  superconductivity [104, 105], in particular with connection to resonating valence bond (RVB) physics [18, 11]. As we demonstrated in Sec. 2.3, the  $t$ – $J$  model emerges as an effective low-energy description of the Hubbard model in the limit  $t \ll U$ , giving rise to a super-exchange  $J = 4t^2/U$  [70, 38]. The validity of the model in this context therefore necessitates  $J/t \ll 1$ . For high- $T_c$  superconductors the regime of interest is  $J \sim 0.3t$  for a two-dimensional (2D) square lattice system close to half-filling [106].

Despite its long history, there is increasing motivation to re-examine  $t$ – $J$  model and explore its properties over a wider parameter space. A significant case for this will be presented in Chapter 6, where we show that periodically driving the Hubbard model breaks the perturbative connection between  $t$  and  $J$ , allowing  $J/t$  to be controlled by the drive, and the physics with  $J/t > 1$  to be explored [16]. Complementary to solid-state systems, the direct implementation of the Hubbard model and an experimental resolution of its low-temperature phase diagram has been a long-standing goal

of experiments with ultra-cold fermionic quantum gases in optical lattices [107, 108]. As we shall discuss further in Chapter 5, in these synthetic solids, strong periodic driving (such as lattice shaking) is also routinely used to engineer the band structure [109] and microscopic interactions of the system [110], as demonstrated recently for the super-exchange [111, 112, 113]. Thus, mapping out the complete phase diagram of the  $t$ - $J$  model provides a fuller picture of the strongly-correlated states one might engineer by driving the Hubbard model.

Motivated by these developments, in this chapter we map out the ground-state phase diagram of the  $t$ - $J$  model in 1D over a wide range of  $J/t$  and fillings. While much of the focus on the  $t$ - $J$  model is in 2D systems, the 1D system nonetheless possesses a rich phase diagram. Indeed, it exhibits many of the phases associated with correlated materials in higher dimensions, such as insulating, spin-gapped and superconducting phases. Moreover, in 1D, the DMRG algorithm introduced in Sec. 3.7 allows a precise diagnosis of these phases in an unbiased way for large system sizes, and accurate extrapolation to the thermodynamic limit.

To correctly capture all the physics arising from the  $t$ - $J$  model with varied fillings, we include the singlet-pair-hopping term discussed in Sec. 2.3. Close to half-filling it is often argued that pair-hopping processes are rare [38], and so most previous studies of the  $t$ - $J$  model have neglected this term [114, 115, 76, 116]. However, previous work on the large- $U$  Hubbard model has demonstrated that pair-hopping is essential to understand its optical properties when doped away from half-filling [117, 118]. Some earlier works analysing phases of the  $t$ - $J$  model have taken pair hopping into account [119, 120, 121, 122, 123], but were restricted to mean-field approximations (which tend to overestimate correlations) or used exact diagonalisations on very small systems. A key contribution of our work is that we address the  $t$ - $J$  model without these limitations.

We find the inclusion of pair-hopping leads to a dramatically different ground state phase diagram. In particular, it has a significant impact on superconductivity by pushing the metal-superconducting boundary to lower values of  $J/t$  at dilute fillings. Closer to half-filling, the pair-hopping simultaneously increases the size of the spin-gapped region and leads to the suppression of superconductivity, in line with mean-field calculations in two-dimensions [123]. We explain this effect by considering a simplified model of constrained hardcore bosons. This constrained model motivates us to consider ladder systems where two  $t$ - $J$  chains are coupled together in different geometries, where constraints may play an even more significant role in the physics.

This chapter is structured as follows. In Sec. 4.1 we recall the  $t$ - $J$  model and discuss the pair-hopping term. In Sec. 4.2 we present a selection of phase-diagrams and discuss how we characterise the various phases. We then introduce in Sec. 4.3 a constrained hardcore boson model and compare its properties to those of the  $t$ - $J$  model. In Sec. 4.5 we present DMRG results for two  $t$ - $J$  chains which are coupled together in different geometries. Finally, we conclude in Sec. 4.6.

## 4.1 The $t$ - $J$ model

As we demonstrated in Sec. 2.3, in the limit  $t \ll U$  of the Hubbard model, double-occupancies are energetically suppressed. However, second-order processes, where different singly-occupied configurations are connected by virtual excitations to and from these doubly-occupied states, give rise to the  $t$ - $J$  model describing the effective low-energy dynamics. The  $t$ - $J$  model Hamiltonian may be written formally as [119]

$$\begin{aligned} \hat{H}_{tJ\alpha} = & -t \sum_{\langle ij \rangle \sigma} (\hat{f}_{i,\sigma}^\dagger \hat{f}_{j,\sigma} + \text{H.c.}) \\ & -J \sum_{\langle ij \rangle} \hat{b}_{ij}^\dagger \hat{b}_{ij} - \alpha J \sum_{\langle ijk \rangle} (\hat{b}_{ij}^\dagger \hat{b}_{jk} + \text{H.c.}), \end{aligned} \quad (4.1)$$

where  $t$  is the single-particle hopping amplitude,  $J = 4t^2/U$  is the strength of the super-exchange interaction and  $\alpha$  is a dimensionless constant of order unity. This model is built from projected fermionic annihilation operators for a spin- $\sigma$  fermion on lattice site  $j$ , defined as  $\hat{f}_{j,\sigma} = \hat{c}_{j,\sigma} \mathbb{P}_0$ , where  $\hat{c}_{j,\sigma}$  is the corresponding canonical fermionic annihilation operator. Recall that  $\mathbb{P}_0$  is a projector that eliminates double-occupations and is given by  $\mathbb{P}_0 = \prod_j (1 - \hat{n}_{j,\uparrow} \hat{n}_{j,\downarrow})$ , where  $\hat{n}_{j,\sigma} = \hat{c}_{\sigma,j}^\dagger \hat{c}_{\sigma,j}$  is the number operator for spin- $\sigma$  fermions on site  $j$ . The operator

$$\hat{b}_{i,j} = \frac{1}{\sqrt{2}} (\hat{f}_{i,\downarrow} \hat{f}_{j,\uparrow} - \hat{f}_{i,\uparrow} \hat{f}_{j,\downarrow}),$$

annihilates a spin-singlet on lattice sites  $i$  and  $j$ .

The  $t$ - $J$  model captures two significant pieces of physics. First, it subjects the motion of electrons in a tight-binding band with hopping amplitude  $t$  to a local constraint that excludes double-occupancies. Specifically, unlike  $\hat{c}_{j,\sigma}$ , the projection means that  $\hat{f}_{j,\sigma}$  operators do *not* obey the canonical fermionic anticommutation relations. This induces a non-Fermi liquid metallic state and accounts for density dependent band-narrowing effects [70]. Second, neighbouring electrons experience an antiferromagnetic Heisenberg super-exchange with amplitude  $J$ . This induces real-space singlet

pairing of electrons, which can subsequently hop with amplitude  $\alpha J$ , and accounts for the formation of superconducting and magnetically ordered insulating states.

As we showed in Sec. 2.3, the parameter  $\alpha$  is equal to  $1/2$  for a  $t$ - $J$  model arising from the equilibrium Hubbard model. To distinguish the Hamiltonian in Eq. (4.1) from the typically studied  $t$ - $J$  model, which takes  $\alpha = 0$ , we refer to it as the  $t$ - $J$ - $\alpha$  model from now on. We note that  $t$ - $J$ - $\alpha$  models arising from more complicated multi-band Hubbard models may not have  $\alpha = 1/2$ . Moreover, as we shall discuss in Chapter 6, and further in Appendix E, by adding a strong periodic driving term to the Hubbard model, we can obtain  $t$ - $J$ - $\alpha$  models where  $J/t$  and  $\alpha$  may be controlled by varying the driving strength. Consequently, in this chapter we consider the regime  $0 \leq J/t \leq 8$  and  $0 \leq \alpha \leq 1/2$  not accessible from equilibrium.

One can obtain a qualitative picture of the phases of the model via a simple energetics argument [124]. Solving the two electron problem, one finds that the binding energy of a nearest-neighbour singlet pair is given by [120]

$$E_{\text{pair}} = -J - 2\alpha J - \frac{4t^2}{J + 2\alpha J}. \quad (4.2)$$

Thus, in the dilute limit, comparing  $E_{\text{pair}}$  to the energy for two free electrons  $E_{\text{free}} = -4t$ , suggests that pair formation will occur for  $J/t \geq 2/(1 + 2\alpha)$ . These nearest-neighbour singlet pairs may subsequently quasi-condense to form a superconductor.

For yet larger  $J/t$ , the formation of phase-separated electron-rich and hole-rich regions might be expected [76]. The exact solution of a Heisenberg spin-chain gives the antiferromagnetic bond energy  $E_{\text{bonds}} = -2J \ln(2)$ . For  $\alpha = 1/2$  we see that  $E_{\text{pair}} < E_{\text{bonds}}$  for all values of  $J/t$ , meaning that singlet pairs will *never* freeze into larger antiferromagnetic clusters. As the pair hopping term increases the mobility of bound pairs, it is expected to destabilise antiferromagnetic clusters, even when  $J/t \gg 1$ . In the following sections we will discuss how we quantitatively determine the various phase boundaries.

## 4.2 Phase diagram

To compute the ground state phase diagram of the  $t$ - $J$ - $\alpha$  model, we use the finite system DMRG algorithm [74, 20] described in Chapter 3, as implemented in the open source Tensor Network Theory (TNT) library [69]. Further details of the DMRG calculation are provided in Appendix C. We consider a 1D chain of  $L$  sites containing a number of “up” and “down” fermions  $N_{\uparrow}$  and  $N_{\downarrow}$  respectively, where  $N_{\sigma} = \langle \sum_j \hat{n}_{j,\sigma} \rangle$ , and  $\langle \cdot \rangle$  denotes the expectation value with respect to the ground state. Fixing this

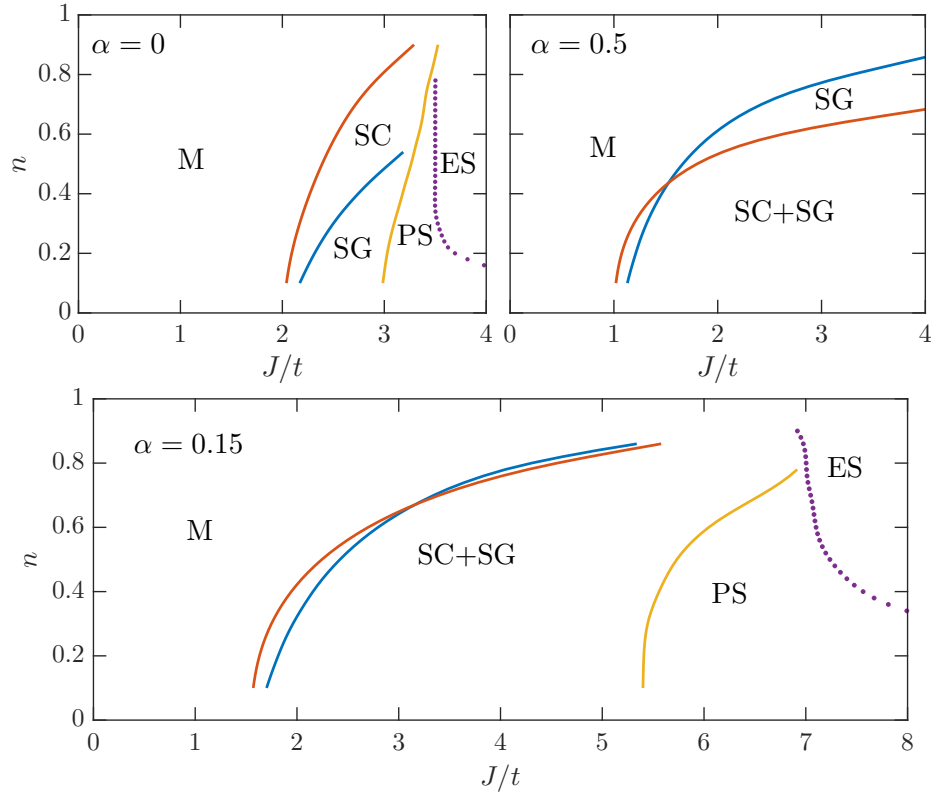


Figure 4.1: The phase diagrams for (a)  $\alpha = 0$ , i.e. the standard  $t$ - $J$  model, (b)  $\alpha = 0.15$ , and (c)  $\alpha = 1/2$ . Metal (M) Superconducting (SC), phase-separated (PS), electron solid (ES), and spin-Gapped (SG) phases are marked. Note that the PS and ES phases have vanished for  $\alpha = 0.5$ , which we have verified for up to  $J/t = 100$ .

filling results in a mean number of fermions per site  $n = (N_{\uparrow} + N_{\downarrow})/L$ . Note that except when determining the spin-gap in Sec. 4.2.3, we take  $N_{\uparrow} = N_{\downarrow}$ .

The main correlation functions of interest are the density-density correlations

$$N_{ij} = \langle \hat{n}_i \hat{n}_j \rangle - \langle \hat{n}_i \rangle \langle \hat{n}_j \rangle,$$

with  $\hat{n}_j = \hat{n}_{j\uparrow} + \hat{n}_{j\downarrow}$ , the spin-spin correlations

$$S_{ij} = \langle \hat{S}_i^z \hat{S}_j^z \rangle,$$

with  $\hat{S}_i^z = (\hat{n}_{i,\uparrow} - \hat{n}_{i,\downarrow})/2$ , and the nearest-neighbour singlet-pairing correlations

$$P_{ij} = \langle \hat{b}_{i,i+1}^{\dagger} \hat{b}_{j,j+1} \rangle.$$

We also compute the corresponding structure factors, i.e. the Fourier transforms of these quantities,

$$X(q) = \frac{1}{L} \sum_{jk} X_{jk} e^{iq(j-k)}, \quad (4.3)$$

where  $X$  is any of  $N$ ,  $S$ , or  $P$ . In the following subsections, Sec. 4.2.1–4.2.4, we explain the physics in at play in each of the phases, and how they are diagnosed using the correlation functions above.

Our main results, the phase diagrams for the  $t$ – $J$ – $\alpha$  model in the  $n$ – $J/t$  plane, are presented in Fig. 4.1. For  $\alpha = 0$ , we reproduce the results of Moreno *et al* [76]. We also show the phase diagrams for  $\alpha = 0.15$  and  $\alpha = 1/2$ , mapping the full range of phases induced by the pair-hopping, including metallic (M), superconducting (SC), spin-gapped (SG), and phase-separated (PS) phases and electron solid (ES) phases.

For all three values of  $\alpha$  shown in Fig. 4.1, the ground state for small  $J/t$  is a correlated metal. As the strength of the superexchange interaction increases, antiferromagnetic pairs begin to form, and the system crosses into a superconducting phase, which exhibits a slow algebraic decay of singlet correlations. Further information about the nature of pairs in the system is provided by the presence or absence of a spin-gap. As we discuss in Sec. 4.3, the presence of a finite spin-gap indicates that all fermions in the system are bound into nearest-neighbour singlet pairs. Contrary to the small exact diagonalisation results of Ammon *et al* [120], we find that superconductivity does not survive at all filling fractions. We do, however, find that the spin gap extends outside of the superconducting region, indicating a gas of preformed pairs. For weaker values of the pair hopping  $\alpha = 0$  and  $\alpha = 0.15$ , at sufficiently large  $J/t$ , the superexchange interaction  $J$  wins over kinetic energy  $t$  and  $\alpha J$ , and the system phase-separates.

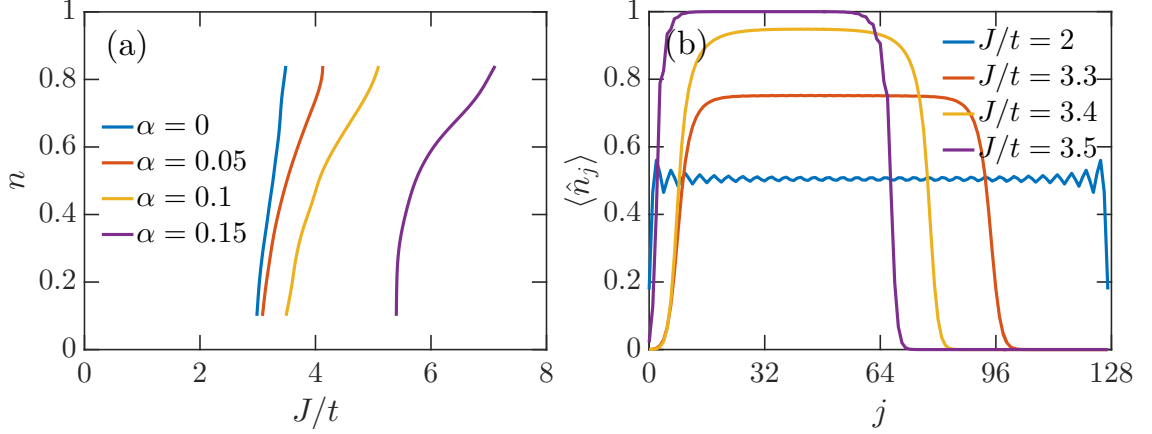


Figure 4.2: (a) Phase diagram plot of  $J$  vs  $n$  indicating the phase separation boundary at various values of  $\alpha$ . (b) Examples of the ground-state real-space fermion density  $\langle \hat{n}_i \rangle$  for  $\alpha = 0$ ,  $n = 0.5$  on  $L = 128$  sites, at various values of  $J/t$ .

#### 4.2.1 Phase-separated region

As we showed in Sec. 2.3, the second term in Eq. (4.1) is commonly rewritten as the antiferromagnetic Heisenberg coupling,

$$\hat{H}_{\text{Heis}} = \frac{J}{2} \sum_{\langle ij \rangle} \left( \hat{S}_i^x \hat{S}_j^x + \hat{S}_i^y \hat{S}_j^y + \hat{S}_i^z \hat{S}_j^z - \frac{\hat{n}_i \hat{n}_j}{4} \right), \quad (4.4)$$

where  $\hat{S}_j^x = (\hat{f}_{j,\downarrow}^\dagger \hat{f}_{j,\uparrow} + \hat{f}_{j,\uparrow}^\dagger \hat{f}_{j,\downarrow})$ ,  $\hat{S}_j^y = i(\hat{f}_{j,\downarrow}^\dagger \hat{f}_{j,\uparrow} - \hat{f}_{j,\uparrow}^\dagger \hat{f}_{j,\downarrow})$ , and  $\hat{S}_j^z = (\hat{n}_{j,\uparrow} - \hat{n}_{j,\downarrow})$  are the spin-1/2 Pauli operators acting on the spin degree of freedom at site  $j$ . When written in this form, it is clear that in the absence of pair-hopping, the  $t$ - $J$  model will exhibit competition between the delocalising effect of the single-particle hopping  $t$  and the attractive Heisenberg-like interaction  $J$ . When  $t \ll J$ , we expect this attractive interaction to dominate, and the fermions to separate into antiferromagnetic clusters and hole-rich regions. This is known as phase separation [125]. To quantitatively characterise the transition boundary, we compute the inverse compressibility.

The compressibility,  $\kappa$ , of a system is defined by the thermodynamic relation

$$\kappa^{-1} = -V \left( \frac{\partial P}{\partial V} \right)_N. \quad (4.5)$$

That is, the  $\kappa$  tells us how much pressure  $P$  we need to apply in order to change the volume  $V$  of the system given a fixed particle number  $N$ . When the system undergoes phase separation, the fermions collapse inwards, and so no change in pressure is required in order to change the system's volume. The compressibility therefore

diverges. Using the definition of pressure

$$P = - \left( \frac{\partial E}{\partial V} \right)_N, \quad (4.6)$$

we obtain

$$\kappa^{-1} = V \left( \frac{\partial^2 E}{\partial V^2} \right)_N. \quad (4.7)$$

Finally,  $V = N/n$ , and so  $\left( \frac{\partial}{\partial V} \right)_N = -\frac{n}{V^2} \left( \frac{\partial}{\partial n} \right)_N$ , and making the definition  $E \equiv e_0 V$ , where  $e_0$  is the ground state energy per unit volume, we obtain

$$\begin{aligned} \kappa^{-1}(n) &= n^2 \frac{\partial^2 e_0(n)}{\partial n^2} \\ &\approx n^2 \frac{[e_0(n + \Delta n) + e_0(n - \Delta n) - 2e_0(n)]}{(\Delta n)^2}, \end{aligned} \quad (4.8)$$

where  $e_0(n)$  is the ground state energy of the system per site at a filling  $n$ . Since the compressibility diverges at the onset of phase separation,  $\kappa^{-1}$  crosses zero. The phase separation boundary is shown in Fig. 4.2(a) for selected values of  $\alpha$ . We see clearly that the phase separation is suppressed with increasing  $\alpha$ . We further find that phase separation disappears completely for  $\alpha = 1/2$ , in agreement with Ref. [120].

Where phase separation does occur, and if  $J/t$  is sufficiently large, the system can become fully separated into an particle-rich region with  $\langle \hat{n}_j \rangle \approx 1$ , and a hole-rich region with  $\langle \hat{n}_j \rangle \approx 0$ . This is illustrated in Fig. 4.2(b) for  $\alpha = 0$ . In this plot,  $J/t = 2$  is metallic, while the rest are phase-separated, and  $J/t = 3.5$  indicates an electron solid phase with regions of  $\langle \hat{n}_i \rangle = 1$ , and  $\langle \hat{n}_i \rangle = 0$ .

We find that the phase-separated phase presents a number of issues for the DMRG calculation, consistent with Ref. [76]. Firstly, the antiferromagnetic island is off-centre for larger  $J/t$ . This is because the phase-separated ground state is highly degenerate, i.e. ignoring boundary effects, the cluster of fermions has very nearly the same energy regardless of where it is located in the lattice<sup>1</sup>. Relatedly, we find that for large systems DMRG encounters metastability issues deep in the phase-separated phase. The results for  $J/t = 3.5$  in Fig. 4.2(b) are therefore not expected to be quantitatively representative of the true ground state (as can be seen by the lack of reflection symmetry in the antiferromagnetic cluster). Because of this, a full extrapolation of the electron solid phase boundary to the thermodynamic limit is not possible. Rather, in Fig. 4.1, we show the approximate boundary as the contour where  $\max_j \langle \hat{n}_j \rangle > 0.999$  for  $L = 128$  as a dotted line.

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<sup>1</sup>In our results, the fermions tend to cluster on the left because the DMRG algorithm always finishes with a leftward minimisation sweep, breaking the reflection symmetry of the system.

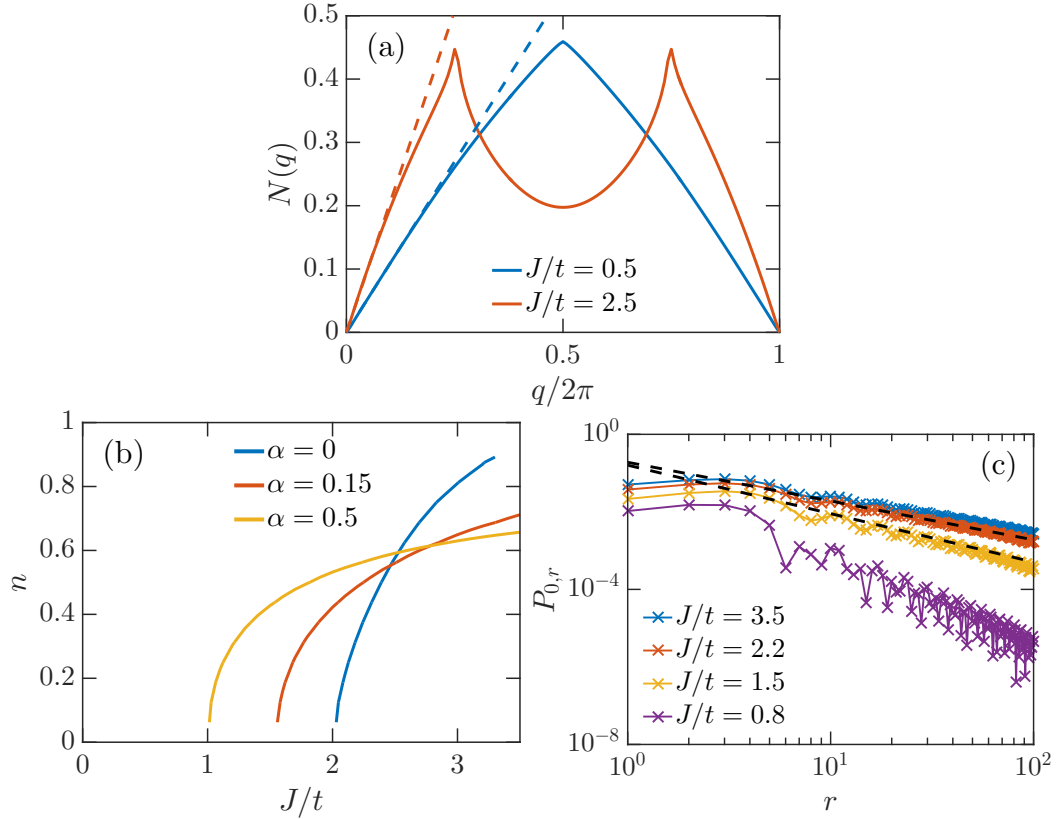


Figure 4.3: (a) The density structure factor  $N(q)$  for  $\alpha = 0.5$ ,  $L = 128$  sites. The dotted lines show the linear fit as  $q \rightarrow 0$ , from which  $K_\rho$  is extracted. (b)  $K_\rho = 1$  contours for  $\alpha = 0, 0.15$ , and  $0.5$ , extrapolated to the thermodynamic limit. (c) The real-space singlet correlations  $P_{0,r}$  are marked with crosses, with a solid line as a guide for the eye. Computed for  $L = 128$ ,  $\alpha = 0.5$ ,  $n = 0.5$ , at various values of  $J/t$ . The upper and lower black dotted lines indicate the power law decays  $0.19r^{-1}$  and  $0.16r^{-1.25}$  respectively.

#### 4.2.2 Superconducting region

We are primarily interested in the effect of the pair-hopping on the superconducting region. If the system is not phase separated, the one-dimensional  $t$ - $J$ - $\alpha$  model may be mapped onto two different effective low-energy, exactly-solvable models known as the Tomonaga-Luttinger Liquid (TLL) and the Luther-Emery Liquid (LEL) [76, 126, 127]. The TLL has gapless spin and charge excitations, whereas the LEL has gapless charge excitations, but an energy gap between the ground state and the lowest-lying spin excitation. The central quantity in both models is the so-called Luttinger parameter  $K_\rho$ . For  $K_\rho < 1$ , the TLL/LEL has repulsive interactions, whereas if  $K_\rho > 1$ , the TLL/LEL has attractive interactions, and thus superconducting correlations

dominate.

We extract  $K_\rho$  by computing the ground-state density structure factor, and exploiting the linear dependence at small  $q$  values, which we show in Fig. 4.3(a). The linear dependence is given by [127, 76]

$$N(q) \approx \frac{K_\rho |q|}{\pi} \quad \text{as, } q \rightarrow 0, \quad (4.9)$$

for both the TLL and LEL. By performing a linear fit for small values of  $q$ , we obtain a value of  $K_\rho$  at a given system size  $L$ . By computing this as a function of  $L$ , extrapolating to the  $L \rightarrow \infty$  limit, and finding where  $K_\rho = 1$ , we determine the superconducting phase boundary, which we show in Fig. 4.3(b) for a few values of  $\alpha$ . We determine the standard error from the extrapolation, as discussed in Appendix C. The typical standard error is  $\sim 0.001$ , which leads to error bars on the contour lines in Fig. 4.1 which are smaller than the line itself.

We see clearly that the effect of the pair hopping is to shift the metal–superconducting phase boundary to lower values of  $J/t$  at small fillings, and suppress SC at large fillings. We expect this observation to persist in higher dimensions, and it indeed is corroborated by two dimensional renormalised mean-field theory studies [123]. In Fig. 4.3(c), we show some examples of the real-space singlet correlations  $P_{0,r}$  at low fermion densities. Between  $J/t = 0.8$  and  $J/t = 0.5$ , as the system enters the spin-gapped region, we see a clear change in behaviour as  $P_{0,r}$  goes from oscillatory and rapid (but still algebraic) decay to a much slower decaying behaviour with suppressed oscillations. The changes are indicative of a gapless metal, to spin-gapped metal, to spin-gapped superconductor transition.

### 4.2.3 Spin-gapped region

The spin gap is defined as the energy gap between the “singlet” ground state, and the lowest-lying triplet excitation,

$$E_{\text{SG}} = E_0(S^z = 1) - E_0(S^z = 0), \quad (4.10)$$

where  $S^z = (N_\uparrow - N_\downarrow)/2$ . In any finite system  $E_{\text{SG}}$  will also be finite, vanishing only in the thermodynamic limit. It also closes rather slowly as a function of system size, and so it is important to accurately extrapolate to  $L \rightarrow \infty$  [76]. The typical standard error in this extrapolation of the spin gap is  $\sim 0.001t$ . The contours drawn in Fig. 4.1 are for  $E_{\text{SG}}(L \rightarrow \infty) < 0.005t$ . The computed standard error is again sufficiently small that error bars in Fig. 4.1 would be smaller than the spin gap contour line itself.

As we shall demonstrate in Sec. 4.3, the presence of a finite spin-gap alters the nature of the superconducting ground state, and it becomes possible to think of the superconductor as a Bose condensate of locally bound singlet pairs. Luttinger liquid theory predicts that the long range behaviour of the singlet correlations will be

$$P_{0,r} \sim r^{-(1+1/K_\rho)}, \quad \text{and} \quad P_{0,r} \sim r^{-1/K_\rho}, \quad (4.11)$$

in the TLL and LEL respectively [126].

#### 4.2.4 Magnetic Correlations

From the Heisenberg term Eq. (4.4), it is clear that the superexchange interaction will induce antiferromagnetic correlations in the ground state. At precisely half-filling, i.e.  $n = 1$ , the electrons become completely immobile and we are left only with the spin degree of freedom, which is governed solely by the Heisenberg Hamiltonian with an antiferromagnetic ground state [38].

Away from half-filling, the presence of holes obscures the underlying magnetic order as the single particle and pair hopping delocalises the spins. Rather than perfect antiferromagnetic correlations (i.e. a spin wave with quasimomentum  $q = \pi$ ), the ground state contains a spin wave at  $q = n\pi$ . This is identified by the location of the peak in the spin structure factor, which is shown in Fig. 4.4(a) for various fillings at  $J/t = 1$ . In Fig. 4.4(b) we show the spin structure factor for  $n = 0.5$  at various  $J/t$ . Upon entering the spin-gap, the sharp peaks, which suggest quasi-long range magnetic order, are suppressed and are instead replaced by a broad peak at  $q = \pi$ . This peak has the approximate form  $S(q) \approx 1 - \cos(q)$ , which is the form given by a free gas of antiferromagnetically bound pairs [120].

In real-space, the antiferromagnetic correlations can be better revealed by looking at the string correlator

$$S_r^s = \left\langle \hat{S}_i^z \left( \prod_{j=1}^{r-1} (-1)^{(1-\hat{n}_{i+j})} \right) \hat{S}_{i+r}^z \right\rangle. \quad (4.12)$$

To reveal underlying antiferromagnetic order in the Hubbard/ $t$ - $J$ - $\alpha$  models, we simply have to remove the holes from the system and look at the so-called “squeezed space” representation. This is achieved by the string correlator by keeping track of how many holes there are between the spins and appropriately flipping the sign of the correlator.

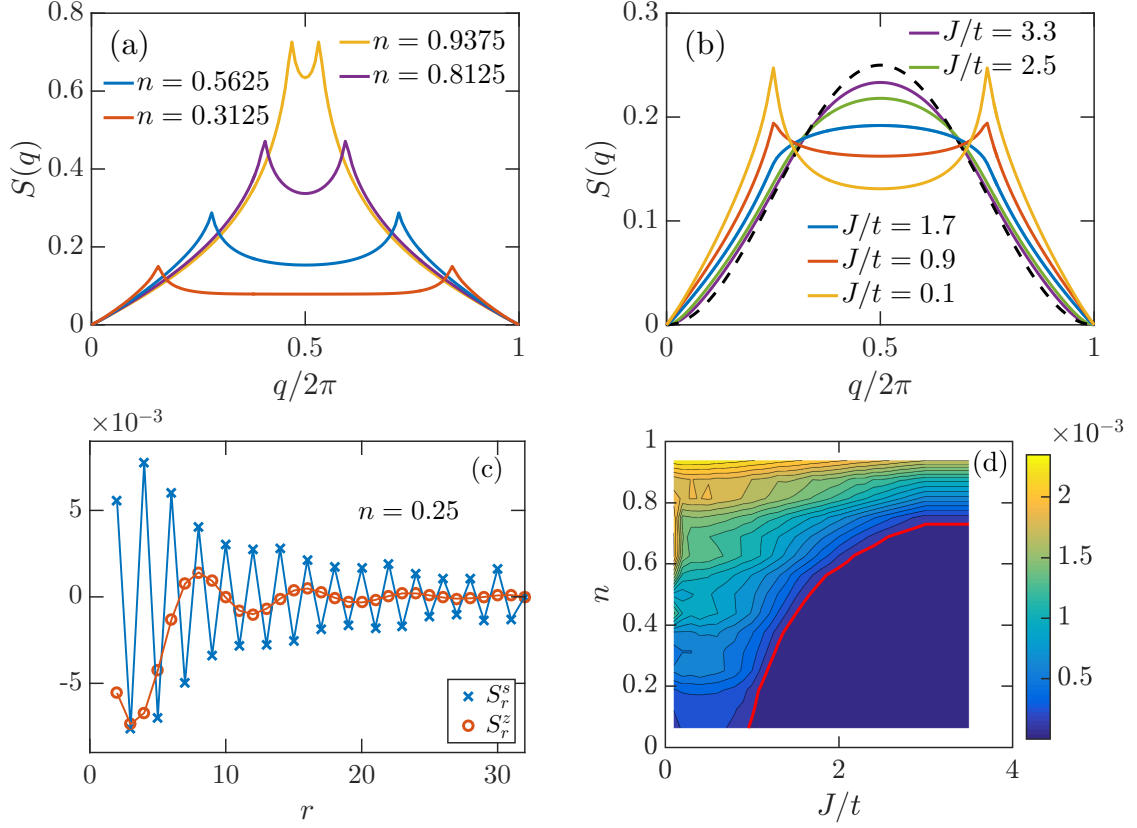


Figure 4.4: Spin structure factor  $S(q)$  for  $L = 128$  sites with  $\alpha = 0.5$ . In (a)  $S(q)$  at  $J/t = 0.1$  at various fillings  $n$  is shown, while (b) shows  $S(q)$  for  $\alpha = 1/2$  and  $n = 0.5$  at various values of  $J/t$ . For reference, the black dashed line indicates  $(1/8)(1 - \cos(q))$ , the structure factor for a free gas of bound pairs. In (c) we show the real-space spin correlations along with the spin-string correlator. Finally, in (d), we show a contour plot of the string correlator  $S_r^s$  evaluated at separation  $r = 50$  for  $\alpha = 1/2$ .

For example, if one were to perform a projective measurement of the spin at each site on the lattice, a particular configuration might be

$$|\uparrow\rangle|\downarrow\rangle|0\rangle|0\rangle|\uparrow\rangle|0\rangle|\downarrow\rangle|0\rangle|\uparrow\rangle$$

$$\Downarrow$$

$$|\uparrow\rangle|\downarrow\rangle|\uparrow\rangle|\downarrow\rangle|\uparrow\rangle$$

Where in the second line we remove the holes  $|0\rangle$  to reveal the underlying antiferromagnetism. This is very closely related to the Haldane insulator (HI) phase of the extended Bose-Hubbard model (EBHM) [128]. There, instead of spin, one keeps track

of density fluctuations about a homogeneous background with fixed  $\bar{n}$ , i.e. looks at the string correlation

$$C_r = \left\langle \delta \hat{n}_i \left( \prod_{j=1}^{r-1} (-1)^{\delta \hat{n}_{i+j}} \right) \delta \hat{n}_{i+r} \right\rangle. \quad (4.13)$$

In the HI phase of the EBHM, the density fluctuations have the same kind of “antiferromagnetic” correlations as the spins in the Hubbard/ $t$ - $J$  models, if we make the identification

$$|\bar{n}\rangle \sim |0\rangle, \quad |\bar{n}-1\rangle \sim |\downarrow\rangle, \quad |\bar{n}+1\rangle \sim |\uparrow\rangle. \quad (4.14)$$

we obtain identical “spin” configurations to those obtained in the Fermi-Hubbard and  $t$ - $J$  models [129].

We compare one instance of the spin-spin correlation function  $S_r^z$  and the string correlation  $S_r^s$  in Fig. 4.4(c). We see that the spin-spin correlator oscillates with a period  $2k_F$ , indicating antiferromagnetism incommensurate with the lattice period. When we effectively “factor out” the holes using the string correlator, the perfect antiferromagnetism is restored, and the amplitude of the correlations is significantly enhanced.

In Fig. 4.4(d), we show a contour plot of the values of  $S_r^s$  at a separation  $r = 50$ . It can clearly be seen that the long-range string correlations are strongly suppressed inside the spin gap region. Indeed, we find that in the region of small  $J/t$ , where the  $t$ - $J$ - $\alpha$  model is a good approximation to the Hubbard model [108], there is quasi-long ranged magnetic string order. However, *inside* the spin-gapped region, both the spin and string correlators decay exponentially, indicating that the antiferromagnetic order has been lost. We can easily understand this by considering the spin-gapped phase as a gas of bound singlet pairs, which we will discuss in more detail in Sec. 4.3. As each singlet pair’s spin degree of freedom is maximally entangled, monogamy of entanglement means that the constituent fermions cannot have any spin correlations beyond their adjacent partner.

### 4.3 Effective Bosonic Model

We have so far demonstrated that, counterintuitively, a finite pair-hopping  $\alpha > 0$  leads to suppressed superconductivity at large fillings, coinciding with an increased spin-gap region. To better understand this observation, we now look at the spin-gapped region in more detail. We study a simple effective bosonic model for singlet pairs inside the spin gap. We will see that this model, due to kinetic constraints arising

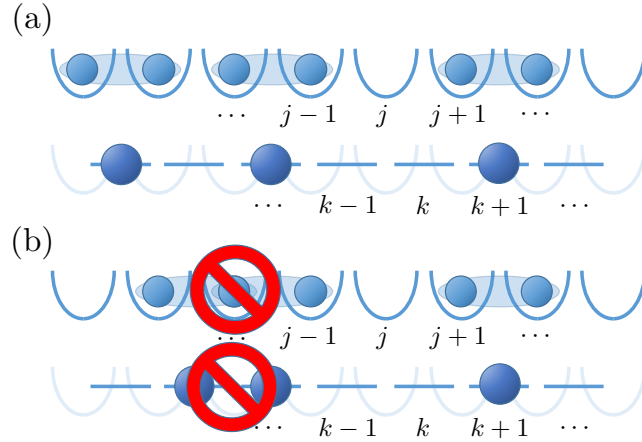


Figure 4.5: (a) Schematic showing how a singlet pair of electrons may be represented in out effective model by a single hardcore boson. (b) Schematic showing how a "no-nearest-neighbour" constraint arises from the "no-double-occupancy" condition of the  $t$ - $J$ - $\alpha$  model.

from strong correlations, has a phase transition from a superfluid ground state to a non-superfluid singlet gas as a function of the filling fraction.

Inside the spin-gap region, we expect that fermions are all bound into nearest-neighbour singlet pairs, which are created and annihilated by the operators  $\hat{b}_{i,i+1}^\dagger$ , and  $\hat{b}_{j,j+1}$ . It is easy to see that when the bonds  $(i, i+1)$ , and  $(j, j+1)$  do not overlap

$$[\hat{b}_{i,i+1}, \hat{b}_{j,j+1}^\dagger] = 0. \quad (4.15)$$

When the bonds *do* overlap, they no longer obey bosonic commutation relations, a complication we shall ignore for now and justify later. As illustrated in Fig. 4.5(a), we define a new Hilbert space for the system consisting of  $L - 1$  "sites", which represent the bonds of the original lattice. These "sites" may be occupied (or not) by a boson representing a singlet pair in the spin-gapped  $t$ - $J$ - $\alpha$  model and thus we have  $nL/2$  particles in the system. The operators  $\hat{a}_j^\dagger$  and  $\hat{a}_j$  respectively create and annihilate hardcore bosons on "site"  $j$ , and  $\hat{m}_j = \hat{a}_j^\dagger \hat{a}_j$  is the bosonic number operator. However, not all configurations of this effective lattice model represent valid configurations in the  $t$ - $J$ - $\alpha$  model, as illustrated in Fig. 4.5(b). Since the  $t$ - $J$ - $\alpha$  model does not allow double-occupations, two nearest-neighbour singlet pairs cannot overlap. This manifests itself in the effective bosonic model as the constraint that we cannot have two adjacent "sites" occupied by hardcore bosons. This constraint is implemented by the projector  $\mathbb{P}_{\text{nn}} = \prod_j (1 - \hat{m}_j \hat{m}_{j+1})$ , which kills any state containing bosons on adjacent sites. This effective boson model is closely related to quantum

lattice dimer models [130] thought to have relevance to high- $T_c$  superconductivity in two dimensions. In the limit  $J/t \rightarrow \infty$ , the Hamiltonian for the effective model is

$$\hat{H}_{\text{eff}} = \mathbb{P}_{\text{nn}} \left[ -J \sum_j \hat{m}_j - \alpha J \sum_j \left( \hat{a}_j^\dagger \hat{a}_{j+1} + \text{H.c.} \right) \right] \mathbb{P}_{\text{nn}}. \quad (4.16)$$

This can be seen as a Hamiltonian for hardcore bosons hopping on a lattice with an infinite nearest-neighbour repulsion or, equivalently, a Heisenberg XXZ model with infinite  $z$ - $z$  coupling. This Hamiltonian therefore admits an exact solution via the Bethe ansatz [131]. Since the total number of bosons is conserved in this Hamiltonian, and we are working at a fixed filling fraction  $n$ , the first term is a constant  $nLJ/2$ , and thus can be ignored. The parameter  $\alpha J$  then just rescales the energies and does not modify the ground state. This leaves the filling fraction  $n$  as the only free parameter in the model. Despite the restriction  $\mathbb{P}_{\text{nn}}$  on the hopping, we still expect the bosons to be able to quasi-condense into a superfluid state when the filling is sufficiently small,  $n < n_{\text{crit}}$ . This superfluid of bosons then corresponds to spin-gapped superconductivity in the  $t$ - $J$ - $\alpha$  model.

To study the ground state phases of this model, we implement DMRG for the Hamiltonian with four-site interactions (see Sec. 3.6.3) and compute the ground-state correlations. Despite the increased range of the interactions, we find that the smaller local physical dimension leads to a significant computational speedup compared with a full simulation of the  $t$ - $J$ - $\alpha$  model.

The boson structure factor  $B(q)$  is Eq. (4.3) applied to the single particle density matrix (SPDM)

$$\rho_{jk} = \langle \hat{a}_j^\dagger \hat{a}_k \rangle, \quad (4.17)$$

and is essentially the momentum distribution of the bosons. This is shown as crosses in Fig. 4.6(a), where we see that when the filling is small, the bosons do not see the extremely strong local repulsive interaction, and so they macroscopically occupy the  $q = 0$  quasi-momentum state. However, as the filling increases, the repulsive interaction plays a stronger role, and the peak broadens as the bosons are forced, by the interactions, to occupy higher momentum states. In the same figure, we compare this with the singlet structure factor of the  $t$ - $J$ - $\alpha$  model with  $J/t = 5$  (solid lines), finding a very close agreement between the two.

Similarly, in the real-space boson density is shown in Fig. 4.6(b). At smaller fillings, small oscillations at a frequency  $\pi n$  can clearly be seen. This is because in one dimension, hardcore bosons are related to fermions via the Jordan–Wigner transformation [132], and so the real-space density profile inherits the Friedel oscillations from

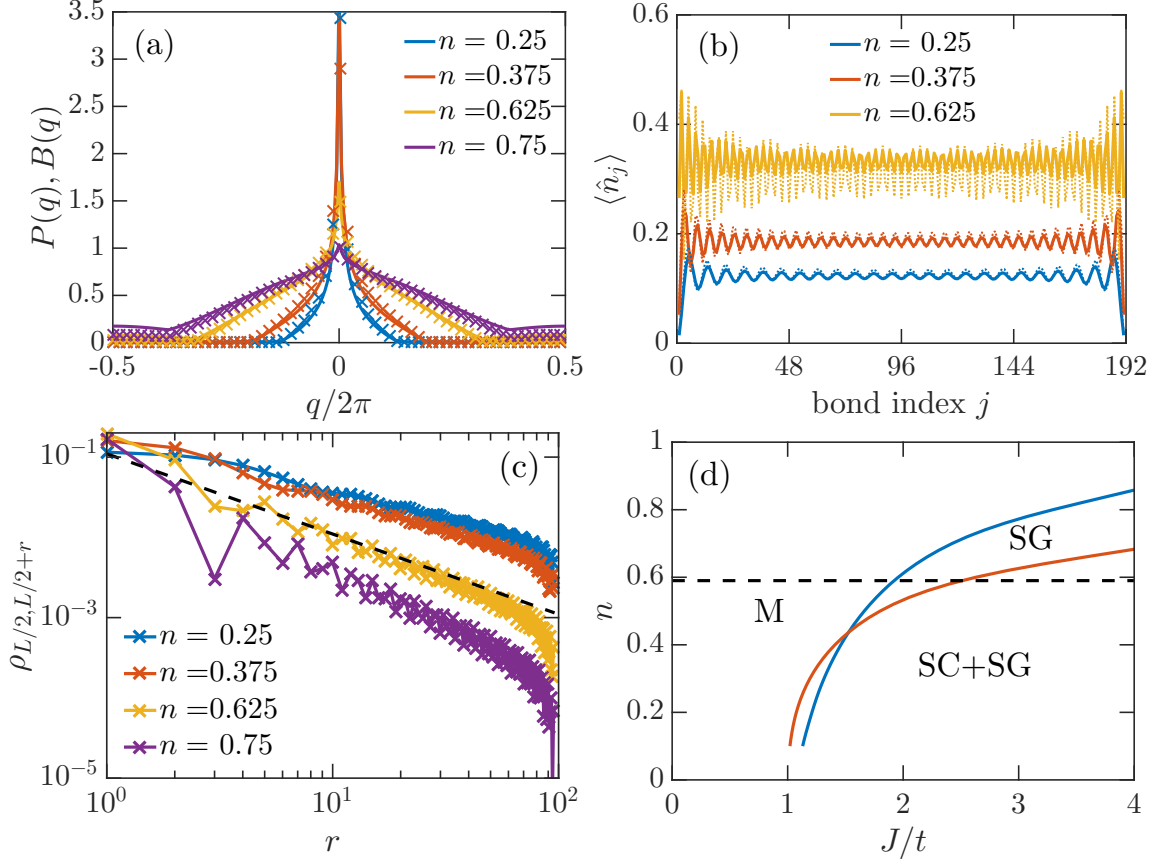


Figure 4.6: A comparison between the  $t$ - $J$ - $\alpha$  model and the projected boson model.  $t$ - $J$ - $\alpha$  model with  $J/t = 5$ , and  $\alpha = 1/2$  computed with  $L = 192$  lattice sites. The singlet structure factor  $P(q)$  is shown in (a) as the solid line, with the boson structure factor  $B(q)$  shown with crosses. We compare the real space densities of singlets and bosons in (b), with the singlets shown with the solid line, and the bosons marked with the dotted line. In (c) a slice of the single boson density matrix as a function of separation  $r$  is marked with crosses, with solid lines as a guide to the eye. For reference, a black dashed line indicates the line  $0.11r^{-1}$ . In (d) we duplicate the  $t$ - $J$ - $\alpha$  model phase diagram at  $\alpha = 0.5$  from Fig. 4.1, but now include the superfluid phase boundary of the effective boson model marked as a black dotted line.

this. Once again, these closely match the oscillations in the real-space singlet density in the  $t$ - $J$ - $\alpha$ . The very close agreement between the two models may be surprising since, as pointed out previously, the singlet creation and annihilation operators do not obey bosonic commutation relations when the singlets overlap. However, note that in the effective bosonic model, we project out states which contain bosons on neighbouring sites, resolving this apparent inconsistency. Moreover, despite the fact that the Hamiltonian in Eq. (4.16) is only rigorously valid in the limit  $J/t \rightarrow \infty$ , the very close numerical agreement between the ground states of the model with the  $t$ - $J$ - $\alpha$  model suggest a wider domain of applicability.

Whether a bosonic lattice system is superfluid or not is determined by the decay of the off-diagonal elements in the SPDM. To determine the critical filling of the superfluid transition, we now look at the Luttinger parameter for bosons  $K_b$  [133]. One can show that for  $r \gg 1$ , the SPDM is

$$\rho_{0,r} \sim r^{-K_b/2}, \quad (4.18)$$

which we show in Fig. 4.6(c). As in the fermionic case, we can extract  $K_b$  from the bosonic density structure factor,

$$M(q) \approx \frac{|q|}{2\pi K_b} \quad \text{as, } q \rightarrow 0, \quad (4.19)$$

Where  $M(q)$  is Eq. (4.3) applied to the correlation function

$$M_{i,j} = \langle \hat{m}_i \hat{m}_j \rangle - \langle \hat{m}_i \rangle \langle \hat{m}_j \rangle.$$

We find that the critical filling is  $n_{\text{crit}} \approx 0.59$ , which we mark on a copy of the  $\alpha = 0.5$   $t$ - $J$ - $\alpha$  phase diagram, showing a qualitative agreement for the superconductor-preformed pair transition at large  $J/t$ . Eventually, at maximum filling  $n = 1$ , the ground state is a density wave,

$$|\psi_0\rangle = \cdots |1\rangle |0\rangle |1\rangle |0\rangle |1\rangle |0\rangle \cdots, \quad (4.20)$$

where all quasi-momentum states are equally occupied.

In the vicinity of the  $t$ - $J$ - $\alpha$  phase diagram where the effective boson model is valid (i.e. the region with a significant spin-gap),  $n_{\text{crit}}$  provides an estimate of the largest filling at which one can have superconductivity. We expect the single-particle hopping  $t$ , which we have neglected in the effective boson model, to increase the propensity of the system to superconduct, and so  $n_{\text{crit}}$  is expected to provide a lower bound on this maximum filling. We find that this number is in approximate agreement

with the  $t$ - $J$ - $\alpha$  model at  $J/t \gg 1$ , as we indicate in Fig. 4.6(d). Eventually, at maximum filling  $n = 1$ , the ground state is a (pair) density wave with every other bond being occupied by a hardcore boson. The close agreement between these two models indicates that the effective model provides a quantitative description of pair condensation in the  $t$ - $J$ - $\alpha$  model. The effective bosonic model makes it clear that the loss of superconductivity close to half-filling is due to the kinetic constraints imposed by the non-overlap of singlet pairs.

In addition, we find that DMRG calculations for the projected boson model converge much more rapidly than the  $t$ - $J$ - $\alpha$  model, while accurately describing many of its properties. In  $t$ - $J$ - $\alpha$  models where DMRG is slow to converge, it may be possible to accelerate these calculations in the spin-gapped regime by “coarse-graining” to an effective bosonic model for the pairs, before interpolating to the full fermionic model [134].

## 4.4 Discussion

In this chapter so far, we have shown that the effect of the often ignored pair-hopping  $\alpha J$  in the  $t$ - $J$ - $\alpha$  model is to enhance mobility of pairs, which manifests itself in the ground state phase diagram in a number of ways. Firstly, this pushes the metal-superconducting boundary to lower values of  $J/t$  in dilute systems and destabilises the phase-separated region. As we will discuss in Chapter 6, this has significant implications for driven Hubbard systems, as it means that driving-induced singlet pairing may be induced at significantly smaller driving strengths. Secondly, at larger fillings, superconductivity is suppressed despite the increased pair hopping. We now understand this in the following way: by lowering the energy of bound singlets, the pair-hopping increases the size of the spin-gapped region up to much larger values of  $n$ . Inside the spin-gap region, the physics may be described by a simple model of hardcore bosons with a kinetic constraint whose origins lie in the “no double-occupation” projection of the  $t$ - $J$  model. Due to these restrictions, the bosons may not condense above a critical filling  $n_{\text{crit}}$ , and so superconductivity in the  $t$ - $J$ - $\alpha$  model cannot occur inside the spin-gap above this filling. This is consistent with the  $\alpha = 0.5$  phase diagram, which shows a larger spin-gapped region than superconducting region.

It is known that including next-nearest-neighbour hopping terms in one dimensional chains (equivalent to a two-leg ladder system) can enhance the size of the spin-gap region [135]. This raises the intriguing possibility that kinetic constraints

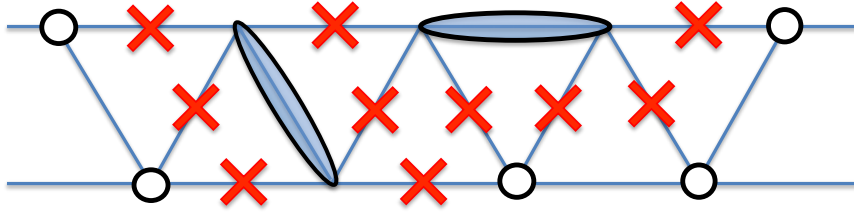


Figure 4.7: Schematic of the  $t$ - $J$ - $\alpha$  model on a triangular ladder. Singlets are indicated by blue ovals, while empty sites are shown by empty circles. With just two singlets placed on the ladder, most of the bonds can no longer be occupied by singlets, as indicated by crosses.

in the spin-gapped phase might play an important role in fully two-dimensional systems, and in particular of high- $T_c$  superconductors. We begin to investigate this in the following Sec. 4.5.

## 4.5 $t$ - $J$ - $\alpha$ Ladder systems

We already saw in Sec. 4.3 that in a one-dimensional chain, the restriction that pairs cannot overlap leads to the suppression of superconductivity at large fillings. As we show in Fig. 4.7, when two of these chains are coupled together, the constraints may become even more severe, potentially inhibiting superconductivity over a wider range of parameters. Furthermore, experiments have shown the absence of a superconducting phase in a spin-gapped ladder [136], and others have shown that superconducting phases in ladders can coincide with the collapse of the spin-gap [137]. This lends further support to the idea that dynamical constraints within the spin-gap lead to the suppression of superconductivity in systems with a ladder geometry.

The suppression of transport due to dynamical constraints is somewhat reminiscent of systems which exhibit “glassy” dynamics [138]. One might expect that in these restricted bosonic models, superfluidity (and thus superconductivity in the corresponding  $t$ - $J$ - $\alpha$  models) depends rather sensitively on the coupling between the chains. Counterintuitively, decoupling the chains, and thus relaxing the constraints might enhance the propensity of such a strongly correlated system to superconduct.

The  $t$ - $J$  model has been studied extensively in a ladder geometry, principally through DMRG calculations [77, 139, 140, 141, 142]. However, to our knowledge, there have so far been no studies which include the pair-hopping  $\alpha J$  in ladder systems. As we already saw in the one dimensional chain, these terms can strongly modify the

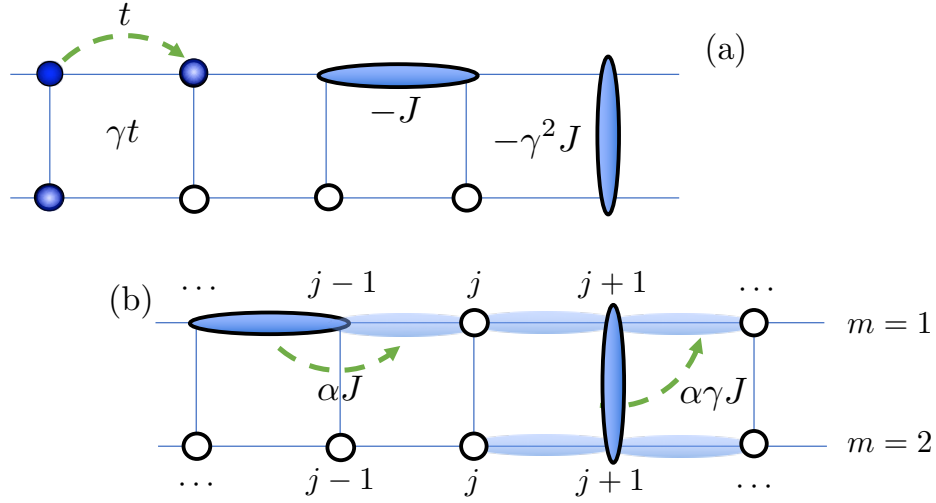


Figure 4.8: Schematic of the rectangular  $t$ - $J$ - $\alpha$  ladder. Empty lattice sites are represented by open circles. Filled circles represent single fermions, while filled ovals represent bound singlet pairs on nearest-neighbour bonds. In (a) we show the intra- and inter-leg hopping processes, with the latter suppressed by a factor  $\gamma$ . We also show the intra- and inter-leg singlet binding, the latter suppressed by a factor  $\gamma^2$ . In (b) we show various allowed pair-hopping processes, suppressed by a factor  $\gamma$  for each inter-leg virtual hop.

physics, suppressing phase separation and imposing constraints by enlarging the spin-gap, and so we expect these terms to be similarly important in higher dimensions. In this section, we couple two such  $t$ - $J$ - $\alpha$  chains together to form a ladder with either rectangular or triangular plaquettes. We show that, depending on the geometry of the ladder, the superconducting correlations carried by the chains may be suppressed if the inter-chain coupling is too strong.

#### 4.5.1 Ladder Hamiltonians

Specifically, we study two geometries, the “rectangular” ladder and the “triangular” ladder. The rectangular ladder Hamiltonian is

$$\hat{H}_{tJ\alpha}^R = \hat{H}_t^R + \hat{H}_J^R + \hat{H}_\alpha^R, \quad (4.21)$$

where

$$\hat{H}_t^R = -t \sum_j \sum_{m=1,2} \left( \hat{f}_{j,\sigma}^{\dagger(m)} \hat{f}_{j+1,\sigma}^{(m)} + \text{H.c.} \right) - \gamma t \sum_{j,\sigma} \left( \hat{f}_{j,\sigma}^{\dagger(1)} \hat{f}_{j,\sigma}^{(2)} + \text{H.c.} \right), \quad (4.22)$$

$$\hat{H}_J^R = -J \sum_j \sum_{m=1,2} \hat{b}_{j,j+1}^{\dagger(m,m)} \hat{b}_{j,j+1}^{(m,m)} - \gamma^2 J \sum_j \hat{b}_{j,j}^{\dagger(1,2)} \hat{b}_{j,j}^{(1,2)}, \quad (4.23)$$

$$\begin{aligned} \hat{H}_\alpha^R = & -\alpha J \sum_j \sum_{m=1,2} \left( \hat{b}_{j,j+1}^{\dagger(m,m)} \hat{b}_{j,j+1}^{(m,m)} + \text{H.c.} \right) \\ & -\alpha \gamma J \sum_j \sum_{m=1,2} \left( \hat{b}_{j,j}^{\dagger(1,2)} \hat{b}_{j,j+1}^{(m,m)} + \text{H.c.} + \hat{b}_{j,j}^{\dagger(1,2)} \hat{b}_{j-1,j}^{(m,m)} + \text{H.c.} \right). \end{aligned} \quad (4.24)$$

Here,  $\hat{f}_{j,\sigma}^{(m)}$  annihilates a spin- $\sigma$  fermion on leg  $m$  and rung  $j$ , and

$$\hat{b}_{i,j}^{(m,n)} = \frac{1}{\sqrt{2}} \left( \hat{f}_{i,\downarrow}^{(m)} \hat{f}_{j,\uparrow}^{(n)} - \hat{f}_{i,\uparrow}^{(m)} \hat{f}_{j,\downarrow}^{(n)} \right),$$

annihilates a spin-singlet across the lattice sites specified at  $i, n$  and  $j, m$ . In Fig. 4.8, we show each of the processes in the rectangular ladder. In Eq. (4.21), single particle hopping terms *between* the legs are suppressed by an anisotropy factor  $\gamma$ . Therefore, second order processes which involve one virtual inter-leg hop are all suppressed by a factor  $\gamma$ , while processes which involve two virtual inter-leg hops are suppressed by a factor  $\gamma^2$ .

Similarly, the triangular ladder Hamiltonian is

$$\hat{H}_{tJ\alpha}^T = \hat{H}_t^T + \hat{H}_J^T + \hat{H}_\alpha^T, \quad (4.25)$$

where

$$\begin{aligned} \hat{H}_t^T = & -t \sum_j \sum_{m=1,2} \left( \hat{f}_{j,\sigma}^{\dagger(m)} \hat{f}_{j+1,\sigma}^{(m)} + \text{H.c.} \right) \\ & -\gamma t \sum_{j,\sigma} \left( \hat{f}_{j,\sigma}^{\dagger(1)} \hat{f}_{j,\sigma}^{(2)} + \text{H.c.} + \hat{f}_{j,\sigma}^{\dagger(1)} \hat{f}_{j-1,\sigma}^{(2)} + \text{H.c.} \right), \end{aligned} \quad (4.26)$$

$$\hat{H}_J^T = -J \sum_j \sum_{m=1,2} \hat{b}_{j,j+1}^{\dagger(m,m)} \hat{b}_{j,j+1}^{(m,m)} - \gamma^2 J \sum_j \left( \hat{b}_{j,j}^{\dagger(1,2)} \hat{b}_{j,j}^{(1,2)} + \hat{b}_{j,j-1}^{\dagger(1,2)} \hat{b}_{j,j-1}^{(1,2)} \right), \quad (4.27)$$

$$(4.28)$$

$$\begin{aligned} \hat{H}_\alpha^T = & -\alpha J \sum_j \sum_{m=1,2} \left( \hat{b}_{j,j+1}^{\dagger(m,m)} \hat{b}_{j,j+1}^{(m,m)} + \text{H.c.} \right) \\ & -\alpha \gamma J \sum_j \sum_{m=1,2} \left( \hat{b}_{j,j}^{\dagger(1,2)} \hat{b}_{j,j+1}^{(m,m)} + \text{H.c.} + \hat{b}_{j,j}^{\dagger(1,2)} \hat{b}_{j-1,j}^{(m,m)} + \text{H.c.} \right) \\ & -\alpha \gamma^2 J \sum_j \left( \hat{b}_{j,j}^{\dagger(1,2)} \hat{b}_{j,j-1}^{(1,2)} + \text{H.c.} + \hat{b}_{j,j-1}^{\dagger(1,2)} \hat{b}_{j+1,j}^{(1,2)} + \text{H.c.} \right). \end{aligned} \quad (4.29)$$

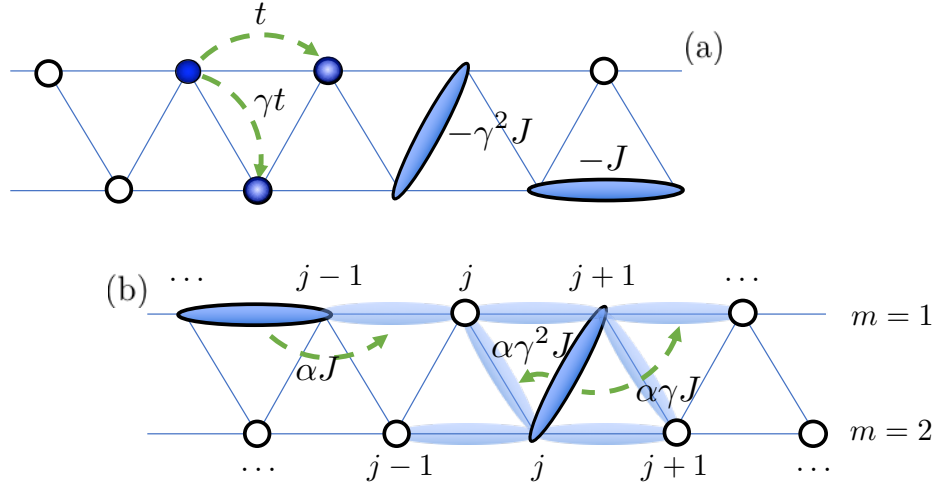


Figure 4.9: Schematic of the triangular  $t$ - $J$ - $\alpha$  ladder. Empty lattice sites are represented by open circles. Filled circles represent single-fermions, while filled ovals represent bound singlet pairs on nearest-neighbour bonds. In (a) we show the intra- and inter-leg hopping processes, with the latter suppressed by a factor  $\gamma$ . We also show the intra- and inter-leg singlet binding, the latter suppressed by a factor  $\gamma^2$ . In (b) we show various allowed pair-hopping processes, suppressed by a factor  $\gamma$  for each inter-leg virtual hop.

We see that the triangular ladder contains all of the processes in the rectangular ladder, but it also contains additional processes due to the higher connectivity, which leads to frustration in the system [143]. These additional frustrating processes lead to stricter constraints in the spin-gap phase.

## 4.5.2 Results

To solve these ladder models, we first map them onto a one-dimensional chain by

$$\hat{f}_{j,\sigma}^{(m)} \rightarrow \tilde{f}_{2j+m-2,\sigma}. \quad (4.30)$$

In terms of the  $\tilde{f}$  operators, the ladder models then become one-dimensional chains with longer-range interactions. Specifically, interactions which are nearest-neighbour in the ladder model become next-nearest-neighbour after the mapping. Similarly, the pair-hopping term, which is a three-site interaction in the ladder, becomes a five-site wide interaction in the effective one-dimensional model. We then construct this Hamiltonian as an MPO using the process described in Sec. 3.6.3, utilising the interface we outline in Appendix B. Finally, we use the standard finite system DMRG algorithm to compute the ground state of the model. Note that the longer-range of the interactions makes this a significantly more challenging model for DMRG to solve.

We begin with two chains deep in the superconducting regime  $J/t = 3$ ,  $\alpha = 0.5$ . To begin to see how varying the anisotropy affects the nature of singlet pairing in the system, we compute the total number of singlets which lie along the legs,

$$N^l = \sum_j \sum_{m=1,2} \langle \hat{b}_{j,j+1}^{\dagger(m,m)} \hat{b}_{j,j+1}^{(m,m)} \rangle, \quad (4.31)$$

and the number of singlets which lie along the rungs, which is given by

$$N_{\text{rect}}^r = \sum_j \sum_{m=1,2} \langle \hat{b}_{j,j}^{\dagger(1,2)} \hat{b}_{j,j}^{(1,2)} \rangle, \quad (4.32)$$

for the rectangular ladder, and

$$N_{\text{tri}}^r = \sum_j \sum_{m=1,2} \langle \hat{b}_{j,j+1}^{\dagger(1,2)} \hat{b}_{j,j+1}^{(1,2)} \rangle + \langle \hat{b}_{j,j-1}^{\dagger(1,2)} \hat{b}_{j,j-1}^{(1,2)} \rangle, \quad (4.33)$$

for the triangular ladder. We plot these in Fig. 4.10(a) and (b) for the rectangular and triangular ladders respectively. We see that the total number of singlets is approximately independent of  $\gamma$ , and so modifying the anisotropy simply changes the fraction of singlets in each orientation. In both cases, as the ladders become more isotropic, the number of singlets in each orientation becomes more equal, as expected. However, in the triangular case, there is a clear crossover point at  $\gamma \approx 0.5$ .

We also plot the half-chain entanglement entropy  $S_E$  as a function of  $\gamma$  in Fig. 4.10(c). In both cases, we see that it decreases with increasing  $\gamma$ . This is partly a reflection of the fact that neighbouring sites along the legs become next-nearest neighbour sites in the mapping to a 1D chain, and hence the MPS requires a larger bond dimension to capture the “long-range” entanglement when the interactions are primarily intra-leg. However, in the triangular ladder, we see a sharp drop in the entanglement entropy around  $\gamma \gtrsim 0.5$ , approximately coinciding with the crossover point in the singlet orientations, suggesting a possible phase transition.

To gain more information specifically on how the superconducting properties of the chains are modified as a function of the anisotropy, we compute the singlet-singlet correlations with the singlets oriented along the legs,

$$P_{i,j}^l = \langle \hat{b}_{i,i+1}^{\dagger(m,m)} \hat{b}_{j,j+1}^{(m,m)} \rangle, \quad (4.34)$$

and along the rungs of the ladder,

$$P_{i,j}^r = \langle \hat{b}_{i,i}^{\dagger(1,2)} \hat{b}_{j,j}^{(1,2)} \rangle. \quad (4.35)$$

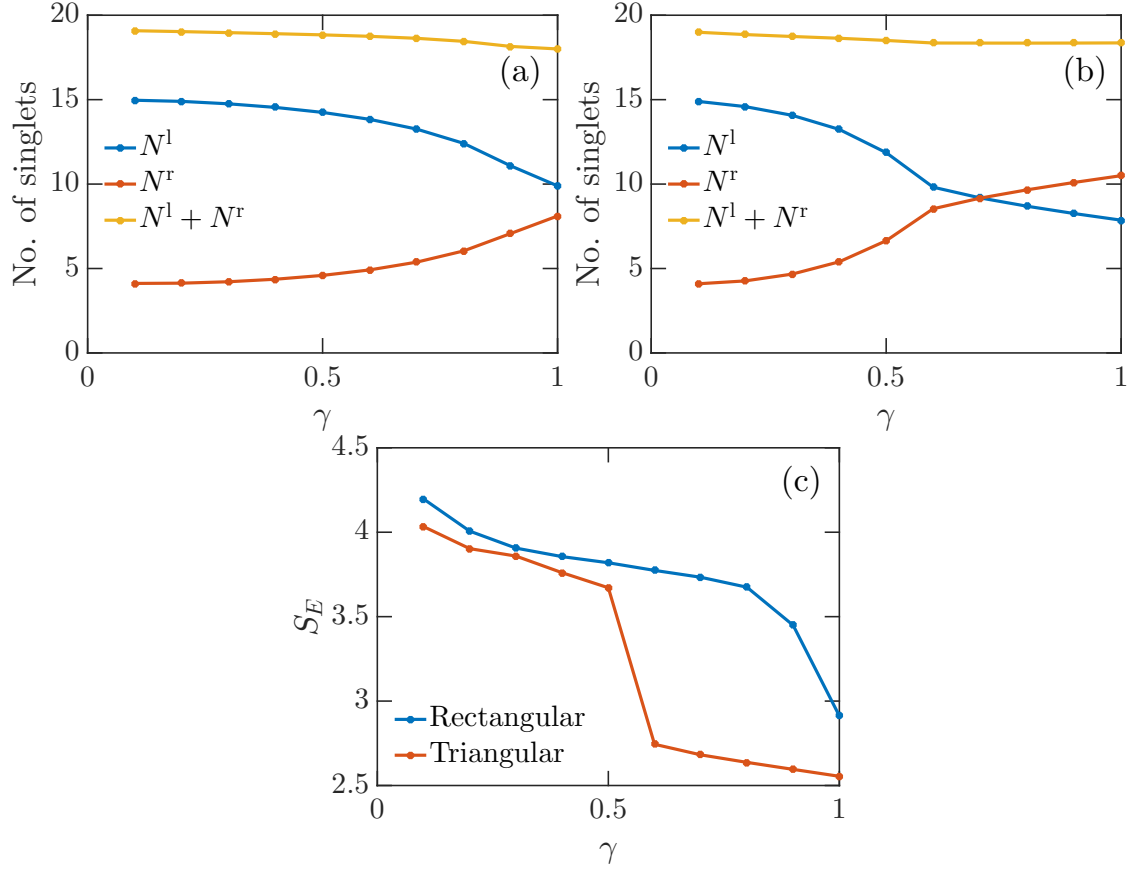


Figure 4.10: DMRG results for the  $t$ - $J$ - $\alpha$  ladder with  $J/t = 3.0$ ,  $\alpha = 0.5$ , using  $2L = 64$  sites and bond dimension  $\chi = 500$ . In (a) and (b) we show the number of singlets which lie along the legs of the ladders  $N^l$ , the number which lie along the rungs  $N^r$ , and the total. The rectangular ladder results are shown in (a), while the triangular results are shown in (b). The half-chain entanglement entropy  $S_E$  for the chains is shown in (c). Data points are marked with dots, with solid lines to guide the eye.

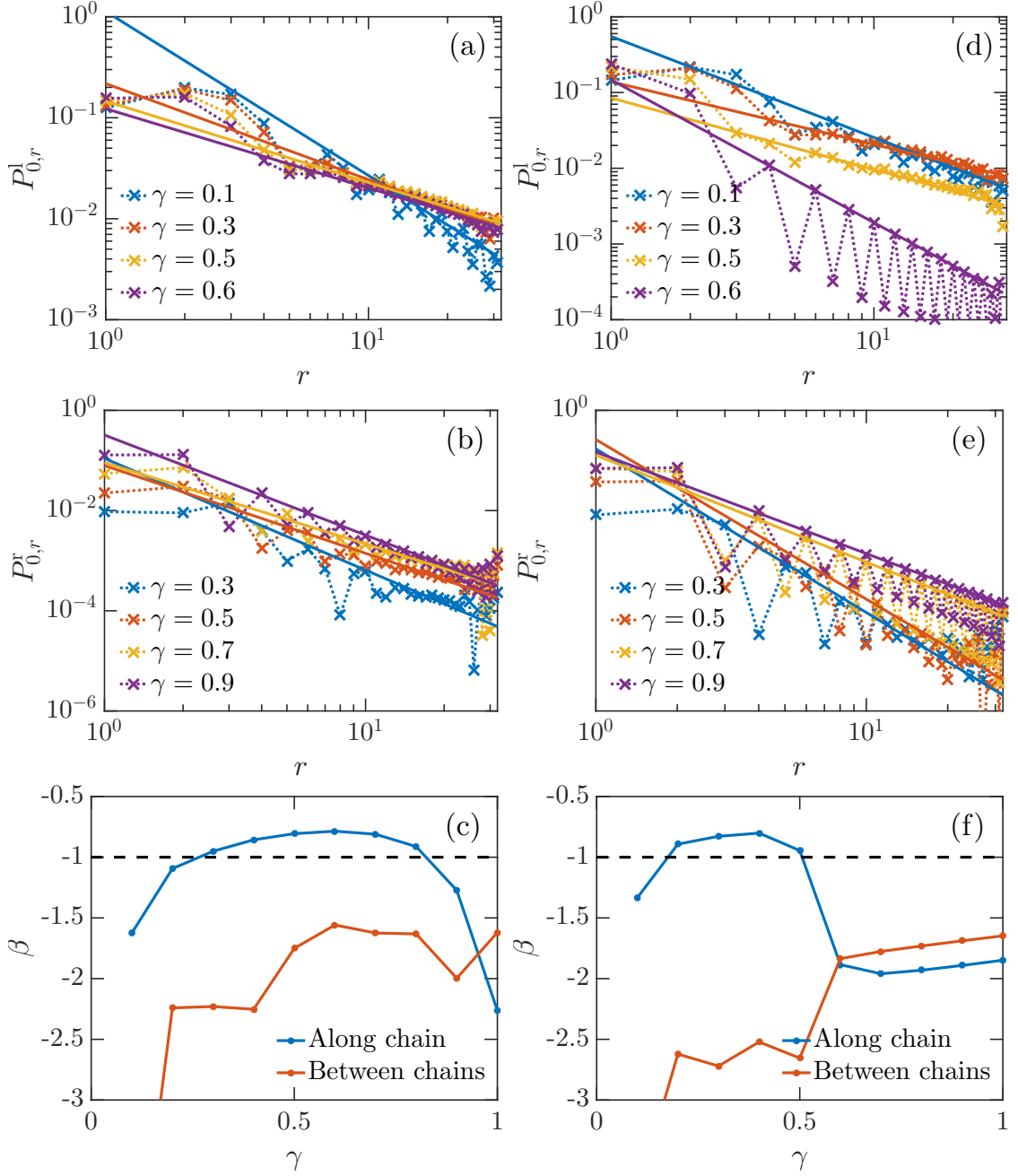


Figure 4.11: Comparison of pair correlations between the rectangular ladder (a)-(c), and the triangular ladder (d)-(f). These results were computed for the same parameters as in Fig. 4.10. The decay of singlet correlations  $P_{0,r}^l$ , where the singlets are oriented in the along the chains, are shown in (a) and (d). In (b) and (e), the decay of singlet correlations  $P_{0,r}^r$ , with the singlets oriented between the chains, is shown. Numerical results are shown as crosses, with dotted lines as a guide to the eye. In (a), (b), (d) and (e), we fit a power law  $P \sim r^\beta$  to the correlations. The power  $\beta$  from this power law is plotted as a function of the anisotropy  $\gamma$  for the rectangular and triangular ladders in (c) and (f) respectively.

We plot  $P_{0,j}^l$  in Fig. 4.11(a) for the rectangular ladder, and Fig. 4.11(d) for the triangular ladder at various values of  $\gamma$ . Likewise, we plot  $P_{0,j}^r$  in Fig. 4.11(b) and (e). The calculated results are shown with crosses, with dotted lines to guide the eye.

In all cases we find an approximate power-law decay for the correlations, consistent with a Luttinger liquid. For each of these correlations, we fit a power-law decay  $P \sim r^\beta$ . We show the fitted power  $\beta$  as a function of the anisotropy as the blue line in Fig. 4.11(c) and (f) for the rectangular and triangular ladders respectively. Recall from Sec. 4.2.2 that states with a Luttinger parameter  $K_\rho > 1$ , and hence a singlet-singlet correlation which decays slower than  $1/r$  is considered superconducting. As a guide, we mark  $\beta = -1$  as a black dashed line.

We observe different behaviours in each of the rectangular and triangular models as  $\gamma$  is varied. For small values of  $\gamma$  we find that in both cases, the correlations are carried predominantly along the legs rather than along the rungs, as expected. In the rectangular ladder, moderate coupling between the chains increases the range of singlet correlations, suggesting enhanced superconducting properties. However, as the chains become isotropic, the correlations gradually switch to being carried equally along both the rungs and the legs, with neither of them reaching the characteristic  $1/r$  decay indicative of superconductivity. The triangular ladder similarly shows enhancement of the leg correlations for small  $\gamma$ 's. However, at  $\gamma \gtrsim 0.5$  we see a sharp transition to a state with suppressed pair correlations, consistent with the sharp drop observed in the entanglement entropy Fig. 4.11(c).

## 4.6 Conclusions and outlook

In this chapter, we have explored in detail the properties of the  $t$ - $J$ - $\alpha$  model. We first computed the ground-state phase diagram of the one-dimensional chain. There we showed that the pair hopping can push the superconducting boundary to lower values of  $J/t$  at dilute fillings. However, the pair hopping also increases the region with a finite spin-gap. The presence of a spin-gap leads to a description of the model by dynamically constrained bosons, whose constraints inhibit superconductivity at large fillings.

Motivated by this, we have performed DMRG calculations on two different ladder geometries, where we conjectured that the dynamical constraints are more important than in the strictly one dimensional chain. We have shown that for both rectangular and triangular ladders, near-isotropic couplings lead to a suppression of long-range singlet correlations consistent with a loss of superconductivity in the chains. In the

case of the triangular ladder, this is seen as a sharp transition around  $\gamma \approx 0.5$ . The precise diagnosis of this phase transition remains as future work.

As we will show in Chapter 5 and Chapter 6, periodic driving, arising, for example, through optical lattice shaking, or through vibrational driving in solids, can suppress single-particle hopping, and suppress or enhance the superexchange and pair hopping. It might therefore be possible to decouple the chains by driving the system, and hence induce superconductivity in systems which would ordinarily suffer from these constraints.

It is not yet clear whether the features we have seen in these ladder systems can be explained via a constrained bosonic model as they were for the one dimensional model in Sec. 4.3. For instance, computing the spin gap requires extrapolating with larger systems than we have computed so far for the ladders. Studying the behaviour of the spin-gap and the resulting constrained bosonic model remain as future work. It is also not clear how this behaviour scales as we add more chains, which may reveal more about the role the physics discussed in this chapter might play in high temperature superconductors. It is likely that this behaviour may be clearly observed directly in two and three dimensions with cold atom experiments, where superexchange physics can be more directly probed [111, 112, 113]. In short, studying the  $t$ - $J$ - $\alpha$  model in higher dimensions could provide significant insights into the behaviour of high- $T_c$  superconductors and periodically driven strongly correlated systems.

## Chapter 5

# Periodically driven systems and Floquet theory

Systems under periodic driving are ubiquitous in physics. From simple driven Harmonic oscillators, to atoms in laser fields, the physics of driven systems underpins many technologies relying on control, switching and stabilisation of physical systems. Even relatively simple classical systems under periodic driving can exhibit striking and counterintuitive behaviour. For instance, high-frequency driven systems can be stable in configurations which are not statically stable. The classic example of this is the Kapitza pendulum [144]. A rigid pendulum with a mass at the end has only one stable equilibrium, i.e. the mass hanging directly down. However, if the pivot of the pendulum is periodically modulated with an amplitude much smaller than its length, and at a frequency much faster than the natural frequency of the pendulum, then the second, previously unstable, equilibrium with the pendulum in an inverted position becomes stable.

A similar effect is exploited in the Paul trap for trapping and manipulating charged particles. Static electromagnetic fields have no potential minima [145], and so they cannot be used to trap charges. If an oscillating quadrupole potential is used, however, then the particle's dynamics are governed by the Mathieu equation [146]. This may be solved exactly using Floquet theory, revealing stable equilibria for the ions [147].

In the broadest sense, Floquet theory is the mathematical framework used for analysing systems of linear ordinary differential equations (ODEs) whose coefficients are periodic functions of time [148]. In this chapter we introduce Floquet theory as applied to quantum mechanical systems, i.e. where the system of ODEs is the time dependent Schrödinger equation. We will see that this leads to an intuitive picture of the dynamics, where the Hamiltonian describing the driven system captures the dynamics of the undriven quantum system, plus additional processes induced by

absorbing/emitting quanta of energy from the drive. In the particular limit of large driving frequencies, we will demonstrate that it is possible to perturbatively derive an effective static Hamiltonian which captures the dynamics of driven system.

The time-periodicity of the Hamiltonian has implications for the unitary propagator  $\hat{U}(\tau_2, \tau_1)$  which evolves a state from time  $\tau_1$  to  $\tau_2 > \tau_1$ . The periodicity of the evolution allows us to write

$$\hat{U}(\tau_2, \tau_1) = \hat{U}(\tau_2, \tau_0 + mT) \hat{U}(\tau_0 + mT, \tau_0) \hat{U}(\tau_0, \tau_1), \quad (5.1)$$

That is, we evolve from  $\tau_1$  to an arbitrary intermediate time  $\tau_1 \leq \tau_0 < T$ , then evolve for an integer number  $m$  driving periods, before concluding the evolution by evolving from  $\tau_0 + mT$  to  $\tau_2$ . The periodicity of  $\hat{H}$  demands that  $\hat{U}(\tau + mT, \tau) = \hat{U}(\tau + T, \tau)^m$ . It is therefore convenient to define an effective *time independent* (Floquet) Hamiltonian  $\hat{H}_F$ ,

$$\hat{U}(\tau_0 + T, \tau_0) = e^{-i\hat{H}_F T}, \quad (5.2)$$

which determines the stroboscopic evolution of the system<sup>1</sup>. Just as in the classical examples, the properties of  $\hat{H}_F$  may be drastically different from those of the undriven Hamiltonian. This leads to the general concept of “Floquet engineering”. The idea is to first take a simple system, governed by a static Hamiltonian  $\hat{H}$ , which is relatively easy to implement physically. Then, one adds a driving term which periodically modulates the parameters of  $\hat{H}$ , such that the generated  $\hat{H}_F$  has interesting or useful physical properties which would be difficult, or may even be impossible to engineer in equilibrium [149, 150].

In recent years, many examples of Floquet engineering have been proposed theoretically [151] and implemented experimentally [109]. For example, systems with topologically trivial band structures can be endowed with a nonzero Chern number [152, 153, 154]. More generally, artificial gauge fields can be engineered for neutral ultracold atomic systems [149, 155]. In the presence of interactions, one can engineer Hamiltonians with even more striking properties. For example, a Bose-Hubbard model with a superfluid ground state can be made Mott insulating by shaking the lattice [151, 109] and, as we shall explore in detail in Chapter 6, a Hubbard model with a metallic ground state can be made superconducting by the appropriate choice of driving term.

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<sup>1</sup>Note that this Floquet Hamiltonian implicitly has a parametric dependence on the intermediate time  $\tau_0$ . However, the Floquet Hamiltonians for each different choice of  $\tau_0$  are related to one another by unitary transformations.

## 5.1 Floquet theory for the Schrödinger equation

In the context of quantum mechanics, Floquet theory concerns Hamiltonians which are periodic in time  $\tau$ ,

$$\hat{H}(\tau + T) = \hat{H}(\tau), \quad (5.3)$$

where  $T = 2\pi/\Omega$  is the driving period. The corresponding time-dependent Schrödinger equation for states  $|\psi(\tau)\rangle$  reads

$$[\hat{H}(\tau) - i\partial_\tau] |\psi(\tau)\rangle = 0, \quad (5.4)$$

where  $\partial_\tau$  is the derivative with respect to time. Floquet's theorem states that due to the time-periodicity of  $\hat{H}$ , there exists a complete set of solutions to this Schrödinger equation [156],

$$|\psi_\alpha(\tau)\rangle = e^{-i\epsilon_\alpha\tau} |\phi_\alpha(\tau)\rangle, \quad (5.5)$$

where  $|\phi_\alpha(\tau + T)\rangle = |\phi_\alpha(\tau)\rangle$  are time-periodic Floquet states. The Floquet states therefore obey the eigenvalue equation

$$[\hat{H}(\tau) - i\partial_\tau] |\phi_\alpha(\tau)\rangle = \epsilon_\alpha |\phi_\alpha(\tau)\rangle, \quad (5.6)$$

where  $\epsilon_\alpha$  are real eigenvalues known as Floquet quasienergies. Because of the periodicity of the Floquet states in Eq. (5.5), the quasienergies are only defined up to  $\epsilon_\alpha \pm m\Omega$  for integer  $m$ . In other words, breaking the continuous time translational symmetry of a time-independent Hamiltonian to the discrete translational invariance of a periodically time-dependent Hamiltonian means that energy is no longer conserved. Rather, a system in a Floquet eigenstate can absorb or emit any integer number of energy quanta  $m\Omega$  while remaining in that same Floquet state.

The quasienergy operator  $\hat{H}_Q = [\hat{H}(\tau) - i\partial_\tau]$  is a Hermitian operator which acts on the combined Floquet-Hilbert space  $\mathcal{T} \otimes \mathcal{H}$ , where  $\mathcal{H}$  is the original Hilbert space of our many-body system, and  $\mathcal{T}$  is the space of square-integrable periodic functions of time with period  $T$ <sup>2</sup>. Vectors in this extended Hilbert space are denoted  $|\chi\rangle$ . The scalar product between these vectors is given by

$$\langle\langle\chi|\xi\rangle\rangle = \frac{1}{T} \int_0^T d\tau \langle\chi(\tau)|\xi(\tau)\rangle, \quad (5.7)$$

where  $|\chi(\tau)\rangle$  and  $|\xi(\tau)\rangle$  are time-periodic vectors in  $\hat{H}$ , and  $\langle\chi(\tau)|\xi(\tau)\rangle$  is the standard scalar product on  $\mathcal{H}$ . Using this inner product, and choosing a particular basis

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<sup>2</sup>Note that the quasienergy operator is sometimes referred to as the Floquet Hamiltonian. However, we will reserve the term “Floquet Hamiltonian” to refer to the effective static Hamiltonian  $\hat{H}_F$  which governs the stroboscopic evolution of the system.

in the Floquet-Hilbert space, we can write the  $\hat{H}_Q$  as a matrix, and diagonalise it to find the quasienergies just as one would with a static Hamiltonian. Once one has the Floquet eigenstates and quasienergies, the dynamics are completely determined, similar to how determining eigenstates and eigenenergies of static Hamiltonians completely determines their dynamics. Concretely, if we expand the initial state  $|\psi(0)\rangle$  in terms of Floquet states,

$$|\psi(0)\rangle = \sum_{\alpha} c_{\alpha} |\phi_{\alpha}(0)\rangle, \quad (5.8)$$

then the state at subsequent times  $|\psi(\tau)\rangle$  is

$$|\psi(\tau)\rangle = \sum_{\alpha} c_{\alpha} e^{-i\epsilon_{\alpha}\tau} |\phi_{\alpha}(\tau)\rangle. \quad (5.9)$$

How are these quasienergies related to the Floquet Hamiltonian  $\hat{H}_F$ ? Let us consider applying the propagator  $\hat{U}(T + \tau, \tau)$  to a state  $|\psi_{\alpha}(\tau)\rangle$  from Eq. (5.5),

$$\begin{aligned} \hat{U}(T + \tau, \tau) |\psi_{\alpha}(\tau)\rangle &= |\psi_{\alpha}(\tau + T)\rangle \\ &= e^{-i\epsilon_{\alpha}(\tau+T)} |\phi_{\alpha}(\tau + T)\rangle \\ &= e^{-i\epsilon_{\alpha}T} (e^{-i\epsilon_{\alpha}\tau} |\phi_{\alpha}(\tau)\rangle) \\ &= e^{-i\epsilon_{\alpha}T} |\psi_{\alpha}(\tau)\rangle. \end{aligned} \quad (5.10)$$

The states  $|\psi_{\alpha}(\tau)\rangle$  are therefore eigenstates of  $U(\tau + T, \tau) \equiv e^{-i\hat{H}_F T}$  with eigenvalue  $e^{-i\epsilon_{\alpha}T}$ , and so the eigenvalues of  $\hat{H}_F$  are, in fact, the quasienergies  $\epsilon_{\alpha}$ . In Sec. 5.2, we shall use this fact to construct the effective Hamiltonian  $\hat{H}_F$  by block-diagonalising the quasienergy operator.

### 5.1.1 Analogy with Bloch's theorem

The Floquet theorem is in close analogy with Bloch's theorem [157], where continuous translational invariance in space is broken to a discrete translational invariance by a periodic potential  $V(x)$  as we discussed in Sec. 2.1. As a result, momentum is no longer conserved, rather only crystal momentum, or quasimomentum, defined up to  $2\pi/a$ . This analogy is laid out more explicitly in Fig. 5.1. We consider again the Hamiltonian for particles in the periodic potential,

$$\hat{H} = \frac{\hat{p}^2}{2m} + V(x), \quad (5.11)$$

where  $V(x + a) = V(x)$ . In (a) we show the dispersion relation for a free particle,  $E_q \sim q^2$ . Due to the discrete translational symmetry of  $\hat{H}$ , we get replicas of the free

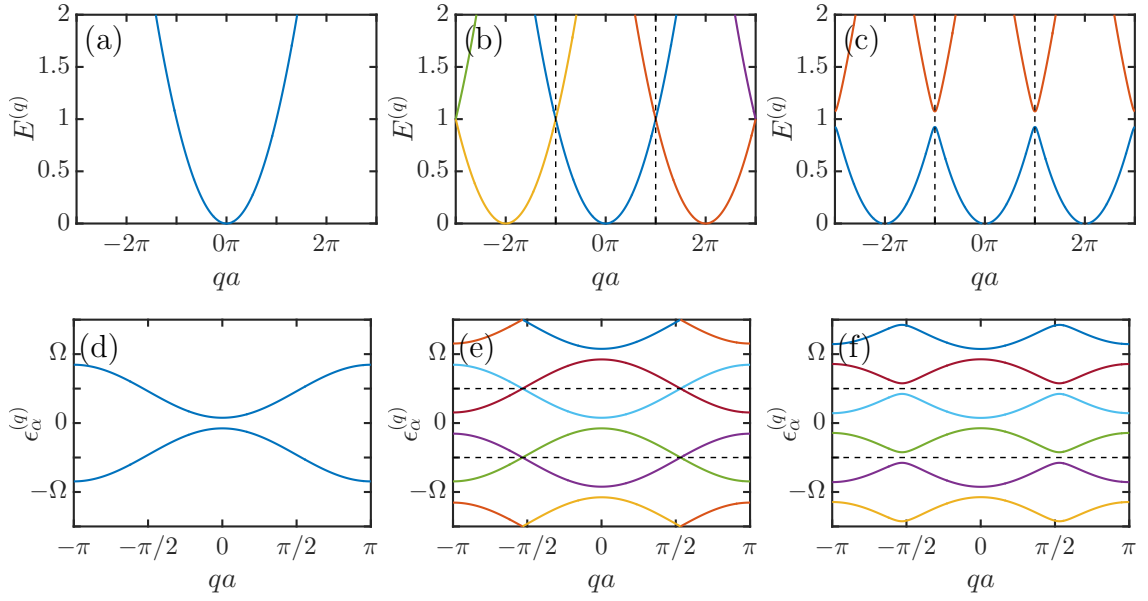


Figure 5.1: We illustrate the analogy between Floquet theory and Bloch's theorem. In (a), a free particle dispersion relation is shown. In (b), due to the periodicity  $V(x + a) = V(x)$ , the dispersion is replicated every  $q \rightarrow q + 2\pi/a$ , with degeneracies at the Brillouin zone boundaries (marked with dotted lines). In (c), the perturbation  $V(x)$  breaks the degeneracy and opens gaps at the zone edges. In comparison, in (d) we show a single Brillouin zone with a pair of bands. In (e), adding a time periodic perturbation  $V(\tau + T) = V(\tau)$ , results in band replicas every  $\epsilon_q \rightarrow \epsilon_\alpha^{(q)} + \Omega$ . In (f), the perturbation couples the bands, and a gap again opens up at the degeneracy points.

particle dispersion at every  $q \rightarrow q \pm 2\pi/a$  in momentum space, with degeneracies at the Brillouin zone boundaries, marked with dotted lines, which we show in (b). The potential  $V(x)$  can in general mix states of different momenta, and so the degeneracy at the zone boundaries is broken, opening up a band gap, which we show in (c). In analogy with this, in Fig. 5.1(d)-(f) we consider a system described by the Hamiltonian

$$\hat{H} = \hat{H}_0 + \hat{V}(\tau), \quad (5.12)$$

where here  $\hat{H}_0$  is the Hamiltonian for a pair of noninteracting electron bands, and  $\hat{V}(\tau + T) = \hat{V}(\tau)$  is a time-periodic driving term. In Fig. 5.1(d), we show this pair of electronic bands. Then, due to the periodicity of  $V(\tau)$ , we get replicas of this band structure every  $\epsilon_\alpha \rightarrow \epsilon_\alpha + m\Omega$  in energy, shown in (e), which can result in degeneracies from the intersection of bands with different photon numbers  $m$ . Finally, if the perturbing driving term  $V(\tau)$  couples these different bands, then an avoided crossing will appear, shown in (f). If  $\Omega$  is chosen such that this gap opens around the Fermi level, then it will turn the system from a conductor to a band insulator. In systems with Dirac cones, driving with circularly polarised light can break time-reversal symmetry and turn the system from a semimetal to a topological insulator [152, 153, 158].

### 5.1.2 Example: Driven two-level atom

To introduce some of the more practical aspects of working with periodically-driven systems, and provide a concrete physical interpretation of the quasienergy operator, here we discuss the classic example of a driven two-level system [156]. The levels are separated in energy by  $\omega_0$ , and the system is driven by an external field at frequency  $\Omega = 2\pi/T$  with an amplitude  $V$ . The Hamiltonian for the system is

$$\hat{H} = \frac{\omega_0}{2} \hat{S}^z + V \cos(\Omega\tau) \hat{S}^x. \quad (5.13)$$

Such a Hamiltonian describes, for instance, an atom in a laser field [159], or a spin-1/2 magnetic dipole in an oscillating magnetic field [160], and is sometimes called the classical Rabi model (CRM). We choose the Floquet basis

$$|\sigma, m\rangle\rangle = |\sigma\rangle e^{-im\Omega\tau}, \quad (5.14)$$

where  $\sigma = \pm 1$  and  $\hat{S}^z |\sigma\rangle = \sigma |\sigma\rangle$  are the energy eigenstates of the undriven two-level system, and  $m$  is an integer. Expanding the quasienergy operator, we obtain

the matrix

$$\langle\langle\sigma, m|\hat{H}_Q|\sigma', n\rangle\rangle = \frac{\omega_0}{2} \left( \langle\sigma|\hat{S}^z|\sigma'\rangle + m\Omega \right) \delta_{m,n} + \frac{V}{2} \langle\sigma|\hat{S}^x|\sigma'\rangle \left( \delta_{1,(m-n)} + \delta_{1,(n-m)} \right). \quad (5.15)$$

Or, written in matrix form,

$$\mathbf{H}_Q = \begin{pmatrix} \ddots & & & & \\ & \frac{\omega_0}{2}\mathbf{S}^z - 2\Omega & \frac{V}{2}\mathbf{S}^x & 0 & 0 \\ & \frac{V}{2}\mathbf{S}^x & \frac{\omega_0}{2}\mathbf{S}^z - \Omega & \frac{V}{2}\mathbf{S}^x & 0 \\ & 0 & \frac{V}{2}\mathbf{S}^x & \frac{\omega_0}{2}\mathbf{S}^z & \frac{V}{2}\mathbf{S}^x \\ & 0 & 0 & \frac{V}{2}\mathbf{S}^x & \frac{\omega_0}{2}\mathbf{S}^z + \Omega \\ & & & & \ddots \end{pmatrix}, \quad (5.16)$$

where  $(\mathbf{S}^{(z/x)})_{\sigma,\sigma'} \equiv \langle\sigma|\hat{S}^{(z,x)}|\sigma'\rangle$  are the Pauli matrices. We see that the matrix  $\mathbf{H}_Q$  has a clear block structure. The blocks on the diagonal are replicas of the undriven Hamiltonian with energy offsets  $\pm m\Omega$ . The first off-diagonal block simultaneously causes transitions between adjacent  $m$  blocks and flips the state of the two-level system. The quasienergy matrix thus has a clear physical interpretation. The dynamics it generates correspond to the atom undergoing transitions to/from its ground and excited state while emitting/absorbing photons of energy  $\Omega$  from the driving field. Although a general Hamiltonian's periodic term may not be due to a light field, and although the external driving is completely classical,  $m$  is still commonly referred to as the “photon number”.

In fact, this physical interpretation of  $\hat{H}_Q$  as capturing the absorption/emission of photons can be made more explicit by considering the corresponding quantum model. We write down the Hamiltonian for this two-level system coupled to a single photonic mode, sometimes called the quantum Rabi model (QRM) [159],

$$\hat{H}_{\text{QRM}} = \frac{\omega_0}{2}\hat{S}^z + \Omega\hat{a}^\dagger\hat{a} + g\hat{S}^x(\hat{a} + \hat{a}^\dagger), \quad (5.17)$$

where  $\hat{a}^{(\dagger)}$  is the annihilation (creation) operator for the bosonic mode, and  $g$  is the coupling strength between the atom and the light field. Then, expanding this in the basis  $\{|\sigma, n\rangle\}$ , where  $n$  is the occupation number of the mode, we obtain

$$\langle\sigma, n|\hat{H}_{\text{QRM}}|\sigma', m\rangle = \frac{\omega_0}{2}\mathbf{S}^z + n\Omega\delta_{m,n} + g\mathbf{S}^x \left( \sqrt{n}\delta_{m,n-1} + \sqrt{n+1}\delta_{m,n+1} \right), \quad (5.18)$$

or, in matrix form,

$$\mathbf{H}_{\text{QRM}} = \begin{pmatrix} \frac{\omega_0}{2}\mathbf{S}^z & g\mathbf{S}^x & 0 & 0 & \cdots \\ g\mathbf{S}^x & \frac{\omega_0}{2}\mathbf{S}^z + \Omega & \sqrt{2}g\mathbf{S}^x & 0 & \\ 0 & \sqrt{2}g\mathbf{S}^x & \frac{\omega_0}{2}\mathbf{S}^z + 2\Omega & \sqrt{3}g\mathbf{S}^x & \\ 0 & 0 & \sqrt{3}g\mathbf{S}^x & \frac{\omega_0}{2}\mathbf{S}^z + 3\Omega & \\ \vdots & & & & \ddots \end{pmatrix}. \quad (5.19)$$

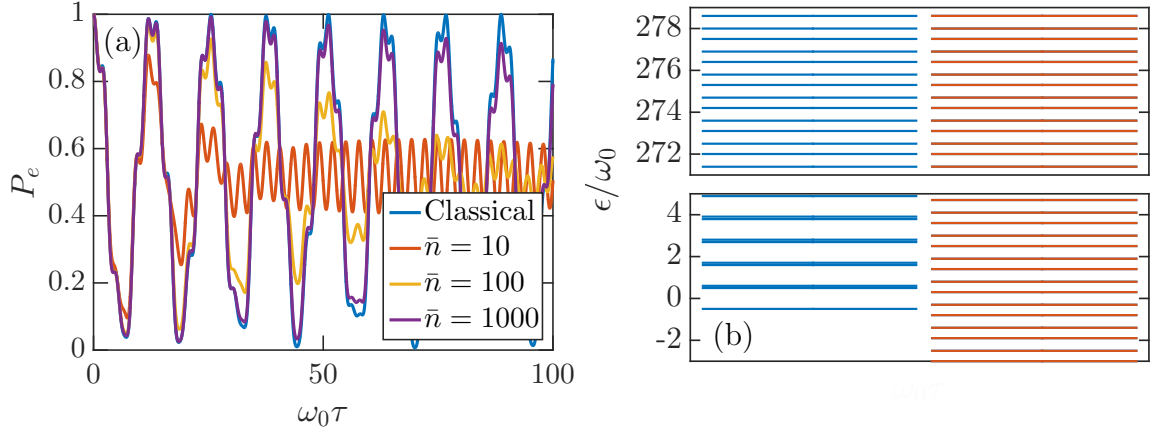


Figure 5.2: A comparison between the semiclassical and fully quantum Rabi models. In (a) we show the dynamics of the excited state population  $P_e$ . The atom is initially placed in its excited state,  $|e\rangle$ , while light field is initialised in a coherent state with a mean number of photons  $\bar{n}$ . In (b) we show a comparison between the energy spectrum of the quantum Rabi model (left, blue), and the quasienergy spectrum of the classical Rabi model (right, red). In both figures the parameters used are  $\Omega = 1.1\omega_0$  and  $V = 0.5\omega_0$ , and  $g = V/(2\sqrt{\bar{n}+1})$ . In (b), we choose  $\bar{n} = 250$ . Note that we have not made the rotating wave approximation, which is not valid for this choice of parameters.

If we then take the photon number to be  $N \gg 1$  (i.e. the “classical limit”), and subtract a constant energy shift  $N\Omega$ , then, making the identification  $V/2 = \sqrt{N+1}g$ , the quasienergy matrix for the CRM is approximately equal to the Hamiltonian matrix for the QRM in the vicinity of the photon number  $n \approx N$ , i.e.  $\mathbf{H}_Q \approx \mathbf{H}_{\text{QRM}}$ . The dynamics generated by the quasienergy operator thus correspond to those generated by the fully quantum model in the limit of large photon numbers.

To illustrate this point, we calculate, using exact numerical diagonalisation, the dynamics of the QRM versus the CRM, and show the results in Fig. 5.2(a). In both cases, the atom is initialised in its excited state. In the quantum case, the light field is initialised in a coherent state with mean photon number  $\bar{n}$ ,

$$|\bar{n}\rangle = \sum_m \sqrt{e^{-\bar{n}} \frac{\bar{n}^m}{m!}} |m\rangle, \quad (5.20)$$

where  $|m\rangle$  is a Fock state containing  $m$  photons. We see that the two models agree closely on short timescales. However, in the quantum case, we get the well known “collapse and revival” of the Rabi oscillations. On a timescale  $1/(V\bar{n})$ , the excited state population  $P_e = |\langle e | \psi(\tau) \rangle|^2$  collapses to  $P_e = 1/2$  before undergoing a revival on a timescale  $\sim 2\pi/(V\sqrt{\bar{n}})$ . Therefore, when we increase  $\bar{n}$  in the coherent state, the quantum system corresponds more closely to the semiclassical result.

The quasienergy spectrum  $\epsilon_\alpha$  may be computed numerically in one of two ways. Firstly, one can construct  $\mathbf{H}_Q$  explicitly, as in Eq. (5.16), introducing a cutoff in the photon number  $-M/2 \leq m \leq M/2$  so as to make the quasienergy matrix a finite  $(M+1) \times (M+1)$  matrix. One can then diagonalise this matrix to compute approximations to the quasienergies, then increasing this cutoff  $M$  until the quasienergies converge. Alternatively, one can numerically integrate the time dependent Schrödinger equation for a time  $T$  to compute  $\hat{U}(\tau + T, \tau)$ . Then, from Eq. (5.10) the eigenspectrum of this operator is

$$u_\alpha = e^{-i\epsilon_\alpha T}, \quad (5.21)$$

emphasising again that if  $\epsilon_\alpha$  is a quasienergy, then  $\epsilon_\alpha + m2\pi/T$  is also a quasienergy. We use this second method to compute  $\{\epsilon_\alpha\}$  for CRM, and compare these to the energy spectrum of the quantum Rabi model in Fig. 5.2(b). Because the Hilbert space has dimension 2, there are only two distinct quasienergies, repeated infinitely. Meanwhile, the QRM naturally has a spectrum which bounded from below, leading to a significant disparity between the spectra at low photon numbers. However, at large energies/photon numbers, the energy spectrum of the QRM closely matches the quasienergy spectrum of the CRM.

## 5.2 Effective Hamiltonians

The numerical strategies used in the previous example to compute the quasienergy spectra are infeasible for many-body systems, where the dimension of  $\mathcal{H}$  is exponentially large. Knowledge of the Floquet spectrum  $\{\epsilon_\alpha\}$  may also not be that physically insightful in terms of the properties of the driven system. It is often more useful to compute the Floquet Hamiltonian  $\hat{H}_F$ , which is the focus of this section.

The choice of Floquet basis states is not unique. We can of course express  $\hat{H}_Q$  in any complete orthonormal basis spanning  $\mathcal{H} \otimes \mathcal{T}$ . We now return to considering a generic quasienergy operator  $\hat{H}_Q$ . If we expand this in the basis

$$|\alpha, m\rangle\rangle = |\alpha\rangle e^{-im\Omega\tau}, \quad (5.22)$$

where  $\{|\alpha\rangle\}$  is an arbitrary orthonormal basis for  $\mathcal{H}$ , and apply the generalised inner

product from Eq. (5.7), we obtain the following form for the quasienergy operator

$$\hat{H}_Q = \begin{pmatrix} \ddots & \vdots & \vdots & \vdots & \vdots & \ddots \\ \cdots & \hat{H}_0 - 2\Omega & \hat{H}_{-1} & \hat{H}_{-2} & \hat{H}_{-3} & \cdots \\ \cdots & \hat{H}_1 & \hat{H}_0 - \Omega & \hat{H}_{-1} & \hat{H}_{-2} & \cdots \\ \cdots & \hat{H}_2 & \hat{H}_1 & \hat{H}_0 & \hat{H}_{-1} & \cdots \\ \cdots & \hat{H}_3 & \hat{H}_2 & \hat{H}_1 & \hat{H}_0 + \Omega & \cdots \\ \ddots & \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix}, \quad (5.23)$$

where

$$\hat{H}_m = \frac{1}{T} \int_0^T \hat{H}(\tau) e^{im\Omega\tau} d\tau \quad (5.24)$$

is the  $m$ th Fourier component of the Hamiltonian. Note that since we have left the basis spanning the Hilbert space  $\mathcal{H}$  arbitrary, the elements of  $\hat{H}_Q$  have retained the form of operators on  $\mathcal{H}$ . Due to the tensor product structure of the Floquet-Hilbert space, we can use a time-periodic unitary transformation to block-diagonalise the quasienergy operator [161], i.e.

$$\hat{H}_Q = \begin{pmatrix} \ddots & \vdots & \vdots & \vdots & \vdots & \ddots \\ \cdots & \hat{H}_F - 2\Omega & 0 & 0 & 0 & \cdots \\ \cdots & 0 & \hat{H}_F - \Omega & 0 & 0 & \cdots \\ \cdots & 0 & 0 & \hat{H}_F & 0 & \cdots \\ \cdots & 0 & 0 & 0 & \hat{H}_F + \Omega & \cdots \\ \ddots & \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix}. \quad (5.25)$$

Note that due to the structure of the quasienergies, (i.e. that they are repeated every  $\Omega$ ), each diagonal block must be the same operator on  $\mathcal{H}$ , shifted by  $m\Omega$ . Moreover, since the eigenvalues of these diagonal blocks are the quasienergies, these operators must be the effective Hamiltonian  $\hat{H}_F$  (up to some unitary transformation).

Unfortunately, it is generally not possible to exactly calculate the unitary transformation which brings this into block-diagonal form, or the exact form of  $\hat{H}_F$ . However, in the limit that  $\Omega$  is large compared to other energy scales in the Hamiltonian, and the off-diagonal blocks  $\hat{H}_m$ ,  $|m| > 1$  are small compared to  $\Omega$ , then the quasienergy operator has a structure very similar to that of the large  $U$  Hubbard model discussed in Sec. 2.3. There, we had distinct blocks in the Hamiltonian separated in energy by  $U$ , and we sought to compute the effect of adding a weak perturbation (the kinetic energy  $t$ ) which coupled these blocks. In this case, we would like to compute the effect of adding perturbations  $\hat{H}_m$ ,  $|m| > 1$  which couple the zero-photon block  $\hat{H}_0$  to blocks of different photon numbers [161].

For simplicity, we take the unperturbed Hamiltonian to be

$$\Omega \hat{H}^{(0)} = \sum_m m \Omega (1 \otimes \mathbb{P}_m). \quad (5.26)$$

Where  $\mathbb{P}_m = |m\rangle \langle m|$  is the projector onto the  $m$  photon sector. The perturbation we apply is then the matrix containing the Fourier components of the Hamiltonian, i.e.

$$h \hat{H}^{(1)} = \sum_{m,m'} \hat{H}_{m-m'} \otimes |m\rangle \langle m'|, \quad (5.27)$$

where  $h \ll \Omega$  is the characteristic energy scale of the Hamiltonian. We recall from Chapter 2 that the effective Hamiltonian within a degenerate manifold (i.e. the  $n$  photon block), split by a perturbation  $\lambda \hat{H}^{(1)}$  is given by

$$\hat{H}_{\text{eff}} = E_n \mathbb{P}_n + \lambda \mathbb{P}_n \hat{H}^{(1)} \mathbb{P}_n + \lambda^2 \sum_{m \neq n} \frac{\mathbb{P}_n \hat{H}^{(1)} \mathbb{P}_m \hat{H}^{(1)} \mathbb{P}_n}{E_n - E_m}, \quad (5.28)$$

where here  $E_n = n\Omega$ . We focus on the zero-photon block<sup>3</sup>, i.e.  $n = 0$ . Substituting in  $\lambda = h$ , the definitions of  $\mathbb{P}_m$  and  $\hat{H}^{(0,1)}$ , we obtain

$$\begin{aligned} \hat{H}_F &\approx \hat{H}_0 + \frac{h^2}{\Omega} \sum_{m \neq 0} \frac{\mathbb{P}_0 \hat{H}^{(1)} \mathbb{P}_m \hat{H}^{(1)} \mathbb{P}_0}{m} \\ &= \hat{H}_0 + \frac{1}{\Omega} \sum_{m \neq 0} \frac{\hat{H}_m \hat{H}_{-m}}{m} \end{aligned} \quad (5.29)$$

$$= \hat{H}_0 + \frac{1}{\Omega} \sum_{m > 0} \frac{[\hat{H}_m, \hat{H}_{-m}]}{m}, \quad (5.30)$$

where in the last line we have grouped the positive and negative  $m$  terms together. Note that for this perturbation to be valid,  $\Omega$  must be larger than any energy scale appearing in the undriven Hamiltonian. It is possible to derive higher-order corrections to  $\hat{H}_F$  by taking higher orders in the degenerate perturbation theory [161], which we shall not discuss here. We see that the advantage of this Floquet approach is that it has turned a complicated time-dependent problem into a static problem which is amenable to standard time-independent perturbation theory. Other approaches to computing the Floquet Hamiltonian include using the Floquet-Magnus expansion [150], which we shall not discuss here. We note that, intuitively, the 0th order Floquet Hamiltonian is given by the 0th Fourier component of the time-dependent Hamiltonian, i.e. its time average

$$\hat{H}_0 = \frac{1}{T} \int_0^T \hat{H}(\tau) d\tau. \quad (5.31)$$

---

<sup>3</sup>Note that due to the periodicity of the spectrum, it does not matter which block we choose (up an overall energy shift).

### 5.2.1 Example: Driven single-band model

We illustrate this high-frequency expansion with the example of a one dimensional tight-binding chain [162],

$$\hat{H} = \hat{H}_t + V \cos(\Omega\tau) \sum_j j \hat{n}_j, \quad (5.32)$$

where

$$\hat{H}_t = -t \sum_j \left( \hat{c}_j^\dagger \hat{c}_{j+1} + \text{H.c.} \right), \quad (5.33)$$

Here  $t$  is the hopping amplitude, and  $V$  and  $\Omega$  are the driving amplitude and frequency, respectively.  $\hat{c}_j^\dagger$  and  $\hat{c}_j$  are the (bosonic or fermionic) creation and annihilation operators for a particle on lattice site  $j$ , and  $\hat{n}_j = \hat{c}_j^\dagger \hat{c}_j$ . Recall from Sec. 2.2 that the Hamiltonian  $\hat{H}_t$  corresponds to, for example, a gas of noninteracting particles trapped in the lowest Bloch band of a one dimensional optical lattice. The driving term  $\hat{H}_V(\tau)$  then corresponds to the lattice being shaken back and forth, in the frame which is co-moving with the lattice [163], as we show in Appendix E. Again expanding the Quasienergy operator in the Floquet basis

$$|\alpha, m\rangle\rangle = |\alpha\rangle e^{-im\Omega\tau}, \quad (5.34)$$

we obtain

$$\hat{H}_Q = \begin{pmatrix} \ddots & \vdots & \vdots & \vdots & \vdots & \ddots \\ \cdots & \hat{H}_t - 2\Omega & V \sum_j j \hat{n}_j & 0 & 0 & \cdots \\ \cdots & V \sum_j j \hat{n}_j & \hat{H}_t - \Omega & V \sum_j j \hat{n}_j & 0 & \cdots \\ \cdots & 0 & V \sum_j j \hat{n}_j & \hat{H}_t & V \sum_j j \hat{n}_j & \cdots \\ \cdots & 0 & 0 & V \sum_j j \hat{n}_j & \hat{H}_t + \Omega & \cdots \\ \ddots & \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix}, \quad (5.35)$$

which has a tridiagonal structure since the driving term in the lab frame has only one Fourier component  $m = \pm 1$ . We can immediately see a problem with this. Namely, that if we are interested in the strongly-driven regime, where  $V \sim \Omega \gg t$ , where the driving is expected to significantly modify the physics of the undriven system, then this basis is unsuitable for performing perturbation theory, since the off-diagonal blocks are not small compared to the spectral gap  $\Omega$  of the diagonal blocks. To find a more suitable basis, we employ a unitary transformation to the Floquet basis

$$\hat{R}(\tau)|\alpha, m\rangle\rangle. \quad (5.36)$$

However, rather than applying this transformation directly to the basis states, we will instead transform the Hamiltonian, i.e.

$$\hat{H}^R = i(\partial_\tau \hat{R})\hat{R}^\dagger + \hat{R}\hat{H}\hat{R}^\dagger. \quad (5.37)$$

In principle, if we found the correct  $\hat{R}(\tau)$ , we could bring the matrix precisely into block-diagonal form in Eq. (5.25) and directly read off the effective Hamiltonian  $\hat{H}_F$ . However, this is generally not possible to do exactly. Instead, we choose an  $\hat{R}(\tau)$  which brings  $\hat{H}_Q$  into a form suitable for performing perturbation theory. A common choice for this is the rotating frame with respect to the driving term,

$$\hat{R}(\tau) = \exp \left( i \int_0^\tau \hat{V}(\tau') d\tau' \right) = \exp \left( i \frac{V}{\Omega} \sin(\Omega\tau) \sum_j j \hat{n}_j \right). \quad (5.38)$$

Applying this transformation to the annihilation operators  $\hat{c}_j$ ,

$$\hat{c}_j \rightarrow \hat{R}(\tau) \hat{c}_j \hat{R}^\dagger(\tau) \quad (5.39)$$

$$= e^{i \frac{V}{\Omega} \sin(\Omega\tau) \sum_k k \hat{n}_k} \hat{c}_j e^{-i \frac{V}{\Omega} \sin(\Omega\tau) \sum_k k \hat{n}_k} \quad (5.40)$$

Since all of the  $\hat{n}_k$ 's mutually commute, and they commute with  $\hat{c}_{j \neq k}$ , this reduces to

$$\hat{c}_j \rightarrow e^{i \frac{V}{\Omega} \sin(\Omega\tau) j \hat{n}_j} \hat{c}_j e^{-i \frac{V}{\Omega} \sin(\Omega\tau) j \hat{n}_j}. \quad (5.41)$$

Expanding the rightmost exponential as a power series, we encounter terms of the form

$$\hat{c}_j \hat{n}_j^l = \hat{c}_j (\hat{c}_j^\dagger \hat{c}_j)^l \quad (5.42)$$

$$= (1 \pm \hat{c}_j^\dagger \hat{c}_j)^l \hat{c}_j, \quad (5.43)$$

where  $l$  is an integer power, and we take the  $+$  sign for bosons and the  $-$  sign for fermions. Applying this to Eq. (5.41), we obtain

$$\hat{c}_j \rightarrow e^{i \frac{V}{\Omega} \sin(\Omega\tau) j \hat{n}_j} e^{-i \frac{V}{\Omega} \sin(\Omega\tau) j (1 \pm \hat{n}_j)} \hat{c}_j. \quad (5.44)$$

Finally, in the bosonic case the  $\hat{n}_j$  terms inside the exponentials cancel, whereas for fermions, since they are followed by a  $\hat{c}_j$ , they must be zero anyway. We thus obtain the result that regardless of the exchange statistics,

$$\hat{c}_j \rightarrow e^{-i \frac{V}{\Omega} \sin(\Omega\tau) j} \hat{c}_j. \quad (5.45)$$

Applying this to our Hamiltonian Eq. (5.32), we obtain

$$\hat{H}^R(\tau) = \hat{R}\hat{H}_t\hat{R}^\dagger \quad (5.46)$$

$$= -t \sum_j \left( e^{-i\frac{V}{\Omega} \sin(\Omega\tau)} \hat{c}_j^\dagger \hat{c}_{j+1} + \text{H.c.} \right). \quad (5.47)$$

Notice that the rotating frame transformation Eq. (5.38) is constructed such that the driving term is exactly cancelled, and is instead imprinted as an oscillating complex phase on the hopping term. Therefore, when we now expand in the Floquet basis in Eq. (5.36), the blocks in the quasienergy operator (i.e. the Fourier components of the Hamiltonian) become

$$\hat{H}_{m,m'} = -t \sum_j \left( \mathcal{J}_{m'-m}(\nu) \hat{c}_j^\dagger \hat{c}_{j+1} + \mathcal{J}_{m-m'}(\nu) \hat{c}_{j+1}^\dagger \hat{c}_j \right) + m\Omega \delta_{m,m'}, \quad (5.48)$$

where  $\nu = V/\Omega$ , and we have used the Jacobi-Anger expansion,

$$e^{iz \sin(\theta)} = \sum_{n=-\infty}^{\infty} \mathcal{J}_n(z) e^{in\theta}, \quad (5.49)$$

where  $\mathcal{J}_n(z)$  is the  $n$ th order Bessel function of the first kind. The rotating-frame driving now has an infinite number of Fourier components. Now our quasienergy operator has diagonal blocks separated in energy  $\Omega$ , and which are coupled by off-diagonal blocks whose elements are bounded by  $t \ll \Omega$ . We can therefore use the high frequency expansion Eq. (5.29). To zeroth order, the effective  $\hat{H}_F$  is given by the time-average of the rotating-frame Hamiltonian.

$$\hat{H}_F = -\mathcal{J}_0(\nu)t \sum_j \left( \hat{c}_j^\dagger \hat{c}_{j+1} + \text{H.c.} \right). \quad (5.50)$$

Looking again at Eq. (5.48), we note that since  $\mathcal{J}_{-n}(\nu) = (-1)^n \mathcal{J}_n(\nu)$ , we also have that  $\hat{H}_{-m} = (-1)^m \hat{H}_m$ . Since the Fourier blocks for  $\pm m$  only differ by a sign, they commute, and so the first-order correction is given by

$$\frac{1}{\Omega} \sum_{m>0} \frac{[\hat{H}_m, \hat{H}_{-m}]}{m} = 0. \quad (5.51)$$

In fact, it can be shown that the zeroth-order Floquet Hamiltonian is actually exact in this case [149]. We have therefore retained a tight-binding model Hamiltonian, but the driving field has renormalised the hopping amplitude  $t \rightarrow t\mathcal{J}_0(V/\Omega)$ . By increasing the driving strength, we can suppress the kinetic energy of the particles, or even invert the Bloch band by changing the sign of  $t$ . Moreover, by tuning the driving strength

$V$  so that  $t \rightarrow 0$ , then the particles can be completely localised. This is the very well-known “coherent destruction of tunneling” [164], or “dynamical localisation” [162], and has been experimentally demonstrated many times in ultracold atom systems [109, 155, 165, 166].

As an aside, in the Bose-Hubbard model, this effect can be used to induce a superfluid-Mott insulator transition by suppressing  $t/U$  to below its critical value [151]. Explicitly, we turn Eq. (5.32) into a driven Bose-Hubbard model by adding a local interaction term

$$\hat{H}_{\text{int}} = \frac{U}{2} \sum_j \hat{n}_j(\hat{n}_j - 1) \quad (5.52)$$

to Eq. (5.32), where  $U \ll \Omega$ . Since  $\hat{H}_{\text{int}}$  commutes with the driving term, it is not modified by the rotating frame transformation, and thus the quasienergy blocks become

$$\hat{H}_{m,m'} = -t \sum_j \left( \mathcal{J}_{m'-m}(\nu) \hat{c}_j^\dagger \hat{c}_{j+1} + \mathcal{J}_{m-m'}(\nu) \hat{c}_{j+1}^\dagger \hat{c}_j \right) + (\hat{H}_{\text{int}} + m\Omega) \delta_{m,m'}. \quad (5.53)$$

As we point out in the next section, there are subtleties with applying the high-frequency expansion to interacting many-body systems. However, if we disregard this for the moment, then to zeroth order, the high-frequency expansion yields again obtain a Bose-Hubbard model with  $U \rightarrow U$ , but  $t \rightarrow t\mathcal{J}_{m-m'}(V/\Omega)$ . We will discuss the dynamics of the driven Fermi-Hubbard model in great detail in Chapter 6

### 5.3 Floquet Heating

In the examples we have examined so far in Sec. 5.1.2 and Sec. 5.2.1, the energy spectra of the undriven systems have been bounded. This means that provided the driving frequency  $\Omega$  is much larger than the width of the undriven spectrum, there will be no intersections between quasienergy levels originating from different photon number sectors. As such, we expect that slowly modifying the driving strength will adiabatically modify the spectrum of the system. An initial equilibrium state will then be adiabatically modified, and is expected to be stable for long times.

However, the properties of systems whose spectra are unbounded are expected to be qualitatively different in the long-time limit. For example, let us consider a single-band many-body system with interactions, such as the Hubbard model which we introduced in Chapter 2. If the model has a finite interaction strength, then in the thermodynamic limit, the energy spectrum is *not* bounded from above. The

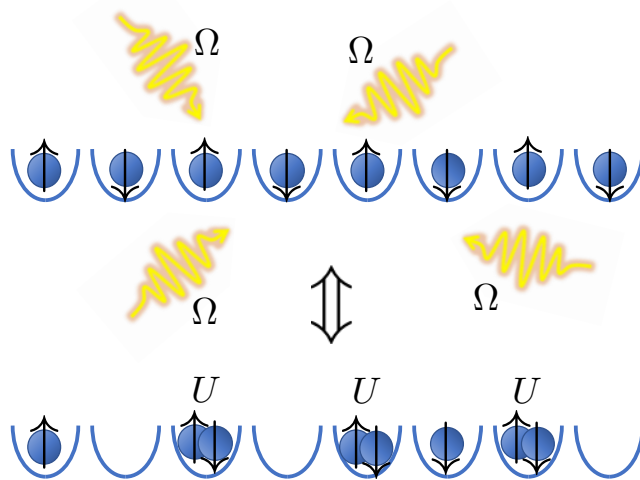


Figure 5.3: We show a cartoon of a collective excitation in the Hubbard model. For any interaction  $U$  and driving frequency  $\Omega$ , there will be a process of  $n$  electronic excitations and  $m$  photons such that  $nU = m\Omega$ , which invalidates the perturbation theory.

system can then, in principle, absorb an unlimited amount of energy from the drive, eventually heating up to an infinite temperature state [167].

It may at first seem counterintuitive that the Schrödinger equation Eq. (5.4) can lead to an infinite temperature state (that is, a mixed state whose density matrix is the identity), since it simply corresponds to unitary evolution of a pure state, and thus the state of the system must always remain a pure state. To resolve this, we appeal to the eigenstate thermalisation hypothesis (ETH) [168, 169]. The ETH states that if one takes an eigenstate of a many-body Hamiltonian, considers a contiguous subsystem and traces out the remainder of the system, then the density matrix of the resulting subsystem is a thermal state of the local Hamiltonian with the temperature set by the energy of the eigenstate. In other words, expectation values of local observables with respect to an eigenstate of the many-body system are indistinguishable from thermal expectation values for the subsystem of interest. From a thermodynamical perspective, this means starting with a single microstate of the full many-body Hamiltonian and tracing out part of the system, essentially treating it as a bath with which energy is exchanged with the remaining subsystem. Then a canonical ensemble of the remaining subsystem is obtained, with a well-defined temperature set by the energy of the initial microstate.

How does this square with the high-frequency expansion discussed in Sec. 5.2,

wherein the dynamics appear to be governed by a reasonable-looking local Hamiltonian? For interacting systems, the unbounded spectrum means that there will always be a collective excitation of the many-body system within the  $m = 0$  sector which is resonant with a Floquet replica with a large photon number, as we sketch in Fig. 5.3 for the Hubbard model. Specifically, if we denote states of the Hubbard model with  $n$  doublons  $m$  photons as  $|n, m\rangle\rangle$ , then  $|0, 0\rangle\rangle$  will be resonant with  $|n, -m\rangle\rangle$  for  $n/m \approx \Omega/U$ , i.e. when  $n/m$  is a rational approximant to  $\Omega/U$ . This means that these states will be strongly admixed by the driving. Hence the degenerate perturbation theory, which relies on having unperturbed states with a well-defined photon number  $m$  which are far-separated in energy, will in general fail to converge. Nevertheless, as we saw in the tight-binding example, Eq. (5.48), the off-diagonal blocks governing such couplings scale as  $\sim \mathcal{J}_m(V/\Omega)$ . As such, for large photon numbers, and reasonable values of  $V/\Omega$ , these couplings are strongly suppressed, and so heating tends to be negligible on typical experimental timescales.

The corrections to  $\hat{H}_F$  arising from these large-photon number couplings take the form of higher-order commutators [150, 161], which generate long-range interactions involving strings of local operators. These terms cause a large amount of entanglement between disparate parts of the system to build up over time. Thus, these terms cause the local observables of the system to become indistinguishable from a high temperature thermal state [170]. Recall from Chapter 3 that our MPS ansatz relies on restricted entanglement entropy. Floquet heating therefore also has implications for the simulability of driven systems. We will discuss Floquet heating more specifically for the case of the driven Hubbard model in Chapter 6.

It has been shown through very general arguments for driven many-body systems [171, 172], and through numerical studies of specific models [167] that on short timescales, the dynamics are well described by a short-range Hamiltonian which is approximately given by the high-frequency expansion. The timescale on which this approximation fails and significant heating begins to occur is given by

$$\tau^* \sim e^{-C\Omega/\varepsilon}, \quad (5.54)$$

where  $C$  is numerical constant of order unity and  $\varepsilon$  is an energy scale which bounds the terms in the Hamiltonian. Floquet-engineered Hamiltonians are therefore not useful indefinitely, but are time-limited by the timescale  $\tau^*$ .

It may appear from Eq. (5.54) that we can delay heating for exponentially long times by simply increasing  $\Omega$  to arbitrarily large values. However, while the Floquet heating processes we have discussed thus far are seen in simplified single-band models

such as the Hubbard model, there are experimentally relevant heating effects caused by scattering to higher excited Bloch bands which are not accounted for here [157, 166]. Recall from Chapter 2 that the Hubbard model captures only dynamics within the lowest Bloch band, neglecting higher bands and the continuum of free states. If  $\Omega$  is taken to be similar to the gap  $\Delta_{0,1}$  between the lowest Bloch band and the higher excited bands, then Floquet replicas from adjacent photon sectors can couple to this lowest band, inducing transitions which can result in particles being lost completely [166, 173].

Despite all of these expected heating contributions, there have by now been several experimental implementations of driven Fermionic systems with optical lattices. These variously demonstrate Floquet engineering of topological order [153, 154], and modification of single particle hopping and superexchange in a driven Hubbard model [111, 112, 113], which we will discuss in Chapter 6. The heating effects discussed in this section therefore do not appear to prohibit the observation of interesting Floquet-engineered Hamiltonians. Moreover, the heating effects due to coupling to higher Bloch bands can be reduced by increasing the lattice depth and thus the gap to the higher bands [157], or by modifying the lattice geometry such that the resulting band structure has fewer crossings with low-photon number Floquet replicas [113].

## 5.4 Conclusions

In this chapter we have introduced the basics of Floquet theory and how it is used to treat periodically driven many-body quantum systems. We have seen that a periodically-driven system is governed by an effective Hamiltonian  $\hat{H}_F$ , that these Hamiltonians may have very different properties to undriven Hamiltonians, and that they can be controlled by modifying the driving strength.

The dynamics of the driven system are governed by the quasienergy operator, which has a clear physical interpretation. Diagonal blocks are replicas of the undriven system with differing “photon” numbers  $m\Omega$ . The off-diagonal blocks then couple these blocks via processes induced by the drive. If we rotate to a basis where the off-diagonal terms are small compared to the energy gap  $\Omega$ , the effective static Hamiltonian  $\hat{H}_F$  can then be obtained by performing perturbation theory within one of the diagonal blocks.

Unfortunately, the utility of Floquet engineering is time-limited by heating processes which occur on a timescale  $\tau^*$ , which is exponentially long in the driving

frequency  $\Omega$ . Furthermore, since  $\Omega$  cannot be arbitrarily increased without inducing further heating processes from coupling to neglected higher Bloch bands, this places a fundamental limit on the lifetime of Floquet-engineered states. In optical lattice systems, this can be controlled somewhat by increasing the lattice depth and thus increasing the gap to higher Bloch bands, and in judicious choice of the lattice geometry, such that crossings with higher bands are avoided [113].

In the next chapter we will analyse, in detail, the Hubbard model with a driving term whose frequency is *in-gap*. As we will have  $\Omega < U$ , the high frequency expansion discussed in Sec. 5.2 is not applicable. However a slightly modified version will yield the  $t$ - $J$ - $\alpha$  model from Chapter 4 where pairing is enhanced by virtual photon processes. We shall see that this will allow control over  $t/J$  and  $\alpha$  in the  $t$ - $J$ - $\alpha$  model, allowing us in-turn to switch between metallic and superconducting phases.

## Chapter 6

# Enhanced superexchange pairing in the periodically driven Hubbard model

The results presented in this chapter were published as J.R. Coulthard, S.R. Clark, S. Al-Assam, A. Cavalleri and D. Jaksch. Enhancement of superexchange pairing in the periodically driven Hubbard model. *Phys. Rev. B* **96**, 085104 (2017). J.R.C. performed most of the calculations and made substantial contributions to the manuscript.

In Chapter 5, we discussed periodic driving as a means of controlling many-body quantum systems through Floquet engineering. The examples we gave were primarily focused on optical lattice systems, where Floquet engineering has been demonstrated most cleanly. There, Hamiltonians with periodic driving terms are implemented by oscillating the equilibrium position of the lattice [109, 157] (see also Appendix E), by modulating the depth of the lattice [174], or by modulating the magnetic field controlling the s-wave scattering length (and hence the Hubbard  $U$ ) [110].

In parallel with this, in the context of solid-state systems, advances in THz laser technology now allow for the strong and coherent driving of a single low-energy degree of freedom [175]. This kind of driving can substantially modify the microscopic parameters of the Hamiltonian governing the system, leading to drastic changes in the macroscopic phase of the material. For example, THz driving has been demonstrated to melt long-ranged order, such as charge-density waves [176, 177, 178, 179, 180], magnetic order [181, 182, 5], and orbital order [5, 183]. Even more dramatically, resonantly driving these degrees of freedom opens up the possibility of *inducing* order, such as superconductivity, in the nonequilibrium state [9, 184].

Light-induced states with superconducting-like properties have so far been observed in several cuprates [6, 7, 8] and an alkali-doped fullerene [9]. These systems are all governed by quite different physics, which naturally raises questions as to what the underlying mechanism might be, and how universal the effects are. Thus far, theoretical approaches have focused on, e.g. a minimal Frölich-type model of phonon-mediated superconductivity. In such a model, nonlinear phonon couplings lead to substantially modified electronic structures under driving, which can in turn lead to suppression of the electronic hopping. Self-consistent mean-field calculations have shown that this can lead to fast enhancement of the superconducting order parameter [185].

In this work, we consider a qualitatively different mechanism for light-induced superconductivity in strongly-correlated lattice systems. We show that modulating the on-site energies of a bipartite lattice at a frequency  $\Omega$  inside the Mott gap  $U$  slows down fermionic hopping  $t$  without suppressing the superexchange  $J$  or the pair-hopping  $\alpha J$ . This is because the absorption and re-emission of quanta from the driving field creates virtual charge-density excitations, leading to additional exchange interactions. The additional driving-induced contributions to the superexchange compensate for the suppressed contribution from the hopping. Therefore, while ordinarily  $J \ll t$ , in a driven system  $J$  can become dominant and induce a strong nearest-neighbour singlet pairing effect, and moreover enhance long-range pairing correlations, even in one dimension. We find that on moderate timescales, the resulting non-equilibrium states are not significantly heated by the driving field. In fact, we find that the modulation can *substantially reduce* the temperature of an initial thermal state on experimentally relevant timescales. Moreover, we demonstrate that the nonequilibrium enhancement of pairing is robust to changes in several experimentally relevant parameters, such as the driving strength, driving frequency, ramp time, and lattice fillings.

Specifically, we investigate the Hubbard model with a bare hopping rate  $t$  and a large on-site interaction  $U \gg t$ . We then apply a periodic driving term with frequency  $\Omega$  which modulates the on-site energy in time  $\tau$  with a spatially alternating pattern. We first demonstrate numerically that this leads to an enhancement of singlet pairing for a one-dimensional system with realistic driving parameters,  $t < \Omega < U$ , even when the driving is ramped up on nonadiabatic timescales. We then go on to study the system in Floquet theory [150, 151, 156, 162, 186, 187, 188], as we discussed in Chapter 5. We will derive an effective  $t$ - $J$ - $\alpha$  Hamiltonian which is valid in arbitrary spatial dimensions, and which provides qualitative insights into the non-equilibrium

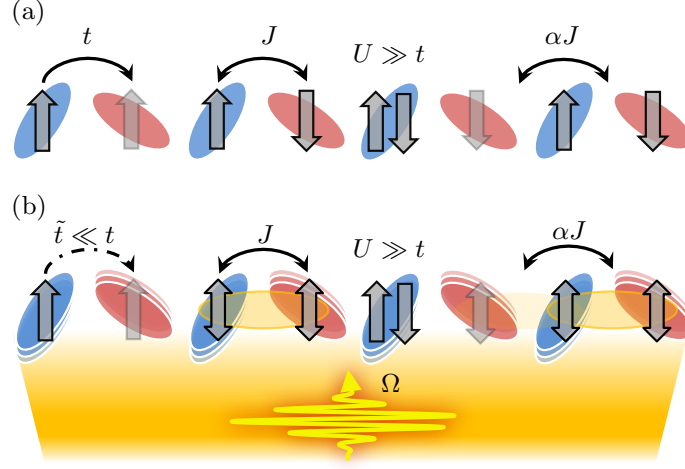


Figure 6.1: (a) A bipartite chain with electron hopping  $t$ , exchange interaction  $J$  and onsite correlation  $U \gg t$ . Singlet pairs move through the lattice with effective hopping rate  $\alpha J$ . (b) Exciting on-site vibrational modes with  $t < \Omega < U$  greatly suppresses hopping  $\tilde{t} \ll t$ , but leaves super-exchange interaction  $J$  and pair hopping  $\alpha J$  approximately unchanged, resulting in an enhancement of nearest-neighbour singlet pairing.

dynamics of the driven system. We note again that  $\Omega$  is not the dominant energy scale in our system, and so the standard high-frequency approximation is not valid.

While motivated by experiments, our primary goal is to explore the fundamental principle of the interplay between strong correlations and strong periodic driving in a simplified setting. This is in contrast to ab-initio calculations, which seek to accurately model the physics of a specific material. Nevertheless, organic superconductors (such as charge transfer salts) are often well-described by Hubbard models and are thus likely candidate materials where the effects we describe are likely to be observed. In these materials, each lattice site of the Hubbard model is a molecule with an IR-active vibrational mode, which we assume has a frequency  $\Omega < U$  [40, 189]. We further assume that these modes are sufficiently massive and excited with a sufficiently large amplitude that the leading order effect is a time-periodic modulation of the on-site electronic energy, neglecting the back-action of the electrons on the oscillators. Note that while the incident laser pulse will excite the molecules coherently and uniformly, we assume that the system has a two-molecule unit cell, as in Fig. 6.1, so that the induced driving terms have a different amplitude and/or phase on each sublattice  $a$  and  $b$ . These unit cells might consist of two different molecules, or two molecules in differing orientations [190].

While the Hamiltonian we study in this chapter is motivated in part by organic salts, it should be noted that the physics we observe is not specific to this sublattice driving. We demonstrate in Appendix E that a different driving term, which is frequently implemented in ultracold atomic setups leads to the same qualitative physics, and can be used to implement the  $t$ - $J$ - $\alpha$  model described in Chapter 4, with control over both  $t/J$  and  $\alpha$ , with very recent experimental work already ongoing in this direction [111, 112, 113].

In this chapter, we combine the methods of the previous three chapters. In Sec. 6.1, we introduce the driven Hubbard model, before obtaining its quasienergy spectrum for a small system via exact diagonalisation. We then use the tensor network methods discussed in Chapter 3 to study the real-time dynamics of the model in one dimension in Sec. 6.2. In Sec. 6.3, we perturbatively derive the Floquet Hamiltonian for the system, whose ground states and thermal states are used to approximate the non-equilibrium states of the driven Hubbard model. Finally, we conclude in Sec. 6.4.

## 6.1 The driven Hubbard model

In this chapter we study the driven Hubbard model, whose Hamiltonian is

$$\hat{H}(\tau) = \hat{H}_{\text{hub}} + \hat{H}_{\text{drive}}(\tau), \quad (6.1)$$

where  $\hat{H}_{\text{hub}} = \hat{H}_{\text{hop}} + \hat{H}_{\text{int}} - \mu \sum_j \hat{n}_j$  and contributions given by

$$\hat{H}_{\text{hop}} = -t \sum_{\langle ij \rangle \sigma} (\hat{c}_{i,\sigma}^\dagger \hat{c}_{j,\sigma} + \text{H.c.}), \quad (6.2)$$

$$\hat{H}_{\text{int}} = U \sum_j \hat{n}_{j,\uparrow} \hat{n}_{j,\downarrow}, \quad (6.3)$$

$$\begin{aligned} \hat{H}_{\text{drive}}(\tau) = & \frac{V_a}{2} \sin(\Omega\tau - \Delta\phi) \sum_{j \in a} \hat{n}_j \\ & + \frac{V_b}{2} \sin(\Omega\tau + \Delta\phi) \sum_{j \in b} \hat{n}_j. \end{aligned} \quad (6.4)$$

Here  $\hat{c}_{i,\sigma}$  with  $\sigma = \uparrow, \downarrow$  is the fermionic annihilation operator for a spin- $\sigma$  electron on site  $j$ ,  $\hat{n}_{j,\sigma} = \hat{c}_{j,\sigma}^\dagger \hat{c}_{j,\sigma}$ ,  $\hat{n}_j = \hat{n}_{j,\uparrow} + \hat{n}_{j,\downarrow}$ , and  $\langle ij \rangle$  denotes nearest-neighbour sites on a bipartite lattice composed of  $a$  and  $b$  sub-lattices. That is, all single particle hopping processes from  $a$  sites go to  $b$  sites and vice-versa. We denote the lattice filling by  $\bar{n} = \sum_j \langle \hat{n}_j \rangle / L$  where  $L$  is the number of lattice sites. The hopping amplitude is  $t$ ,  $U$  the on-site Coulomb repulsion, and  $\mu$  the chemical potential. The driving  $\hat{H}_{\text{drive}}(\tau)$

describes a time  $\tau$  periodic single particle Hamiltonian with driving frequency  $\Omega$ , corresponding sub-lattice driving amplitudes  $V_{a(b)}$ , and a phase difference of  $2\Delta\phi$ . For simplicity we assume  $V_a = V_b = V$  for the driving amplitude, which may be a function of time  $V(\tau)$ , and constant phase  $\Delta\phi = \pi/2$  throughout this chapter. However, the qualitative features of our results are expected more generally (see Appendix D.1). We next begin investigating the properties of  $\hat{H}(\tau)$  by examining its quasienergy spectrum for a small system.

### 6.1.1 Quasienergy spectrum

As we summarised in Chapter 5, one can compute the quasienergy spectrum of a time-periodic Hamiltonian by choosing an appropriate basis in which to expand the quasienergy operator

$$\hat{H}_Q = [\hat{H}(\tau) - i\partial_\tau]. \quad (6.5)$$

Here we again choose the basis

$$|\alpha, m\rangle\rangle = |\alpha\rangle e^{im\Omega\tau}, \quad (6.6)$$

where  $\{|\alpha\rangle\}$  are an arbitrary set of orthonormal basis states for the many-body Hilbert space  $\mathcal{H}$ , and  $m$  is the photon number. Using this basis, the blocks of the quasienergy operator are

$$\hat{H}_{m,m'} = -t \sum_{[j,k],\sigma} \zeta_{j,m-m'} \hat{c}_{j,\sigma}^\dagger \hat{c}_{k,\sigma} + (\hat{H}_{\text{int}} + \mathbb{1}m\Omega) \delta_{m,m'}. \quad (6.7)$$

Note that we have changed the sum over  $\langle i, j \rangle$  to  $[i, j]$  which double-counts the pairs, and dropped the Hermitian conjugate. Here,

$$\zeta_{j,m-m'} = (s_j)^{m'-m} \mathcal{J}_{m'-m}(\nu), \quad (6.8)$$

where  $\nu = V/\Omega$ , and  $s_j = +1$  if the site  $j$  belongs to the  $a$  sublattice, and  $s_j = -1$  if it belongs to the  $b$  sublattice. In Appendix D.1 we compute the elements of the quasienergy operator for the case of general driving  $V_a \neq V_b$  and  $\Delta\phi \neq \pi/2$  and show that it reduces to Eq. (6.7).

As we saw with the examples in Chapter 5, the quasienergy operator expressed in this Fourier basis acquires a clear block structure. The diagonal blocks are replicas of the Hubbard model with the energy shifted by the photon number  $m\Omega$ , and the hopping renormalised by  $\mathcal{J}_0(\nu)$ . Correspondingly, the off-diagonal blocks represent processes whereby a fermion hops to a neighbouring lattice site and absorbs or emits a number of driving quanta  $m' - m$ .

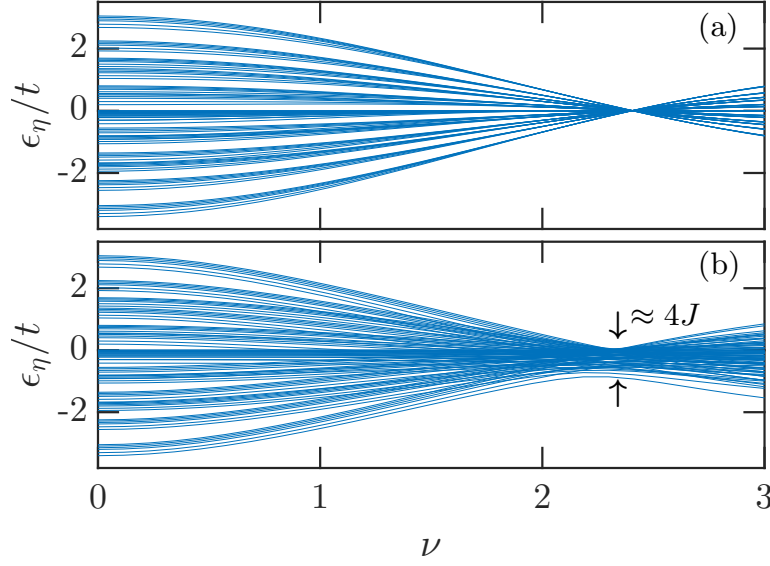


Figure 6.2: The singly-occupied subspace of the Floquet quasi-energy spectrum  $\epsilon_\eta$ , computed exactly for  $L = 6$  sites, with 2 “up” fermions and 2 “down” fermions. In (a), where  $\Omega = 100t$ ,  $U = 20t$ , the quasi-energy spectrum collapses to a single point at  $\nu_0 \approx 2.4$ , signalling complete suppression of  $\tilde{t}$  relative to  $U$ . In (b), where  $\Omega = 6t$ , and  $U = 20t$ , the spectrum does not collapse to a point, but instead strongly resembles the spectrum of a  $t$ - $J$  Hamiltonian with  $J > \tilde{t}$ .

To compute the quasienergy spectrum, we construct its explicit matrix form, introducing a cutoff  $-M \leq m, m' \leq +M$ , and numerically diagonalise it to obtain the quasienergies  $\epsilon_\eta$ . We then increase  $M$  until the quasienergies around the central block converge. We focus on the low-energy part of the  $m = 0$  sector which is adiabatically connected to the singly-occupied sector of the undriven Hubbard model. In Fig. 6.2(a), we show the quasienergy spectrum for extremely high frequency driving  $\Omega \gg U, t$ . In this regime, the diagonal blocks of  $\hat{H}_Q$  are very well separated in energy and therefore decouple. The spectrum is therefore approximately given by a Hubbard model with  $t \rightarrow \tilde{t} = t\mathcal{J}_0(\nu)$ . The width of the spectrum in Fig. 6.2(a) shrinks with increasing  $\nu$  in a manner consistent with this. When the driving strength reaches  $\nu = \nu_0$ , where  $\nu_0$  is the zero of the Bessel function, the spectrum collapses completely to a single degenerate point. This indicates that all of the dynamics of the system, including those induced by the single particle hopping, the superexchange and the pair-hopping are *all* frozen. By increasing  $\nu$  even further, the renormalised hopping amplitude  $\tilde{t}$  becomes negative, and the spectrum broadens again.

For a more realistic in-gap driving  $t < \Omega < U$ , which we show in Fig. 6.2(b),

a qualitatively different result is obtained. The quasienergy spectrum is again suppressed, indicative of a Bessel function renormalisation of  $t$ . However, in contrast to the high-frequency limit, the spectrum does not collapse to a single point, but retains a finite width proportional to  $J = \frac{4t^2}{U}$ , and is shifted down by approximately  $J$ , even when  $\nu = \nu_0$ . This suggests that, rather than being frozen out, the superexchange processes and pair hopping become the dominant factor governing the dynamics at strong driving. In the next section, we present a series of MPS calculations which corroborate this picture for a large one-dimensional system, showing a large, robust increase in the number of nearest-neighbour singlet pairs, and the formation of long-range off-diagonal pair order for  $\nu \lesssim \nu_0$ . We will then use perturbation theory to derive an effective  $t$ - $J$ - $\alpha$  model that accurately describes the properties of the driven state.

## 6.2 Driving enhanced fermion pairing

In this section we consider a one-dimensional Hubbard model, and study its dynamics when the driving amplitude is increased from zero. We first do this for zero-temperature systems of both finite and infinite size, before performing finite temperature calculations for finite-size systems. The numerical methods we employ are DMRG and TEBD introduced in Chapter 3. We provide further technical details of these calculations in Appendix D.2.

### 6.2.1 Zero temperature

We calculate the real-time dynamics for the translationally-invariant infinite system starting from the ground state, using a chemical potential  $\mu = -0.2t$ , resulting in an approximately quarter-filled system. The driving amplitude is ramped up with in-gap driving frequency  $t < \Omega < U$ . We characterise the driving induced non-equilibrium state  $|\psi(\tau)\rangle$  by studying its density-density correlations

$$N_{ij}(\tau) = \langle \hat{n}_i \hat{n}_j \rangle - \langle \hat{n}_i \rangle \langle \hat{n}_j \rangle,$$

the spin-spin correlations

$$S_{ij}(\tau) = \langle \hat{S}_i^z \hat{S}_j^z \rangle,$$

with  $\hat{S}_i^z = (\hat{n}_{i,\uparrow} - \hat{n}_{i,\downarrow})/2$ , and the nearest-neighbour singlet-pairing correlations

$$P_{ij}(\tau) = \langle \hat{b}_{i,i+1}^\dagger \hat{b}_{j,j+1} \rangle.$$

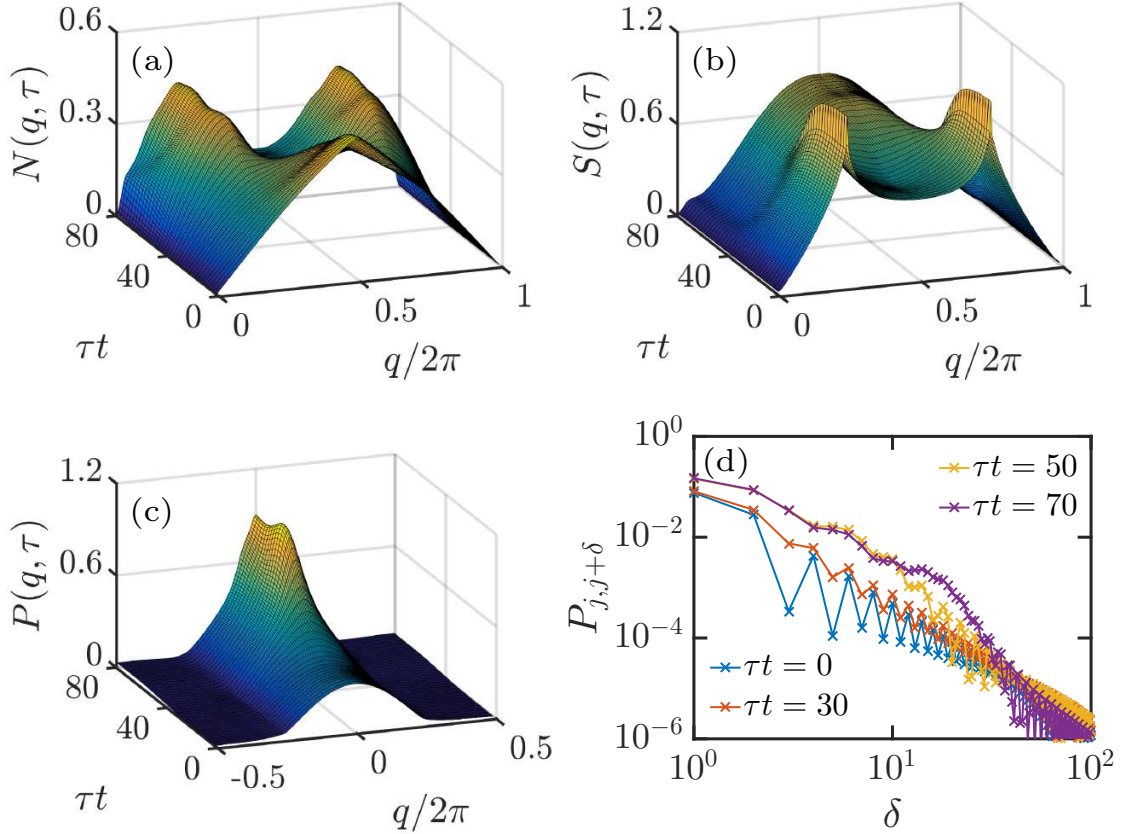


Figure 6.3: An infinite Hubbard chain with  $U = 20t$ ,  $\mu = -0.2t$ , resulting in  $\langle \hat{n} \rangle \approx 1/2$ , and driving frequency  $\Omega = 6t$ . The driving amplitude is ramped according to  $\nu(\tau) = (\nu(\infty)/2) [\tanh((\tau - \tau_0)/\tau_r) + 1]$  with final driving strength  $\nu(\infty) = 2.2$ , ramp time  $\tau_r = 15/t$ , and  $\tau_0 = 25/t$ . The plots show (a) the density-density structure factor  $N(q, \tau)$ , (b) the spin structure factor  $S(q, \tau)$  and (c) the singlet pairing structure factor  $P(q, \tau)$  as a function of quasi-momentum  $q$  and time  $\tau$ . In (a)–(c) we have averaged over the frequency  $\Omega$  oscillations, e.g. that are visible in the line-outs shown in Fig. 6.4(a). Residual low frequency oscillations in these quantities are due to the finite ramping time  $\tau_r$ . In (d) the real-space pairing correlation function  $P_{j,j+\delta}$  at various time slices is shown.

Here the operators  $\hat{b}_{ij}^\dagger$  ( $\hat{b}_{ij}$ ), given by

$$\hat{b}_{ij}^\dagger = \frac{1}{\sqrt{2}}(\hat{c}_{i,\uparrow}^\dagger \hat{c}_{j,\downarrow}^\dagger - \hat{c}_{i,\downarrow}^\dagger \hat{c}_{j,\uparrow}^\dagger), \quad (6.9)$$

create (annihilate) a singlet electron pair at sites  $i$  and  $j$ , and  $\langle \cdot \rangle = \langle \psi(\tau) | \cdot | \psi(\tau) \rangle$ . We mostly concern ourselves with the corresponding structure factors,

$$X(q) = \sum_k X_{j,j+k} e^{iqk}, \quad (6.10)$$

for the translationally-invariant infinite system, where  $X$  is any of the quantities  $N$ ,  $S$  or  $P$ , and  $q$  is the dimensionless quasi-momentum.

The density structure factor  $N(q, \tau)$  is plotted in Fig. 6.3(a). The initial kink at  $q = 4k_F$ , where  $k_F = \bar{n}\pi/2$  is the non-interacting Fermi wave-vector, is suppressed in favour of peaks at  $q = \pm 2k_F$  as the driving increases. This indicates a doubling of the wavelength of Friedel oscillations in the system's density-density correlations. This in turn suggests that the effective number of particles has halved, i.e. the fermions have formed composite bound pairs. We examine the gradient of  $N(q, \tau)$  as  $q \rightarrow 0$ , and interpret this as a time-dependent Luttinger parameter  $K_\rho(\tau)$  [126]. Recall that in equilibrium [127, 76]

$$N(q) \approx \frac{K_\rho q}{\pi}. \quad (6.11)$$

In Fig. 6.3(a), it is clear that the gradient about  $q = 0$  increases as the driving is ramped corresponding to an increase in  $K_\rho(\tau)$ . At large enough driving strengths,  $K_\rho(\tau) > 1$ , indicating the formation of an attractive Luttinger liquid.

Further information about the nature of pairs in the system is obtained via the spin structure factor, which we show in Fig. 6.3(b). Just as we saw in the  $t$ - $J$ - $\alpha$  model studied in Chapter 4, the undriven model has sharp peaks at  $2k_F$ , indicating an incommensurate antiferromagnetic order. When the drive is switched on, these peaks are suppressed and are replaced by a broad peak at  $q = \pi$ . This broad peak indicates short-ranged *commensurate* antiferromagnetic order, with a form similar to  $\bar{n}(1 - \cos q)$  expected for a gas of free nearest-neighbour singlet pairs [191].

The most direct signature of pairing is seen in the singlet structure factor, which we plot in Fig. 6.3(c). As we discussed in Chapter 4, this corresponds to the momentum distribution of the singlet pairs in the system. In the undriven system there is a broad peak about  $q = 0$ , which becomes sharpened by the driving ramp, and its height is increased approximately threefold. This suggests the formation of a quasi-condensate of singlet pairs, consistent with  $K_\rho > 1$ . The  $q = 0$  component of the

singlet structure factor incorporates contributions from both long-range and short-range correlations. To separate these contributions, we plot the real-space singlet correlations in Fig. 6.3(d). The undriven system consists of oscillatory, algebraically decaying correlations. Initially, these oscillations are suppressed by the drive, and are followed by an enhancement of the correlations, which spread through the system at a rate of approximately  $t/4 \sim J$ , which is consistent with an unsuppressed pair-hopping  $\alpha J$  [192]. We find that the pairing enhancement reaches a range of  $20 - 30$  sites on the timescales considered. It is therefore expected that a finite system of a few tens of sites will adequately capture the physics of the driven system. We confirm this explicitly in Appendix D.2, where we compare the results of finite TEBD and iTEBD, finding a negligible difference between the two.

We now turn our attention to the important question of the robustness of the singlet pair enhancement to changes in the driving parameters. In Fig. 6.4(a) we plot the height of the singlet structure factor peak  $P(q=0, \tau)$  at various driving strengths  $\nu$ . The peak oscillates with frequency  $\Omega$  about its mean which is greatly enhanced with increasing driving strength provided  $\nu < \nu_0$ , i.e. so long as we don't drive through the zero of the Bessel function. Correspondingly, the Luttinger parameter  $K_\rho(\tau)$  is shown in Fig. 6.4(b) increases with the driving strength, and exceeds 1 for sufficiently strong driving, again indicating the transition to an attractive Luttinger liquid state.

We show the dependence of the peak height  $P(q=0, \tau)$  in Fig. 6.4(c). The slower the driving ramp, the greater the pairing enhancement. We expect that when the timescale is sufficiently slow, the ground state of the undriven system is adiabatically transferred to the ground state of an effective Floquet Hamiltonian with enhanced pairing. Specifically, the time-derivative of the driving amplitude,  $\dot{\nu} \sim \nu(\infty)/\tau_r$  should be smaller than  $\sim J$ , the size of the energy gap to pair formation. This is clearly not satisfied for the fastest ramps in Fig. 6.4(c), however we still obtain a moderate pairing enhancement at these ramp speeds which is sustained for long times. For the slowest ramps, the peak height begins to saturate, suggesting that the adiabatic limit has been reached.

Finally, in Fig. 6.4(d) we demonstrate the robustness of the pairing effect to different driving frequencies  $\Omega$ . We note that a number of resonances are seen where no singlet-pairing enhancement is observed. These resonances originate from crossings in the quasi-energy spectrum when the ramp is traversed. Since the quasienergy spectrum is periodic and  $\Omega < U$ , high energy states are folded down into the first Brillouin zone  $-\Omega/2 < U - m\Omega < \Omega/2$ , as we show in Fig. 6.5 for a small system. For

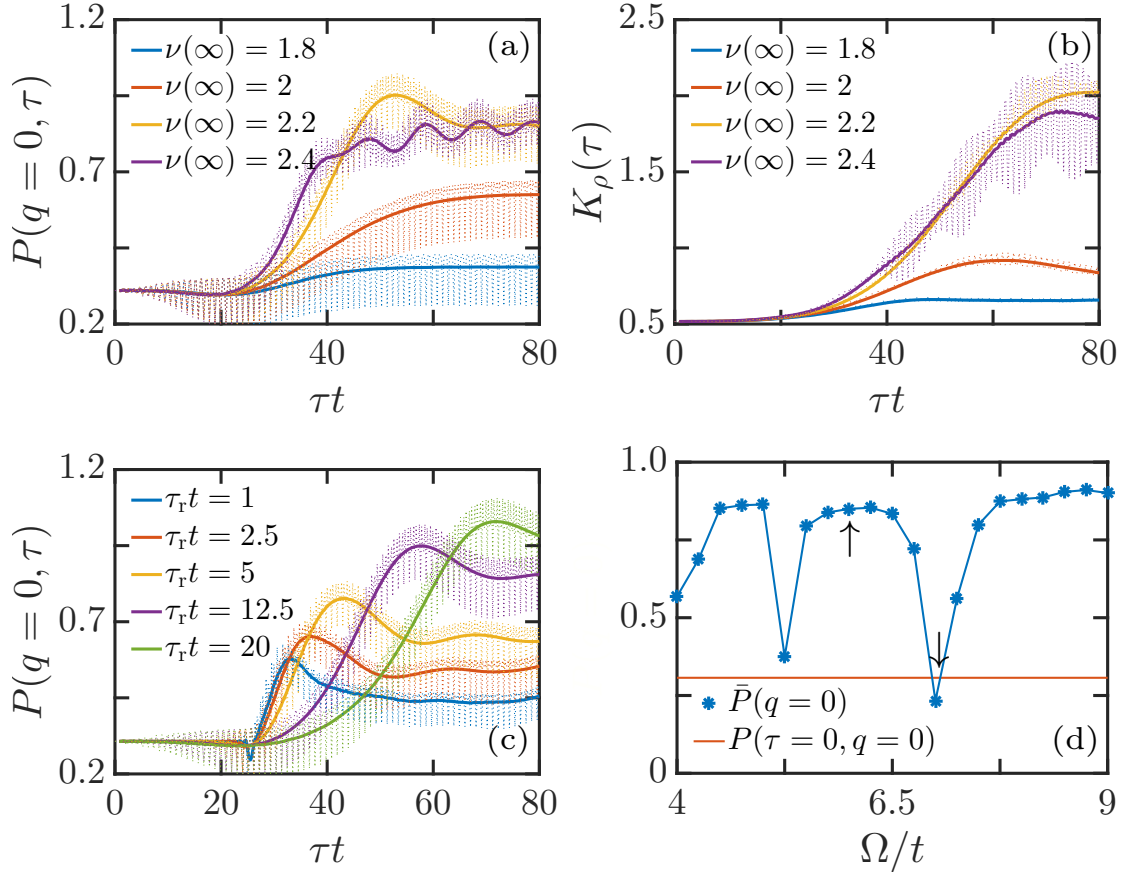


Figure 6.4: (a) The height of the singlet structure factor peak  $P(q=0, \tau)$  at various final driving strengths. The instantaneous value is indicated by a dotted line, while the moving time average is denoted by a solid line. (b) The dynamical Luttinger parameter  $K_\rho(\tau)$  extracted from the slope of  $N(q, \tau)$  at  $q \rightarrow 0$ . (c) The peak of the singlet structure factor  $P(q=0, \tau)$  for various ramp times. (d) The final height of the singlet structure factor averaged from  $\tau = 60/t$  to  $80/t$ ,  $\bar{P}(q=0)$  as a function of the driving frequency  $\Omega$ . The solid blue line is drawn to guide the eye. Arrows mark frequencies  $\Omega = 6t$  and  $\Omega = 7t$ . All parameters not explicitly given in the plots are the same as in Fig. 6.3.

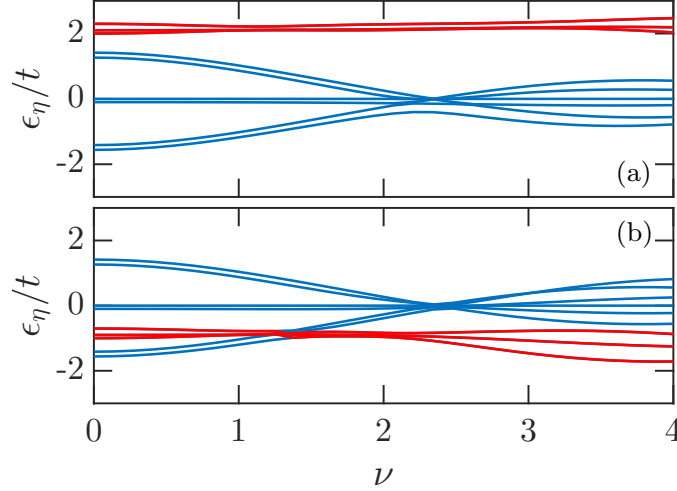


Figure 6.5: The Floquet spectrum  $\epsilon_\eta$  for an  $L = 6$  site system with  $U = 20t$ ,  $\Delta\phi = \pi$ . The doubly-occupied levels are drawn in red, the singly-occupied are drawn in blue. In (a),  $\Omega = 6t$ , and there are no crossings between singly and doubly-occupied states. In (b),  $\Omega = 7t$  and, we observe a crossing between the upper and lower Hubbard bands. The two frequencies shown here correspond to the arrows drawn in Fig. 6.4(d).

$\Omega = 6t$ , the high-energy states which have been folded down into the first Brillouin zone (marked in red) do not intersect the part of the spectrum associated with singly-occupied states (marked in blue), and therefore a sufficiently slow driving ramp will adiabatically follow the Floquet state connected to the undriven ground state. By contrast, in Fig. 6.5(b), where  $\Omega = 7$ , we do have a crossing, and so when the driving is ramped, a strong excitation of doubly-occupied states is expected. We discuss this further in Sec. 6.3.3. However, importantly, away from these resonances, a substantial enhancement of the singlet structure factor peak is observed over a wide range of frequencies  $\Omega < U$ .

### 6.2.2 Finite temperature

While ultracold atom systems can be prepared in very low-temperature states which are quite close to the ground state, it is still extremely challenging to cool Fermionic systems to temperatures  $T < t^2/U$  required to probe the superexchange physics [193, 23, 194]. Similarly, real materials are typically in (sometimes rather high temperature) thermal states. The relevance of our results in the previous section to experiments therefore hinge on whether the mechanism survives at finite temperatures. To answer this question, we use the finite temperature TEBD algorithm discussed in Sec. 3.11.

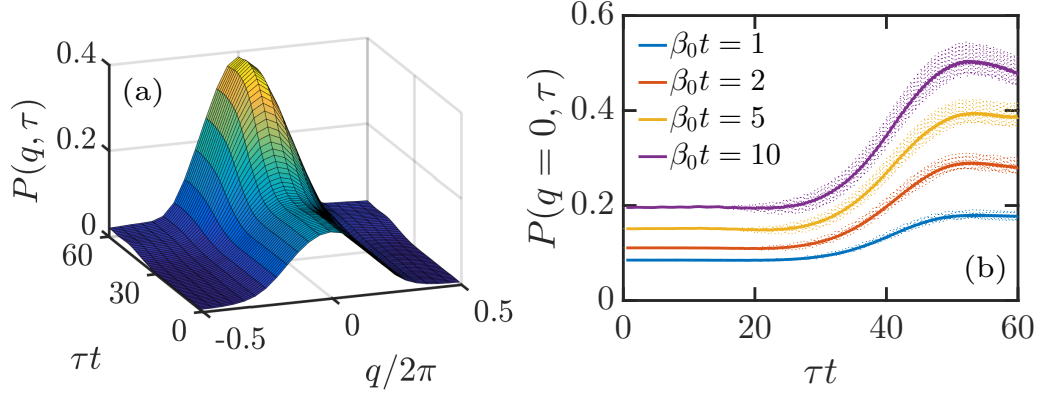


Figure 6.6: (a) The singlet structure factor  $P(q, \tau)$  with an initial temperature  $\beta_0 = 5/t$ . As in Fig. 6.3, we have averaged over the frequency  $\Omega$  oscillations. (b) The height of the peak  $P(q = 0, \tau)$ , for several initial temperatures  $\beta_0$ . The dotted line shows the instantaneous value, while the solid line shows the moving time average. These results were computed for  $L = 24$  sites. All other parameters not explicitly given in the plots are the same as in Fig. 6.3.

We first use imaginary time TEBD to compute thermal states of the Hubbard model at various initial inverse temperatures  $\beta_0$ . We then unitarily evolve this thermal state under the driven Hubbard Hamiltonian  $\hat{H}(\tau)$  as in the previous section. Here we restrict our considerations to a finite system of  $L = 24$  sites.

Figure 6.6(a) demonstrates that the singlet pairing enhancement persists even at finite temperature, although the peak is broadened and has a reduced height compared to the zero temperature cases. In 6.6(b), we again show the height of the singlet structure factor  $P(q = 0, \tau)$ , this time at various initial temperatures  $\beta_0$ . We find that the driven state consistently exhibits an increase in pairing even when the temperature is much greater the pair binding energy, i.e.  $1/\beta_0 \sim t \gg J$ . It may be surprising that driving can induce pairs to form even in such a hot system. In the next section, we will perturbatively derive the effective Floquet Hamiltonian for the system which captures the physics of the driven system. In view of this, the thermal pairing increase can be seen as many-body adiabatic cooling.

In fact, this can already be seen from the quasienergy spectrum in Fig. 6.2(b). As the driving amplitude  $\nu$  approaches  $\nu_0$ , the bandwidth of the quasi-energy spectrum in the  $m = 0$  Floquet sector is greatly reduced. In Fig. 6.4(c), we saw that sufficiently slow driving ramps lead to an approximately adiabatic modification of the spectrum. As a result, the driving reduces the gaps between the many-body

eigenstates of the model while keeping their thermal populations approximately unchanged. To concretely illustrate the effect this has, we consider a toy example of a harmonic oscillator with Hamiltonian  $\hat{H}_{\text{osc}}$ . The oscillator has frequency  $\omega$ , and eigenstates

$$\hat{H}_{\text{osc}} |n\rangle = \omega(n + 1/2) |n\rangle.$$

The thermal density matrix of the oscillator is then

$$\hat{\rho}(\beta_0) = \frac{1}{Z} \sum_n e^{-\beta_0 \omega(n+1/2)} |n\rangle \langle n|, \quad (6.12)$$

where  $Z = 1/\cosh(\beta_0 \omega/2)$ . If we adiabatically change the frequency  $\omega \rightarrow \omega' < \omega$ , then the eigenstates will be modified  $|n\rangle \rightarrow |n'\rangle$ , but the thermal populations will remain unchanged, i.e.

$$\hat{\rho}' = \frac{1}{Z} \sum_{n'} e^{-\beta_0 \omega'(n'+1/2)} |n'\rangle \langle n'|. \quad (6.13)$$

rewriting these populations in terms of the new system parameters, we find

$$\hat{\rho}' = \frac{1}{Z} \sum_{n'} e^{-(\beta_0 \omega/\omega') \omega'(n'+1/2)} |n'\rangle \langle n'| \equiv \frac{1}{Z} \sum_{n'} e^{-(\beta_{\text{eff}}) \omega'(n'+1/2)} |n'\rangle. \quad (6.14)$$

In other words, with respect to the new Hamiltonian, the density matrix looks thermal, but with a temperature which has been reduced by a factor  $\omega'/\omega$ . In the case of our driven Hubbard model, the resulting distribution will not be exactly thermal, since the spectrum is not equally spaced as the harmonic oscillator is. Nevertheless, we expect its properties to be approximately captured by a thermal state with an effective temperature substantially lower than its starting temperature, as we will show further in Sec. 6.3. A similar effect is used in cold-atom systems, where an adiabatic increase of the lattice depth results in a lowering of the temperature [195]. Indeed it has been shown that even for instantaneous quenches, one can obtain cooling in a wide variety of physical systems [196].

### 6.3 Effective $t$ - $J$ model

The numerical results we have presented in the previous section, which bear a strong resemblance to the equilibrium  $t$ - $J$ - $\alpha$  model properties we discussed in Chapter 4, indicate that superexchange and pair-hopping are central in describing the in-gap driven system. Moreover, as we will see in Fig. 6.9(b), negligible double-occupation in the undriven system remains small when the driving is ramped up, provided that

$\Omega$  does not coincide with a crossing in the quasienergy spectrum. This suggests that a  $t$ - $J$ - $\alpha$  model may provide a sufficient description of the driven states in this driving regime [197].

### 6.3.1 Floquet analysis

As we demonstrated in Sec. 2.3, the  $t$ - $J$ - $\alpha$  model emerges from  $\hat{H}_{\text{Hub}}$  by starting with the degenerate manifold of states containing zero doublons, and applying the kinetic energy as a perturbative correction [38]. Here we generalise this approach to also include different Floquet sectors labelled by the photon number  $m$  and perturbatively block-diagonalise the quasienergy matrix, as we did in Sec. 5.2. Recall that the full quasienergy operator has the block structure

$$\hat{H}_Q = -t \sum_{m,m'} \sum_{[j,k],\sigma} \zeta_{j,m-m'} \hat{c}_{j,\sigma}^\dagger \hat{c}_{k,\sigma} \otimes |m\rangle \langle m'| + \sum_m \left( \hat{H}_{\text{int}} + \mathbb{1} m \Omega \right) \otimes |m\rangle \langle m|. \quad (6.15)$$

Here we take the unperturbed Hamiltonian  $\hat{H}^{(0)}$  to be

$$\hat{H}^{(0)} = \sum_m \left( \hat{H}_{\text{int}} + \mathbb{1} m \Omega \right) \otimes |m\rangle \langle m|. \quad (6.16)$$

Which is trivially diagonalised by the Floquet-Fock states

$$\hat{H}^{(0)} |\{n_{j,\sigma}\}, m\rangle\rangle = (n_d U + m \Omega) |\{n_{j,\sigma}\}, m\rangle\rangle \equiv E_{n_d, m}, \quad (6.17)$$

where  $n_d$  is the number of doublons in the configuration  $\{n_{j,\sigma}\}$ , and  $m$  is again the photon number. These states are highly degenerate, as in the undriven Hubbard model. We define the projectors onto these degenerate manifolds in  $\mathcal{H} \otimes \mathcal{T}$  as

$$\mathbb{P}_{n_d, m} = \mathbb{P}_{n_d} \otimes |m\rangle \langle m|, \quad (6.18)$$

where  $\mathbb{P}_{n_d}$  is the projector onto the sector of  $\mathcal{H}$  with  $n_d$  doublons, and  $|m\rangle$  is the state in  $\mathcal{T}$  with photon number  $m$ . We now add the kinetic energy part

$$\hat{H}^{(1)} = -t \sum_{m,m'} \sum_{[j,k],\sigma} \zeta_{j,m-m'} \hat{c}_{j,\sigma}^\dagger \hat{c}_{k,\sigma} \otimes |m\rangle \langle m'| \equiv -t \hat{T}, \quad (6.19)$$

with  $t \ll U, \Omega$  as a perturbation to  $\hat{H}_0$ . We are interested in the part of the system which is adiabatically connected to the  $n_d = 0, m = 0$  manifold. Therefore, the effective Hamiltonian is given by

$$\hat{H}_{\text{eff}} \approx \hat{H}_{\text{eff}}^{(1)} + \hat{H}_{\text{eff}}^{(2)}, \quad (6.20)$$

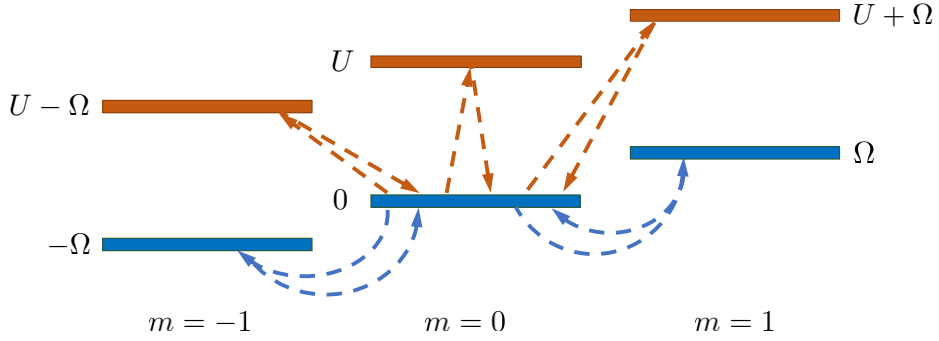


Figure 6.7: A schematic depiction of the processes in  $\hat{H}_{\text{eff}}^{(2)}$  with  $\Omega < U$ . We show the central  $m = 0$  block along with the adjacent  $m = \pm 1$  Floquet replicas. Processes which virtually create and destroy doublons are shown with dotted red arrows, and processes which do not create doublons are represented by blue dotted arrows.

where

$$\begin{aligned}\hat{H}_{\text{eff}}^{(1)} &= -t\mathbb{P}_{0,0}\hat{T}\mathbb{P}_{0,0}, \\ \hat{H}_{\text{eff}}^{(2)} &= -t^2 \sum_{n_d > 0} \sum_m \frac{\mathbb{P}_{0,0}\hat{T}\mathbb{P}_{n_d,m}\hat{T}\mathbb{P}_{0,0}}{n_d U + m\Omega} - t^2 \sum_{m \neq 0} \frac{\mathbb{P}_{0,0}\hat{T}\mathbb{P}_{0,m}\hat{T}\mathbb{P}_{0,0}}{m\Omega}.\end{aligned}\quad (6.21)$$

The projectors in  $\hat{H}_{\text{eff}}^{(1)}$  simply select the  $|0\rangle\langle 0|$  component of the perturbing hopping operator and project out any double-occupations it might create. Specifically,

$$\begin{aligned}\hat{H}_{\text{eff}}^{(1)} &= -t\mathbb{P}_{0,0} \sum_{m,m'} \sum_{[ij],\sigma} \zeta_{j,m-m'} \hat{c}_{j,\sigma}^\dagger \hat{c}_{i,\sigma} \otimes |m\rangle\langle m'| \mathbb{P}_{0,0} \\ &= \mathbb{P}_0 \left[ -t\mathcal{J}_0(\nu) \sum_{[ij],\sigma} \hat{c}_{j,\sigma}^\dagger \hat{c}_{i,\sigma} \right] \mathbb{P}_0 \otimes |0\rangle\langle 0|,\end{aligned}\quad (6.22)$$

where in the last line we have used that  $\zeta_{j,0} = (s_j)^0 \mathcal{J}_0(\nu)$ , which is independent of  $j$ . We therefore recover the single-particle hopping suppression from Sec. 5.2.1, but with the additional constraint that the hopping cannot create doublons due to the large on-site repulsion.

We now focus on the second-order correction,  $\hat{H}_{\text{eff}}^{(2)}$ . In Eq. (6.21), we have separated the sum over all of the  $(n_d, m) \neq (0, 0)$ , manifolds into two terms, depicted schematically in Fig. 6.7. The first term sums over all processes which (virtually) create a nonzero number of doublons, depicted by the red dotted arrows in Fig. 6.7. The second term sum over all processes which create no doublons, but which (virtually) emit or absorb a nonzero number of photons, depicted by the blue arrows. We

first focus on the second term in Eq. (6.21), i.e. the zero-doublon contribution.

$$\hat{H}_p = -t^2 \sum_{m \neq 0} \frac{\mathbb{P}_{0,0} \hat{T} \mathbb{P}_{0,m} \hat{T} \mathbb{P}_{00}}{m\Omega}. \quad (6.23)$$

Substituting the definition of  $\hat{T}$  from Eq. (6.19), and using the photonic part of the projectors  $\mathbb{P}_{0,m}$  and  $\mathbb{P}_{0,0}$ , we obtain

$$\hat{H}_p = -\frac{t^2}{\Omega} \mathbb{P}_0 \sum_{m \neq 0} \frac{1}{m} \left( \sum_{[k,l]b} \zeta_{l,-m} \hat{c}_{l,b}^\dagger \hat{c}_{k,b} \right) \mathbb{P}_0 \left( \sum_{[j,k]a} \zeta_{j,m} \hat{c}_{j,a}^\dagger \hat{c}_{i,a} \right) \mathbb{P}_0 \otimes |0\rangle \langle 0|. \quad (6.24)$$

This Hamiltonian describes processes whereby a fermion hops from site  $i$  to site  $j$ , absorbs/emits a quantum of energy  $\Omega$ , and then a fermion (which may be the same fermion) hops from site  $k$  to site  $l$  and emits/absorbs another photon. This therefore constitutes effectively an infinitely long-range interaction. Note that due to the projectors, none of these hopping processes can create doublons, even virtually. Some simplifications will reveal that the  $+m$  and  $-m$  contributions exactly cancel, and so the long-range interaction does not feature in the effective Hamiltonian. Let us rewrite the sum

$$\begin{aligned} \hat{H}_p = & -\frac{t^2}{\Omega} \mathbb{P}_0 \sum_{m > 0} \left[ \frac{1}{m} \left( \sum_{[k,l]b} \zeta_{l,-m} \hat{c}_{l,b}^\dagger \hat{c}_{k,b} \right) \mathbb{P}_0 \left( \sum_{[j,k]a} \zeta_{j,m} \hat{c}_{j,a}^\dagger \hat{c}_{i,a} \right) \right. \\ & \left. - \frac{1}{m} \left( \sum_{[k,l]b} \zeta_{l,m} \hat{c}_{l,b}^\dagger \hat{c}_{k,b} \right) \mathbb{P}_0 \left( \sum_{[j,k]a} \zeta_{j,-m} \hat{c}_{j,a}^\dagger \hat{c}_{i,a} \right) \right] \mathbb{P}_0 \otimes |0\rangle \langle 0|. \end{aligned} \quad (6.25)$$

We see that the two terms are identical except that the signs of the second subscript in  $\zeta_{l,m}$  have been flipped. Using the definition of  $\zeta_{l,m}$ , we see

$$\begin{aligned} \zeta_{j,-m} &= (s_j)^{-m} \mathcal{J}_{-m}(\nu) \\ &= (-1)^m (s_j)^m \mathcal{J}_m(\nu) \\ &= (-1)^m \zeta_{l,m}, \end{aligned} \quad (6.26)$$

where we have used that  $s_j = \pm 1$ , and so  $(s_j)^{-m} = (s_j)^m$ . We have also used the identity  $\mathcal{J}_m(\nu) = (-1)^m \mathcal{J}(\nu)$ . Each of the two hopping process in the second term acquires a factor  $(-1)^m$  relative to the first term. The two terms are therefore identical and so exactly cancel, i.e.

$$\hat{H}_p = 0. \quad (6.27)$$

We note that interestingly, the fact that this effective long-range interaction is 0 is due to the fact that our driving is classical. Were the driving field quantized, then the

number of photon sectors would be bounded from below, and so there would not be a contribution photon sector  $-m$  to cancel contribution from sector  $+m$ . Moreover, as we saw in Sec. 5.1.2, the matter-photon coupling matrix elements would scale with  $\sqrt{m}$  rather than being constant as in the classical case, and so there will be nonzero contributions for all but the largest photon numbers. In fact, in recent work we considered a Hubbard model coupled to an empty photonic cavity [198]. We indeed found that the quantised light field led to a nonzero long-range interaction of the form Eq. (6.24).

We simplify the second term in Eq. (6.20) by first taking into account of the projectors onto different photon number sectors, considering the product

$$\begin{aligned}
\mathbb{P}_{0,0} \hat{T} \mathbb{P}_{n_d,m} \hat{T} \mathbb{P}_{0,0} &= \mathbb{P}_{0,0} \left( \sum_{p,p'} \sum_{[k,l],\sigma} \zeta_{l,p-p'} \hat{c}_{l,\sigma}^\dagger \hat{c}_{k,\sigma} \otimes |p\rangle \langle p'| \right) \mathbb{P}_{n_d,m} \\
&\quad \times \left( \sum_{q,q'} \sum_{[i,j],\sigma} \zeta_{j,q-q'} \hat{c}_{j,\sigma}^\dagger \hat{c}_{i,\sigma} \otimes |q\rangle \langle q'| \right) \mathbb{P}_{0,0} \\
&= \mathbb{P}_0 \left( \sum_{[k,l],\sigma} \zeta_{l,-m} \hat{c}_{l,\sigma}^\dagger \hat{c}_{k,\sigma} \otimes |0\rangle \langle m| \right) \mathbb{P}_{n_d} \\
&\quad \times \left( \sum_{[i,j],\sigma} \zeta_{j,m} \hat{c}_{j,\sigma}^\dagger \hat{c}_{i,\sigma} \otimes |m\rangle \langle 0| \right) \mathbb{P}_0 \\
&= \mathbb{P}_0 \left( \sum_{[k,l],\sigma} \zeta_{l,-m} \hat{c}_{l,\sigma}^\dagger \hat{c}_{k,\sigma} \right) \mathbb{P}_{n_d} \left( \sum_{[i,j],\sigma} \zeta_{j,m} \hat{c}_{j,\sigma}^\dagger \hat{c}_{i,\sigma} \right) \mathbb{P}_0 \otimes |0\rangle \langle 0|.
\end{aligned} \tag{6.28}$$

The part of this operator which acts on  $\mathcal{H}$  is now almost identical to Eq. (2.29). We can therefore use the same arguments to simplify this expression to

$$\mathbb{P}_{0,0} \hat{T} \mathbb{P}_{n_d,m} \hat{T} \mathbb{P}_{0,0} = \mathbb{P}_0 \left( \sum_{[i,j,k],\sigma} \zeta_{k,-m} \zeta_{j,m} \hat{c}_{k,\sigma}^\dagger \hat{c}_{j,\sigma} \hat{n}_{j,\uparrow} \hat{n}_{j,\downarrow} \hat{c}_{j,\sigma}^\dagger \hat{c}_{i,\sigma} \right) \delta_{n_d,1} \mathbb{P}_0 \otimes |0\rangle \langle 0|, \tag{6.29}$$

where again  $i$  and  $k$  are both sites which are connected to  $j$  by single particle hopping processes. We must therefore have that  $k$  and  $j$  are on different sublattices, and so

$s_j = -s_k$ . Hence,

$$\begin{aligned}\zeta_{k,-m}\zeta_{j,m} &= (s_j)^{-m} \mathcal{J}_{-m}(\nu) (-s_j)^m \mathcal{J}_m(\nu) \\ &= (-1)^m \mathcal{J}_{-m}(\nu) \mathcal{J}_m(\nu) \\ &= (\mathcal{J}_m(\nu))^2,\end{aligned}\tag{6.30}$$

where in the last line we have used the identity  $(-1)^m \mathcal{J}_{-m}(\nu) = \mathcal{J}_m(\nu)$ . Substituting this, and Eq. (6.30) into  $\hat{H}_{\text{eff}}^{(2)}$ , we obtain

$$\begin{aligned}\hat{H}_{\text{eff}}^{(2)} &= \mathbb{P}_0 \left[ -t^2 \sum_{n_d > 0} \sum_m \mathcal{J}_m^2(\nu) \sum_{[i,j,k],\sigma} \frac{\left( \hat{c}_{k,\sigma}^\dagger \hat{c}_{j,\sigma} \hat{n}_{j,\uparrow} \hat{n}_{j,\downarrow} \hat{c}_{j,\sigma}^\dagger \hat{c}_{i,\sigma} \right) \delta_{n_d,1}}{n_d U + m \Omega} \right] \mathbb{P}_0 \otimes |0\rangle \langle 0| \\ &= \mathbb{P}_0 \left[ -\frac{t^2}{U} \sum_{m \neq 0} \left( \frac{\mathcal{J}_m^2(\nu)}{1 + m \Omega / U} \right) \sum_{[i,j,k],\sigma} \hat{c}_{k,\sigma}^\dagger \hat{c}_{j,\sigma} \hat{n}_{j,\uparrow} \hat{n}_{j,\downarrow} \hat{c}_{j,\sigma}^\dagger \hat{c}_{i,\sigma} \right] \mathbb{P}_0 \otimes |0\rangle \langle 0|,\end{aligned}\tag{6.31}$$

which, as we showed in Sec. 2.3, can be rewritten as

$$\hat{H}_{\text{eff}}^{(2)} = \mathbb{P}_0 \left[ -\tilde{J} \sum_{\langle ij \rangle} \hat{b}_{i,j}^\dagger \hat{b}_{i,j} - \frac{\tilde{J}}{2} \sum_{\langle i,j,k \rangle} \left( \hat{b}_{i,j}^\dagger \hat{b}_{j,k}^\dagger + \text{H.c.} \right) \right] \mathbb{P}_0,\tag{6.32}$$

where we have dropped the explicit projection onto the zero-photon subspace  $|0\rangle \langle 0|$ , and defined a renormalised superexchange interaction

$$\tilde{J} = \frac{4t^2}{U} \sum_{m \neq 0} \left( \frac{\mathcal{J}_m^2(\nu)}{1 + m \Omega / U} \right).\tag{6.33}$$

Putting this all together, we obtain the effective  $t$ - $J$ - $\alpha$  Hamiltonian,

$$\begin{aligned}\hat{H}_{\text{eff}} &= \mathbb{P}_0 \left[ -\tilde{t} \sum_{\langle ij \rangle \sigma} (\hat{c}_{i,\sigma}^\dagger \hat{c}_{j,\sigma} + \text{H.c.}) - \tilde{J} \sum_{\langle ij \rangle} \hat{b}_{ij}^\dagger \hat{b}_{ij} \right. \\ &\quad \left. - \frac{\tilde{J}}{2} \sum_{\langle ijk \rangle} \left( \hat{b}_{ij}^\dagger \hat{b}_{jk}^\dagger + \text{H.c.} \right) \right] \mathbb{P}_0.\end{aligned}\tag{6.34}$$

with the renormalised parameters

$$\tilde{t} = t \mathcal{J}_0(\nu), \quad \text{and} \quad \tilde{J} = \frac{4t^2}{U} \sum_m \left( \frac{\mathcal{J}_m^2(\nu)}{1 + m \Omega / U} \right).\tag{6.35}$$

We now inspect  $\tilde{J}$  in two limits. First,  $\Omega \gg U \gg 1$ . In this limit, only the  $m = 0$  term contributes to the renormalised superexchange, and so

$$\tilde{J} \rightarrow \frac{4(t \mathcal{J}_0(\nu))^2}{U}.\tag{6.36}$$

In other words, in the large- $\Omega$  limit, we obtain a Hubbard model with a suppressed hopping  $t\mathcal{J}(\nu)$ , and  $U$  unchanged. Then since  $U \gg t$ , in the zero-doublon manifold we obtain an effective  $t$ - $J$ - $\alpha$  model where both  $t$  and  $J$  are suppressed, consistent with the quasienergy spectrum Fig. 6.2(a). The opposite limit,  $U \gg \Omega$ , requires more careful consideration. When  $m \ll \Omega/U$ , we can neglect the second term in the denominator. When  $m \gtrsim \Omega/U$ , we can no longer do this. However,  $\mathcal{J}_m(\nu)$  decays extremely rapidly with  $m$  for  $\nu < \nu_0$ , and so these terms do not contribute to the sum anyway. We can therefore write

$$\begin{aligned}\tilde{J} &\rightarrow \frac{4t^2}{U} \sum_m \mathcal{J}_m^2(\nu) \\ &\approx \frac{4t^2}{U} = J.\end{aligned}\tag{6.37}$$

In other words, in the limit  $t \ll \Omega \ll U$ , the dynamics of the driven system are described by a  $t$ - $J$ - $\alpha$  model where  $t \rightarrow \tilde{t}$  is suppressed, but  $J$  is approximately unchanged, and  $\alpha$  remains  $\alpha = 1/2$ . Moreover, the Floquet analysis has revealed why  $J$  is unchanged. In this regime, the superexchange has two contributions,

$$\tilde{J} = \tilde{J}_{\text{kin}} + \tilde{J}_{\text{light}},\tag{6.38}$$

where

$$\tilde{J}_{\text{kin}} = \frac{4(t\mathcal{J}_0(\nu))^2}{U}.\tag{6.39}$$

That is, because the single-particle hopping is suppressed by the drive, the superexchange, induced by the single-particle hopping is also suppressed. However, this suppression is compensated for by additional photon-assisted superexchange processes

$$\tilde{J}_{\text{light}} = \frac{4t^2}{U} \sum_{m \neq 0} \frac{\mathcal{J}_m(\nu)}{1 + m\Omega/U},\tag{6.40}$$

so that the superexchange remains approximately unchanged. Therefore, by driving, we can make the superexchange and pair hopping dominant.

Before continuing, we note that our degenerate perturbation theory breaks down if the model is resonantly driven, i.e.  $m\Omega = U$ . The resonantly driven case was discussed in [197], where it was shown that resonant driving leads to a Floquet Hamiltonian where doublons are coherently created and destroyed by the absorption and emission of driving quanta.

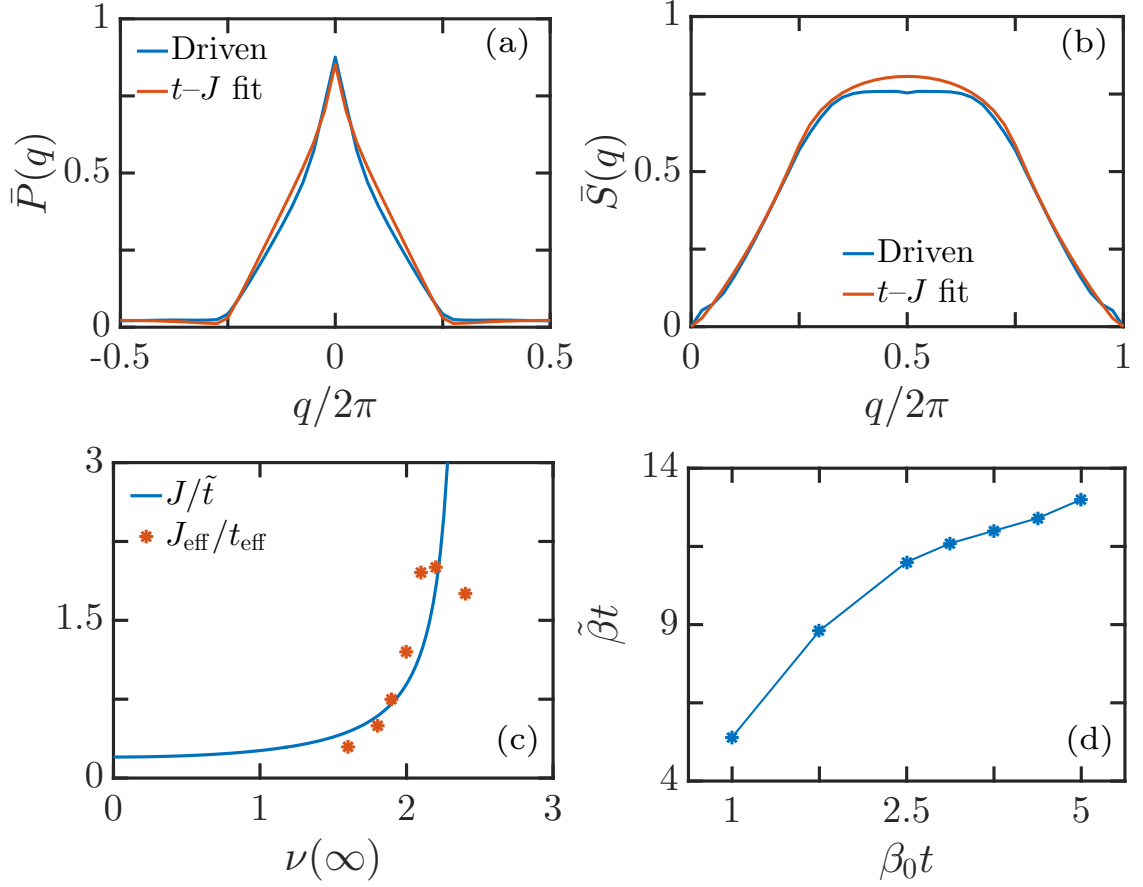


Figure 6.8: The time average between  $\tau t = 60 - 80$  of the driven state's structure factors for (a) singlet pairing  $\bar{P}(q)$  and (b) spin  $\bar{S}(q)$  from Fig. 6.3(b)–(c) are shown alongside the same quantities for a  $t$ - $J$  ground state with  $\alpha = 1/2$  and an effective  $J_{\text{eff}}/t_{\text{eff}}$  that gives the closest match to  $\bar{P}(q)$ . For  $\nu(\infty) = 2.2$ , the effective  $J_{\text{eff}}/t_{\text{eff}} = 2.0$ . Repeating this fit for the sequence of driving strengths  $\nu$  shown in Fig. 6.4(a) gives  $J_{\text{eff}}/t_{\text{eff}}$  plotted in (c), with the solid curve reporting the prediction of Eq. (6.37). In (d)  $\bar{P}(q)$  of the driven initial thermal state at inverse temperature  $\beta_0$  was compared to  $t$ - $J$  model thermal states, with  $J$  fixed to its equilibrium value and the ratio  $J/t$  fixed by the results in Fig. 6.8(c), to extract an effective inverse temperature  $\beta_{\text{eff}}$ . A solid line is drawn to guide the eye. The computations for (a)–(c) were carried for  $L = 40$  sites, and for (d) were carried out with  $L = 24$  sites.

### 6.3.2 Comparison to the $t$ - $J$ - $\alpha$ model

The numerical results we have presented already in Fig. 6.3 and Fig. 6.4 are consistent with the equilibrium properties of the  $t$ - $J$ - $\alpha$  model which we studied in Chapter 4 over a wide range of  $J/t$  values. The Floquet analysis in Sec. 6.3.1 has revealed why this is. By slowly ramping up the driving, we are effectively adiabatically modifying the Hubbard Hamiltonian to a  $t$ - $J$ - $\alpha$  Hamiltonian with  $J > t$ , and therefore traversing

the phase diagram of the model from the metallic phase to the superconducting phase.

We make this comparison more quantitatively in Fig. 6.8. In (a) and (b), we show the spin structure factors and singlet structure factors from Fig. 6.3(b) and (c) respectively. We find that the structure factors of the driven Hubbard model are closely reproduced by the ground state of the  $t$ - $J$ - $\alpha$  model with  $J/t \approx 2$ . For the purposes of this comparison, we computed the driven Hubbard states and the  $t$ - $J$ - $\alpha$  ground states with finite size TEBD and DMRG respectively, for  $L = 40$  sites. In Appendix D.2 we explicitly compare the iTEBD results to the finite TEBD results and find a negligible influence from finite-size effects.

We repeat this fitting procedure of the singlet structure factors for the zero temperature driven Hubbard states to singlet structure factors of the  $t$ - $J$ - $\alpha$  ground states to determine an effective superexchange to hopping ratio  $J_{\text{eff}}/t_{\text{eff}}$ . We plot these as the red points in Fig. 6.8(c) along with the analytic prediction  $J/(t\mathcal{J}_0(\nu))$  from Eq. (6.37). These results show decent agreement with this prediction, and indicate that the superconducting phase can be reached with a driving strength of  $\nu(\infty) \approx 2$ . In Fig. 6.8(d), we fit results obtained from driving initial thermal states of the Hubbard model at different initial inverse temperatures  $\beta_0$  to thermal states of the  $t$ - $J$ - $\alpha$  model with  $J$  fixed to its equilibrium value, and the ratio  $J/t$  determined by the zero-temperature fit in Fig. 6.8(c). In doing so, we extract an effective inverse temperature  $\beta_{\text{eff}}$  which is substantially colder than the initial temperature, supporting our interpretation of the pairing enhancement in Fig. 6.6(d) as being due to adiabatic cooling.

### 6.3.3 Floquet heating

As we discussed in Sec. 5.3, it can be expected that periodically driving a many-body system will cause Floquet heating, even far away from resonances that we see in e.g. Fig. 6.4(d). Higher-order finite-frequency corrections to  $\hat{H}_{\text{eff}}$  will in general be non-local and multi-body. At long times, this will generate entanglement between disparate parts of the system, and so the density matrix of a contiguous subset of the system will have a larger entropy. In the long-time limit, if the subsystems become maximally entangled, then all local observables will resemble those of an infinite temperature thermal state.

Despite operating in a finite-frequency regime, where these finite-frequency corrections might be expected to be quite large, our numerical results do not show significant heating effects. The long-time, time-averaged correlations emerging from the driven Hubbard model, while exhibiting a small quantitative deviation, e.g. in

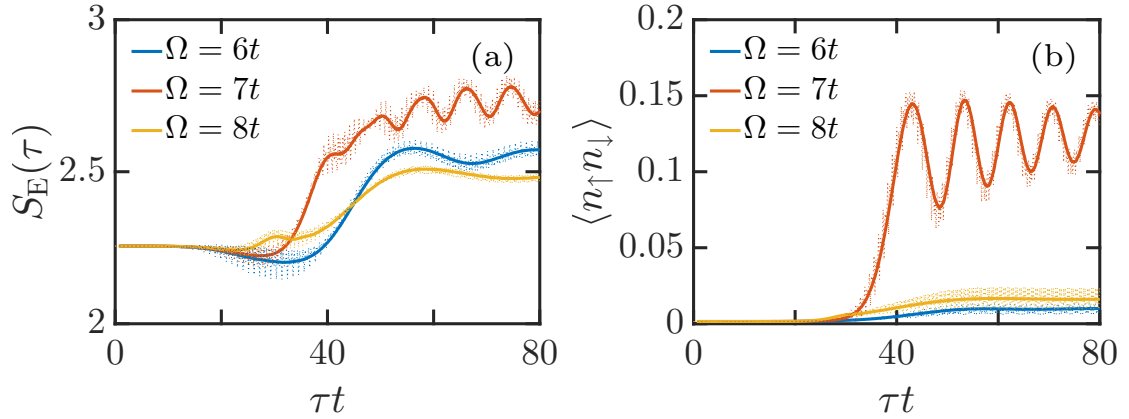


Figure 6.9: (a) The entanglement entropy  $S_E$  between a two-site block and the rest of the zero temperature, infinite system as a function of time is shown. (b) The average double-occupancy per site  $\langle n_\uparrow n_\downarrow \rangle$  is plotted. The dotted line shows the instantaneous value, while the solid line shows the moving time average. The system parameters not explicitly stated are the same as those in Fig. 6.3. Frequencies  $\Omega = 6t$  and  $\Omega = 7t$  shown here correspond to the arrows drawn in Fig. 6.4(d).

Fig. 6.8(a)–(b), nonetheless are well captured by an effective  $t$ – $J$ – $\alpha$  model. This suggests that the Floquet heating rate in our system is small, and rather, our results are more consistent with prethermalisation in driven systems [199, 200, 201, 167].

To quantify the Floquet heating rate in more detail, we return to the zero-temperature, iTEBD calculation, and compute the entanglement entropy between a two-site block and the rest of the infinite system defined as

$$S_E(\tau) = -\text{Tr} [\rho_C(\tau) \log_2(\rho_C(\tau))], \quad (6.41)$$

Note that this is different from the half-chain entanglement entropy used in Ref. [167]. When we compute the half-chain entropy we see a linear increase with time after the driving ramp. However, we can attribute this linear increase in half-chain entanglement entropy to the spread of correlations observed in Fig. 6.3(d). There we saw an increase in the long-range correlations which spread approximately linearly at a rate  $\sim J$ . This leads to an increase in the half-chain entanglement entropy that is not attributable to heating.

The entanglement entropy  $S_E$  is shown in Fig. 6.9(a) for different driving frequencies. We see that the entropy increases during the driving ramp, and so the two-site block is more entangled with its environment. This is expected for two reasons. Firstly, the after the driving ramp there is a large number of singlets. These are

entangled objects which can sit across the boundary of the two-site block, thus increasing  $S_E$ . Secondly, the development of long-range singlet correlations corresponds to further entanglement between the central two-site block and the “environment”.

How much of this entanglement growth can we attribute the heating? One would expect that if Floquet heating was significant, the the entanglement entropy would continue to grow until it saturated at the maximum possible value  $S_E = \log_2(d^2) = 4$ , which would be reached when the state of the two-site block locally resembles an infinite temperature state. In Fig. 6.9(a) we see that in all cases, the entanglement entropy saturates far below this theoretical maximum, indicating that Floquet heating does not play a significant role on the timescales we consider.

The largest growth in  $S_E(\tau)$  is seen for  $\Omega = 7t$ , which was already identified in Fig. 6.4(d) as resonance. The additional entanglement makes the resonantly driven case more difficult to capture with an MPS ansatz due to a rapid growth of truncation error after the ramp [202]. However, the entanglement still remains well below the theoretical maximum value  $S_E = 4$ . This is because the destruction of singlet correlations observed in Fig. 6.4(d) is not due to Floquet heating processes, but rather due to resonant excitation of doublons [167]. We show the average number of doublons per site as a function of time in Fig. 6.9(b). For the resonant frequency  $\Omega = 7t$ , the number of doublons greatly increases and oscillates, clearly showing that the  $t$ - $J$ - $\alpha$  model description has broken down. On the other hand, for frequencies away from the resonance, the doublon fraction rises slightly but remains small and does not increase with time, supporting our description of the driven states by  $t$ - $J$ - $\alpha$  ground states. In summary, we find no evidence of Floquet heating on the timescales we consider. In such a broad time window, it is likely that dissipation and environmental couplings, which we do not model here will, dominate and so Floquet heating is therefore unlikely to be of dominant practical importance in experiments.

It should be noted, however, that since we have worked entirely within the framework of the driven Hubbard model and neglected all higher Bloch bands, in reality there will be additional heating processes which are not contained within our model, even in comparatively “clean” optical lattice systems [166, 113]. However, as we assume that  $\Omega < U$ , we must also have that  $\Omega$  is smaller than the gap to higher Bloch bands, otherwise our initial undriven Hubbard model would not be valid. We therefore expect such heating rates to be small enough that enhanced pairing may be observed in experiments, as has been demonstrated in [111, 112, 113].

## 6.4 Conclusions

In this chapter we have investigated a driven Fermionic Hubbard model in detail. We have shown that in-gap driving can slow down the fermions while retaining the normally weak superexchange, making  $J$  the dominant energy scale. We have demonstrated numerically that in a one-dimensional setting, this effect manifests itself as a strong, controllable increase in pair correlations, similar to what would be expected from a  $t$ - $J$ - $\alpha$  model where  $J/t$  was increased to unphysical values. Moreover, this was found to be robust to changes in the driving strength, ramp time, and driving frequency, and to substantial initial temperatures.

This work naturally raises many interesting further questions. The Floquet analysis revealed additional infinite-range interactions which were nonzero in the classical limit, but would be very significant in the limit of a quantised driving field with only a few photons. We have already begun to investigate this limit in the context of a Hubbard model coupled to a photonic cavity [198]. Theoretical calculations and experimental observations of the ET organic salts showed that the vibrational modes driving the systems were excited to only a few quanta [189, 40]. This suggests that quantum corrections to the Floquet picture studied here, including the addition of the infinite-range interaction, could be important in experiments.

In thermal equilibrium, strictly one-dimensional systems with local interactions are known to lack long-range order such as superconductivity at any finite-temperature due to the Mermin-Wagner theorem [203]. Quasi-2D systems such as cuprate superconductors are not bound by such restrictions, and pairing correlations are expected to emerge at much smaller values of  $J/t$ . Moreover, experiments in THz-driven solid state systems have observed signatures of superconductivity at temperatures well above the equilibrium critical temperature of the material. Studying the effect of our driving scheme in higher dimensions, where they have a finite critical temperature, is therefore crucial to realising its full potential as a means of engineering useful superconducting states in solid-state systems.

In the context of ultracold atom systems, a series of experiments have already been performed [111, 112, 113], which have observed some of the effects we have studied in this chapter. Future work will focus on Floquet engineering the  $t$ - $J$ - $\alpha$  model in two and three dimensional lattices.

# Chapter 7

## Conclusions and outlook

In this thesis we have explored periodic driving as a means to engineer useful states of strongly correlated Fermion systems. Specifically, in Chapter 6, we have studied the doped Fermi-Hubbard model under periodic driving, finding that the driving results in a strong and robust increase in singlet-pair correlations indicative of superconductivity. This could provide a new mechanism by which superconducting states can be engineered with THz driving of certain classes of quantum materials, specifically those which are accurately described by Hubbard models with local vibrational modes.

The increase in pair correlations results from the driving modifying the Hamiltonian describing the system from that of a purely repulsive Hubbard model to a  $t$ - $J$ - $\alpha$  model with  $J/t > 1$ . We showed further in Appendix E that in an optical lattice setup where the lattice is shaken, the  $t$ - $J$ - $\alpha$  model can be implemented with  $J/t \gtrsim 1$ . Moreover, unlike the sublattice driving considered in Chapter 6, the pair-hopping can also be modified by shaking the optical lattice. This allows the  $t$ - $J$ - $\alpha$  model to be engineered in optical lattices over a wider range of parameters than was previously possible, e.g. by simply adjusting parameters of the Hubbard model. Our results therefore increase the range of candidate Hamiltonians for high- $T_c$  superconductors which may be simulated using optical lattices, in the manner discussed in Chapter 1. This would be particularly useful in two dimensions, where current theoretical approaches are limited.

Our results naturally raises many interesting questions to be answered in future research. Firstly, while in Chapter 6, we found no evidence of Floquet heating on the timescales we considered, the model we considered was limited by not taking into account higher Bloch bands. Experimental studies on Floquet system have found these bands to be play an important role in experimental heating rates [166, 113]. Future theoretical work which addresses these additional heating contributions would be very useful in identifying the lattice geometries and driving regimes where heating

can be minimised, and provide means of extending the lifetimes of Floquet engineered states.

In Chapter 5, we discussed the connection between Floquet driving and fully quantum mechanical coupling to a bosonic driving field, using the example of a two-level system. Later, in Chapter 6 when we studied the driven Hubbard model, we noted that long-range interacting terms which drop out of the Floquet Hamiltonian do so because the driving is classical. We have already begun to explore this in [198], where we study a Hubbard model coupled to an empty photonic cavity. There we showed that virtual transitions to and from higher photon sectors can enhance  $J/t$  in a manner similar to the Floquet driving we studied in this thesis. Further exploring driven systems in the quantum limit of the driving field is a promising avenue for future research as it may 1) allow us to avoid Floquet heating processes which are inevitable with classical driving, and 2) allow us to engineer a wider array of Hamiltonians involving, for example, the infinite-range interactions which were found to vanish in the case of the classically driven model in Sec. 6.3.1.

In Chapter 4, we explored the phase diagram of the one-dimensional  $t$ - $J$ - $\alpha$  model, with particular focus on the effect of the pair-hopping  $\alpha$ . We found that the addition of pair-hopping pushes the superconducting phase to lower values of  $J/t$  at dilute fillings. This, in-turn, allows the superconducting phase to be realised at lower values of  $J/t$ . At larger fillings we showed that this led to dynamical constraints being imposed on the model due to the non-overlap of pairs, which inhibits superconductivity. We speculated that these constraints may also be important in higher dimensions. We began to investigate this in the latter part of Chapter 4 by considering a ladder system comprised of two one-dimensional chains coupled in different geometries. We showed that, counterintuitively, this coupling can suppress long-range pair correlations, in line with our conjecture.

As we discussed in the conclusion of Chapter 4, work must be done to better understand the role of these constraints in ladder systems. In addition to the immediate future work laid out in Chapter 4 regarding more carefully understanding the sharp suppression of pair correlations in the triangular ladder, the additional dimension afforded to us in a ladder geometry affords us further tools for studying superconductivity in the  $t$ - $J$ - $\alpha$  model. For example, a second dimension allows us to study a magnetic flux threaded through the plaquettes, and thus directly diagnose superconductivity through the Meissner effect [204, 205].

By driving inter-chain vibrations in a ladder system, it should be possible using the mechanism discussed in Chapters 5 and 6 to engineer a Floquet Hamiltonian

where the inter-chain coupling is suppressed. This, in-turn, could relax the kinetic constraints on the singlets and re-enable the superconducting phase. This could further broaden the class of systems in which light-induced superconductivity may be realised.

# Appendix A

## Jordan–Wigner transformation

As we outlined in Chapter 3, our tensor network numerics relies on the fact that we can express the full many-body Hilbert space  $\mathcal{H}$  as the tensor product of smaller Hilbert spaces which reflect local degrees of freedom (for instance, lattice sites), i.e.

$$\mathcal{H} = \mathcal{H}_1 \otimes \mathcal{H}_2 \otimes \cdots \otimes \mathcal{H}_L \quad (\text{A.1})$$

where  $L$  is the number of lattice sites in the system. However, fermionic operators are manifestly nonlocal due to their anticommutation relations. For simplicity, we consider spinless fermions, though this is easily generalised to fermions with spin. To be concrete, if  $\{\hat{c}_j\}$  and  $\{\hat{c}_j^\dagger\}$  were purely local operators acting only on the Hilbert space  $\mathcal{H}_j$ , then for  $j \neq k$  we would trivially have

$$\hat{c}_j^\dagger \hat{c}_k = \hat{c}_k \hat{c}_j^\dagger \neq -\hat{c}_k \hat{c}_j^\dagger \quad (\text{A.2})$$

since  $\hat{c}_j^\dagger$  and  $\hat{c}_k$  act on different parts of the Hilbert space. Therefore, purely local operators cannot obey the required canonical anticommutation relations. Instead, we make the transformation [3]

$$\begin{aligned} \hat{c}_i &= \left( \prod_{j < i} \hat{s}_j^z \right) \hat{s}_i^- \\ \hat{c}_i^\dagger &= \left( \prod_{j < i} \hat{s}_j^z \right) \hat{s}_i^+, \end{aligned} \quad (\text{A.3})$$

where  $\hat{s}_j^z$ ,  $\hat{s}_j^+$ , and  $\hat{s}_j^-$  are spin-1/2 operators which do act purely locally on the Hilbert space  $\mathcal{H}_j$ . With this transformation, using that  $\hat{s}_i^- \hat{s}_i^z = -\hat{s}_i^z \hat{s}_i^-$ , we have

$$\begin{aligned} \{\hat{c}_j, \hat{c}_i\} &= \left( \prod_{k < j} \hat{s}_k^z \right) \hat{s}_j^- \left( \prod_{l < i} \hat{s}_l^z \right) \hat{s}_i^- + \left( \prod_{l < i} \hat{s}_l^z \right) \hat{s}_i^- \left( \prod_{k < j} \hat{s}_k^z \right) \hat{s}_j^- \\ &= 0. \end{aligned} \quad (\text{A.4})$$

The transformation Eq. (A.3) is known as the Jordan-Wigner transformation. With this, the nonlocal structure of the fermionic operators is laid out explicitly. This may be cumbersome to deal with when constructing MPOs. Fortunately, for terms containing even powers of creation and annihilation operators (e.g. all particle-number conserving Hamiltonians), the parity operators  $s_k^z$  cancel. For example, a nearest-neighbour hopping term may be written as

$$\begin{aligned}
\hat{c}_j^\dagger \hat{c}_{j+1} &= \left( \prod_{l < j} \hat{s}_l^z \right) \hat{s}_j^+ \left( \prod_{k < j+1} \hat{s}_k^z \right) \hat{s}_{j+1}^- \\
&= \left( \prod_{l < j} (\hat{s}_l^z)^2 \right) \hat{s}_j^+ \hat{s}_j^z \hat{s}_{j+1}^- \\
&= \hat{s}_j^+ \hat{s}_j^z \hat{s}_{j+1}^-.
\end{aligned} \tag{A.5}$$

The Jordan-Wigner strings have therefore cancelled in pairs and restored the nearest-neighbour interaction. For longer-range terms, this generalises to

$$\hat{c}_j^\dagger \hat{c}_{j+r} = \hat{s}_j^+ \left( \prod_{k=j}^{j+r-1} \hat{s}_k^z \right) \hat{s}_{j+r}^-. \tag{A.6}$$

For longer range interactions involving many fermionic operators, the Jordan-Wigner can be quite cumbersome. We therefore built a system which automatically performs this task, among others, when creating MPOs, which we discuss in Appendix B.

# Appendix B

## Automatic construction of MPOs

In this appendix, we elaborate on the connection between MPOs, finite state machines and regular languages, and discuss how we exploit this to create a simple yet powerful scripting language which allows one to create almost any operator as an MPO in the TNT library. As we outlined in Chapter 3, central to performing ground state calculations [206] and time-evolution calculations with long-range interactions [207, 208] is the MPO representation of the Hamiltonian. However, especially for long-range interacting systems with multi-body interactions, constructing these MPOs can be extremely cumbersome and error-prone. Previously, the process was

1. Apply the Jordan-Wigner transformation to  $\hat{H}$  so that it is expressed explicitly in a tensor product space.
2. Express the resulting Hamiltonian as an efficient FSM (see Sec. 3.6.3).
3. If one is using  $U(1)$  symmetries, identify which quantum numbers to assign to the internal legs of the MPO<sup>1</sup>.
4. Input this as a MPO in the TNT library.

Particularly for complicated long-range interacting Hamiltonians, like the  $t$ - $J$ - $\alpha$  model on a ladder, which we discuss in Sec. 4.5, this process can be arduous and error-prone. Automation of MPO construction is therefore highly desirable, and is fortunately possible due to the grammatical structure of expressions for physical Hamiltonians. For example, consider the Hubbard model with an on-site potential  $V_j$ ,

$$\hat{H} = \sum_j \left( U_j \hat{n}_{j,\uparrow} \hat{n}_{j,\uparrow} + V_j \hat{n}_j - t_j \hat{c}_{j,\uparrow}^\dagger \hat{c}_{j+1,\uparrow} + \text{H.c.} - t_j \hat{c}_{j,\downarrow}^\dagger \hat{c}_{j+1,\downarrow} + \text{H.c.} \right) \quad (\text{B.1})$$

---

<sup>1</sup>We will not discuss this aspect in this thesis. For an explanation see, for example, Refs. [206] and [209]

Where we have written the parameters  $U_j$ ,  $t_j$  and  $V_j$  as parameters which possibly vary as a function of lattice position. We can see that this Hamiltonian expression has a very clear grammar. Specifically, each term begins with a parameter (e.g.  $U_j$ ), followed by a sequence of operators (e.g.  $n_{j,\uparrow}$ ). The operators have a name (e.g.  $n_{\uparrow}$ ), labelling how the operator acts, along with a site label, (e.g.  $j + 1$ ) along with a label indicating which site the operator acts on relative to others in the term. We can write this grammar as follows:

```
HAMILTONIAN = TERM [ '+' TERM ] *
TERM = PARAM OPERATOR [ OPERATOR ] *
OPERATOR = OP_NAME '_' { j ' ' [ '+' INTEGER ] ' } ' .
```

Let us explain the notation used here, which is a variation of the extended Backus–Naur form (EBNF) [210]. The first line means that the operator consists of a term, followed by an number of further terms separated by a  $+$ . The square brackets denote that the enclosed expression is optional. The  $*$  at the end denotes that there may possibly be an unlimited number of these optional terms. The second line expresses the structure of the terms. It says that a term in the operator is a parameter followed by an operator followed by a potentially unlimited number of additional operators. Each operator consists of a name, with a “position” attached to it labelling which site it acts on relative to the other sites in the term. Note that by substituting the definitions of **TERM** and **OPERATOR** into **HAMILTONIAN**, we can write the grammar as a single EBNF expression. It turns out that a grammar which may be written as a single EBNF expression is regular, and so can be implemented by finite state machines [210]. This in turn means that our Hamiltonians automatically have FSM representations.

Once the grammar of a language is defined, it is simple to write a parser for it using the method of recursive descent [210]. For the above example, the parser looks like

```
function parse_hamiltonian()
    parse_term();
    while (next_token() == '+')
        parse_term();
    end
end
```

```

function parse_term()
    parse_param();
    parse_operator();
    while (next_token() == token_name)
        parse_operator();
    end
end

function parse_operator()
    parse_op_name();
    expect_token('{j}');
    if (next_token() == '+')
        parse_int();
    end
    expect_token('}');
end

```

This parser has exactly the same structure as the grammar we defined above. The top level function “descends” to the next level, parsing expressions at a smaller and smaller granularity until the entire expression has been parsed. Here the function `parse_op_name()` parses a name and compares it to a dictionary which the user has defined. Each name corresponds to a  $d \times d$  matrix (the representation of the operator in a user-defined basis). The `parse_hamiltonian()` function essentially translates the plain-text Hamiltonian definition into a sum of tensor product strings of operators.

We already saw how to construct FSMs for sums of operator strings in Sec. 3.6.3. We can therefore easily construct the MPO once we have parsed the expression. We can also determine the appropriate quantum numbers to attach to the internal legs [206, 209]. Furthermore, we can traverse the FSM, identifying and removing redundant edges and vertices until a compact representation is obtained [209]. We also automatically perform the Jordan–Wigner transformation, so the expressions in our Hamiltonian grammar may be expressed directly in terms of fermionic operators.

We have implemented this parser in MATLAB as an interface for the TNT library [69]. This greatly increases the user-friendliness of the library and allows for DMRG calculations to be initiated simply by defining operators and parameter arrays, and then writing L<sup>A</sup>T<sub>E</sub>X-like expressions. For example, the Hubbard model is written as

$$\begin{aligned}
 &U_{\{i\}} \text{ nup}_{\{i\}} \text{ ndn}_{\{i\}} + t_{\{i\}} \text{ cdup}_{\{i\}} \text{ cup}_{\{i+1\}} + \text{H.c.} \\
 &+ t_{\{i\}} \text{ cddn}_{\{i\}} \text{ cdn}_{\{i+1\}} + \text{H.c.}
 \end{aligned}$$

Here `+ H.c.` is a convenient macro which inserts the Hermitian conjugate of the term immediately preceding it. As a more complicated example, the  $t$ – $J$ – $\alpha$  model is written as

```

t_{i} cdup_{i} cup_{i+1} + H.c.
+ t_{i} cddn_{i} cdn_{i+1} + H.c.
+ Jb2_{i} sp_{i} sm_{i+1} + H.c.
+ J_{i} sz_{i} sz_{i+1} + mJb4_{i} n_{i} n_{i+1}
+ maJb2_{i} cdup_{i} ndn_{i+1} cup_{i+2} + H.c.
+ maJb2_{i} cddn_{i} nup_{i+1} cdn_{i+2} + H.c.
+ aJb2_{i} cdup_{i} sm_{i+1} cdn_{i+2} + H.c.
+ aJb2_{i} cddn_{i} sp_{i+1} cup_{i+2} + H.c.

```

Note that the pair hopping terms contain both spin and fermionic operators, for which the Jordan–Wigner transformation is handled correctly. Finally, we note that the grammar we actually implement is slightly more sophisticated than the simple example shown above. For example, we can express Hamiltonians with long-range interactions, such as the Ising model with a  $1/r^3$  coupling.

$$\hat{H} = \sum_i \left( J_i^z \sum_r \frac{1}{r^3} \hat{s}_i^z \hat{s}_{i+r}^z + h_i^x \hat{s}_i^x \right). \quad (\text{B.2})$$

In our scripting language, we write this as

```

Jz_{i} \sum_{r} [ 1./(r).^3 ] sz_{i} sz_{i+r}
+ hx_{i} sx_{i}

```

The interface parses this expression, finds the optimal approximation of the function of  $r$  enclosed in the square brackets as a sum of exponentials, then constructs the MPO using the methods discussed in Sec. 3.6.3, which can again correctly take into account  $U(1)$  symmetries and fermionic operators.

# Appendix C

## Details of DMRG Calculations in Chapter 4

In this appendix, we summarise some technical details of the DMRG calculation presented in Chapter 4. The advantage of using a finite-size algorithm rather than infinite-DMRG is that we may use symmetries to exactly fix the number of fermions in the system  $N_{\uparrow}$  and  $N_{\downarrow}$ , which allows the precise determination of quantities such as the spin gap and compressibility.

The drawback of studying such a finite system with open boundaries is that it requires us to consider the interplay between finite-size and finite-entanglement scaling [93]. As we detail in the following, we find that our results are dominated by finite-size effects rather than finite-entanglement artefacts, and so we extrapolate only to  $L \rightarrow \infty$  for the largest value of  $\chi$  used.

We show some typical finite-size extrapolations in Fig. C.1(a) and (b). In (a), we show the spin gap at  $\alpha = 0.5$ ,  $n = 7/32$  as a function of inverse system size  $1/L$  for various values of  $J/t$ . The solid lines are quadratic fits for different interaction strengths. The crosses are data points for different system sizes and values of  $\chi = 100 - 500$  (increasing  $\chi$  makes almost no difference to the results and thus the multiple crosses appear as a single cross). Similarly, we show the extrapolation of the Luttinger parameter in Fig. C.1(b), where the lines and crosses have the same meaning as in (a). In (d) and (e) we repeat these plots for the system parameters  $\alpha = 0.15$ ,  $n = 1/2$ .

Additionally, we include an error bar at the  $1/L \rightarrow 0$  point in each plot (a)-(d), indicating the standard error from the quadratic least-squares fit, where we treat the values computed for  $\chi = 500$  as essentially exact for each system size. The error is sufficiently small that, due to the line thickness, these error bars cannot be seen on most of the plots.

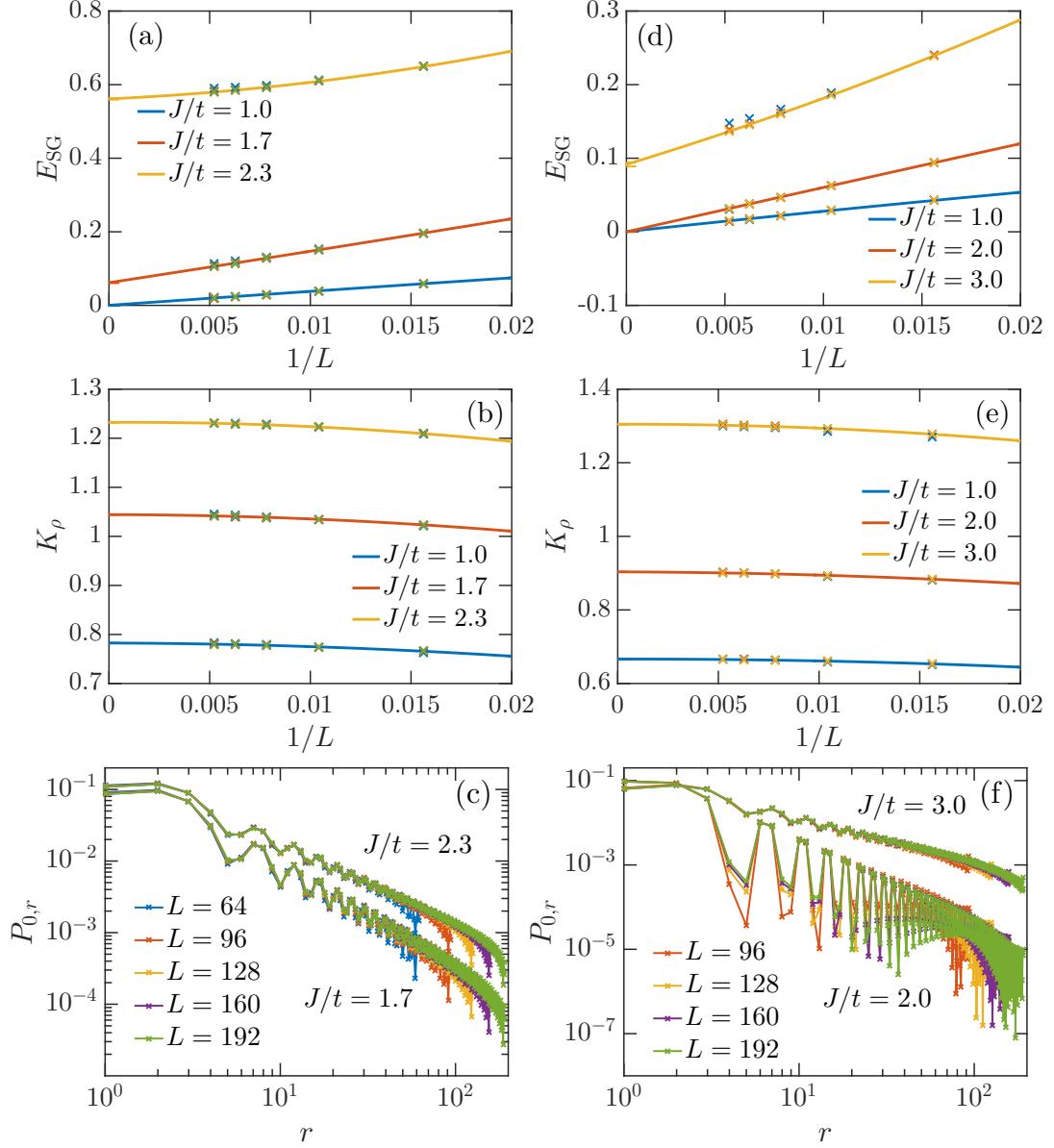


Figure C.1: Examples of the finite size extrapolation. The system parameters for the left column (a)-(c) are  $\alpha = 0.5$ ,  $n = 7/32$ , while the parameters for the right column (d)-(f) are  $\alpha = 0.15$ ,  $n = 1/2$ , with  $J/t$  marked on the plots. In (a) and (d) we show the extrapolation of the spin gap, while in (b) and (e) we show the Luttinger Parameter extrapolation. The crosses (which overlap) are computed for bond dimensions  $\chi = 100 - 500$ . In (c) we show the singlet correlations at selected interaction strengths with increasing system size computed for  $\chi = 300$ .

In Fig. C.1(c), we show the nearest-neighbour singlet correlation function at various system sizes for the same parameters as in plots (a) and (b), while (f) shows the singlet correlations for the same parameters as in plots (d) and (e), with  $\chi = 300$ . We see a polynomial decay over a significant range of distances  $r$ , after which an exponential tail develops. Such exponential tails always appear due to finite size and finite entanglement in some combination. The value of  $r$  at which this exponential tail sets in increases as we increase the system size. Furthermore, at these bond dimensions, the typical truncation error is small ( $\sim 10^{-4}$ ). We conclude that at these bond dimensions, finite-size effects dominate over finite-entanglement effects, and thus we extrapolate only in  $L$  and not  $\chi$  [93].

In all phase diagrams in Chapter 4, we compute the ground state at intervals of  $\Delta J = 0.1$ , and  $\Delta n = 1/16$ . For each quantity which determines a phase boundary, a linear interpolation is performed at the boundary of these grid squares to obtain a set of approximate grid points for the phase boundary. We then interpolate these points with a smoothed cubic spline to produce the plotted contour lines.

# Appendix D

## Additional details and calculations for Chapter 6

### D.1 Calculation of the quasienergy matrix for general sublattice driving

In Chapter 6, we analysed the driven Hubbard model, whose Hamiltonian is

$$\hat{H}(\tau) = \hat{H}_{\text{hub}} + \hat{H}_{\text{drive}}(\tau), \quad (\text{D.1})$$

where  $\hat{H}_{\text{hub}} = \hat{H}_{\text{hop}} + \hat{H}_{\text{int}} - \mu \sum_j \hat{n}_j$  and contributions given by

$$\hat{H}_{\text{hop}} = -t \sum_{\langle ij \rangle \sigma} (\hat{c}_{i,\sigma}^\dagger \hat{c}_{j,\sigma} + \text{H.c.}), \quad (\text{D.2})$$

$$\hat{H}_{\text{int}} = U \sum_j \hat{n}_{j,\uparrow} \hat{n}_{j,\downarrow}, \quad (\text{D.3})$$

$$\begin{aligned} \hat{H}_{\text{drive}}(\tau) = & \frac{V_a}{2} \sin(\Omega\tau - \Delta\phi) \sum_{j \in a} \hat{n}_j \\ & + \frac{V_b}{2} \sin(\Omega\tau + \Delta\phi) \sum_{j \in b} \hat{n}_j. \end{aligned} \quad (\text{D.4})$$

There, we presented results for the special case  $V_a = V_b$  and  $\Delta\phi = \pi/2$ . In this section we compute the quasienergy matrix for general sublattice driving and show that it leads to qualitatively similar physics to the special case presented in the main text.

Our goal is to compute the elements of the quasienergy operator in the Floquet basis

$$\langle \alpha | \hat{H}_{m,m'} | \beta \rangle = \langle \langle \alpha, m | [\hat{H}(\tau) - i\partial_\tau] | \beta, m' \rangle \rangle, \quad (\text{D.5})$$

where

$$|\alpha, m\rangle\rangle = |\alpha\rangle e^{im\Omega\tau}. \quad (\text{D.6})$$

Here  $\{|\alpha\rangle\}$  is an arbitrary orthonormal basis in the many-body Hilbert space  $\mathcal{H}$ , and  $m$  is the photon number. Recalling the definition of the inner product on the Floquet-Hilbert space Eq. (5.7), The blocks of the quasienergy operator are given by

$$\hat{H}_{m,m'} = \mathbb{1}m\Omega \delta_{m,m'} + \frac{1}{T} \int_0^T d\tau \hat{H}(\tau) e^{-i(m-m')\Omega\tau}. \quad (\text{D.7})$$

As we already saw in Sec. 5.2.1, it is advantageous to first transform the Hamiltonian  $\hat{H}(\tau)$  to the rotating frame by use of the operator

$$\hat{R}(\tau) = \exp \left( i \int_0^\tau d\tau' \hat{H}_{\text{drive}}(\tau') \right), \quad (\text{D.8})$$

and the transformation

$$\hat{H}^{\text{rot}}(\tau) = i(\partial_\tau \hat{R}) \hat{R}^\dagger + \hat{R} \hat{H}(\tau) \hat{R}^\dagger. \quad (\text{D.9})$$

Using identical arguments as in Sec. 5.2.1, we find that the fermionic annihilation operators transform as

$$\begin{aligned} \hat{c}_{j \in a, \sigma} &\rightarrow e^{-i\Delta_a(\tau)} \hat{c}_{j \in a, \sigma}, \\ \hat{c}_{j \in b, \sigma} &\rightarrow e^{-i\Delta_b(\tau)} \hat{c}_{j \in b, \sigma}, \end{aligned} \quad (\text{D.10})$$

where

$$\Delta_a(\tau) = \frac{V_a}{2\Omega} \cos(\Omega\tau - \Delta\phi), \quad \text{and} \quad \Delta_b(\tau) = \frac{V_b}{2\Omega} \cos(\Omega\tau + \Delta\phi). \quad (\text{D.11})$$

We can already see that local density operators  $\hat{n}_{j,\sigma}$  are not affected by this transformation, and so  $\hat{H}_{\text{int}}$  is also unaffected. Only the hopping operator is transformed, leaving the Hamiltonian as

$$\hat{H}^{\text{rot}}(\tau) = \hat{H}_{\text{hop}}^{\text{rot}}(\tau) + \hat{H}_{\text{int}}, \quad (\text{D.12})$$

where  $\hat{H}_{\text{hop}}^{\text{rot}}(\tau) = \hat{R}(\tau) \hat{H}_{\text{hop}} \hat{R}^\dagger(\tau)$ . The rotating frame transformation has cancelled the explicit driving term and instead imprinted time dependence on the hopping term. The blocks of the quasienergy operator are therefore

$$\hat{H}_{m,m'} = \frac{1}{T} \int_0^T d\tau \hat{H}_{\text{hop}}^{\text{rot}}(\tau) e^{-i(m-m')\Omega\tau} + \left( \hat{H}_{\text{int}} + \mathbb{1}m\Omega \right) \delta_{m,m'}. \quad (\text{D.13})$$

Because of the bipartite structure of the lattice, a hopping process always involves one operator from the  $a$  sublattice, and one from the  $b$  sublattice. We can therefore write

$$\hat{H}_{\text{hop}}^{\text{rot}}(\tau) = -t \sum_{\langle jk \rangle, \sigma} \left( e^{is_j(\Delta_a(\tau) - \Delta_b(\tau))} \hat{c}_j^\dagger \hat{c}_k + \text{H.c.} \right), \quad (\text{D.14})$$

where  $s_j = +1$  if the  $j$  is in the  $a$  sublattice,  $s_j = -1$  if  $j$  on the  $b$  sublattice.

Our strategy, as in Sec. 5.2.1, will be to write these as exponentials of sinusoids, which have a simple Fourier decomposition in terms of Bessel Functions. We can simplify this by writing

$$\Delta_a(\tau) - \Delta_b(\tau) = \frac{(V_a + V_b)}{2\Omega} \sin(\Omega\tau) \sin(\Delta\phi) - \frac{(V_a - V_b)}{2\Omega} \cos(\Omega\tau) \cos(\Delta\phi), \quad (\text{D.15})$$

where we have used the standard cosine addition formula. Thus we have that

$$e^{is_j(\Delta_a(\tau) - \Delta_b(\tau))} = e^{is_j \left( \frac{(V_a + V_b)}{2\Omega} \sin(\Omega\tau) \sin(\Delta\phi) \right)} e^{-is_j \left( \frac{(V_a - V_b)}{2\Omega} \cos(\Omega\tau) \cos(\Delta\phi) \right)}. \quad (\text{D.16})$$

Then, using the Jacob-Anger expansions,

$$e^{iz \sin \theta} = \sum_{m=-\infty}^{\infty} \mathcal{J}_m(z) e^{im\theta}, \quad \text{and} \quad e^{iz \cos \theta} = \sum_{m=-\infty}^{\infty} i^m \mathcal{J}_m(z) e^{im\theta}, \quad (\text{D.17})$$

where  $\mathcal{J}_m(z)$  is the  $m$ th Bessel function of the first kind, we obtain

$$e^{is_j(\Delta_a(\tau) - \Delta_b(\tau))} = \sum_{n=-\infty}^{\infty} (-i)^n \mathcal{J}_n \left( s_j \frac{(V_a - V_b)}{2\Omega} \cos(\Delta\phi) \right) \quad (\text{D.18})$$

$$\times \sum_{n'=-\infty}^{\infty} \mathcal{J}_{n'} \left( s_j \frac{(V_a + V_b)}{2\Omega} \sin(\Delta\phi) \right) e^{i(n+n')\Omega\tau}, \quad (\text{D.19})$$

and so when we compute the quasienergy blocks by extracting the Fourier component, we obtain

$$\hat{H}_{m,m'} = -t \sum_{[j,k],\sigma} \zeta_{j,m-m'} \hat{c}_{j,\sigma}^\dagger \hat{c}_{k,\sigma} + \left( \hat{H}_{\text{int}} + \mathbb{1} m \Omega \right) \delta_{m,m'}, \quad (\text{D.20})$$

where

$$\begin{aligned} \zeta_{j,m-m'} &= \sum_{n=-\infty}^{\infty} (-i)^n \mathcal{J}_n \left( s_j \frac{(V_a - V_b)}{2\Omega} \cos(\Delta\phi) \right) \\ &\times \sum_{n'=-\infty}^{\infty} \mathcal{J}_{n'} \left( s_j \frac{(V_a + V_b)}{2\Omega} \sin(\Delta\phi) \right) \delta_{n+n',m'-m}. \end{aligned} \quad (\text{D.21})$$

The quasienergy operator therefore has the following form. First, the diagonal blocks are replicas of the Hubbard model with the energy different photon numbers  $m$ , and a hopping which has been modified by  $\zeta_{j,0}$ . The off-diagonal blocks describe modified hopping processes which absorb and emit quanta from the drive and thus change the photon number. In Fig. D.1, we plot  $\zeta_{j,0}$  computed as a function of the phase difference  $\Delta\phi$ , and the driving strength  $\nu_a$ , where  $\nu_b = V/\Omega = 2\nu_b$ . In particular,

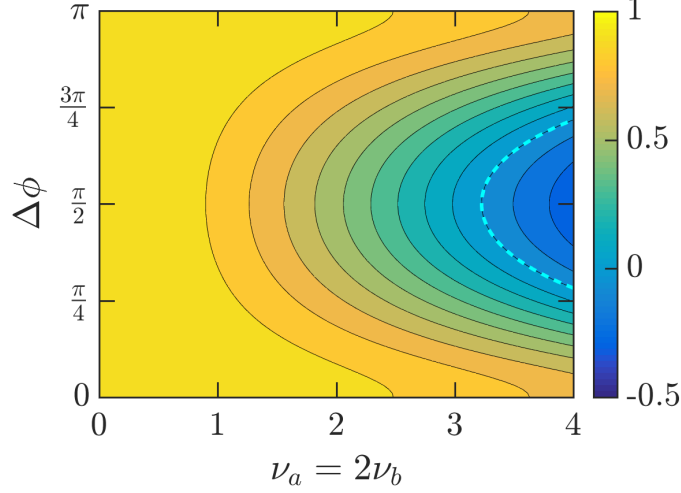


Figure D.1: The coefficient  $\zeta_0$  with unequal  $a$  and  $b$  driving strengths as a function of  $\nu_a$  and  $\Delta\phi$ . The dotted line marks the contour  $\zeta_0 = 0$ , where single particle hopping is suppressed to 0.

we see that  $\zeta_{j,0}$ , which is equal to the suppressed hopping  $\tilde{t}/t$  in the limit  $U \rightarrow \infty$ ,  $\Omega \rightarrow \infty$ , with  $\Omega/U < 1$ .

Finally, we simplify Eq. (D.22) by simplifying to the special case  $V_a = V_b = V$ , and  $\Delta\phi = \pi/2$ . Since  $\mathcal{J}_n(0) = \delta_{n,0}$ , the first sum collapses, and we are left with

$$\zeta_{j,m-m'} = \sum_{n'=-\infty}^{\infty} \mathcal{J}_{n'}(s_j \nu) \delta_{n',m'-m}, \quad (\text{D.22})$$

where  $\nu = V/\Omega$ . Then, using the identity  $\mathcal{J}_n(-z) = (-1)^n \mathcal{J}_n(z)$  and using the Kronecker delta to collapse the infinite sum, we obtain

$$\zeta_{j,m-m'} = (s_j)^{m'-m} \mathcal{J}_{m'-m}(\nu), \quad (\text{D.23})$$

which is the form given in Eq. (6.7).

## D.2 Details of numerical calculations

For the zero temperature calculations, we computed the ground state of the Hubbard system using the infinite time-evolving block decimation (iTEBD) to evolve an initial translationally-invariant infinite matrix product state (iMPS) in imaginary time until a convergence in the singular values is reached [90]. Using a fourth-order Suzuki-Trotter decomposition, and successively refining the timestep to systematically eliminate the Trotter error and bring the final state into canonical form, we

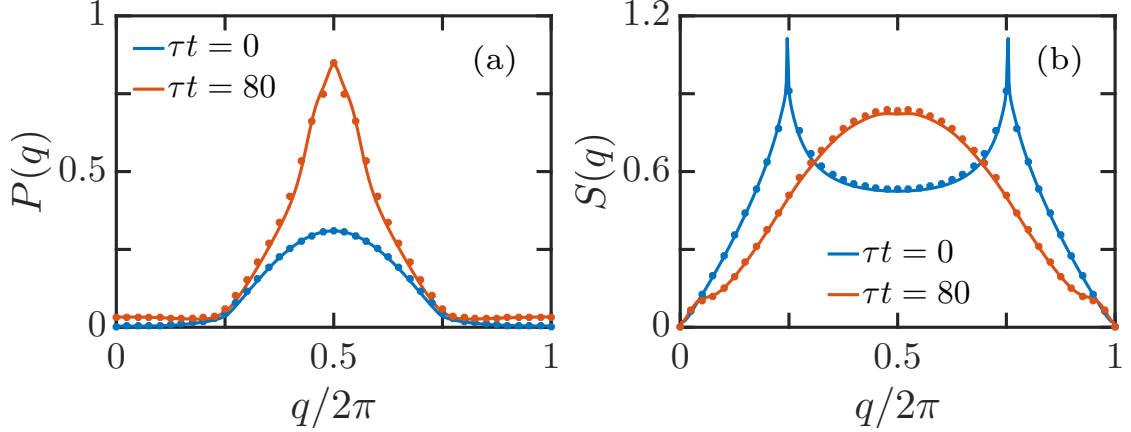


Figure D.2: A comparison of the (a) singlet and (b) spin structure factors at two different times, computed for the same parameters as in Fig. 6.3. The points show results for the finite-size,  $L = 40$  results, while the line shows the infinite-size results.

obtain an iMPS with a bond dimension of  $\chi = 200$ . We subsequently evolve this iMPS using iTEBD, and compute the expectation values given in Sec. 6.2.1.

To accurately capture the driven state our iTEBD calculations were performed with iMPS bond dimensions up to  $\chi = 400$  and a driving frequency dependent timestep  $\Delta\tau = 2\pi/(50\Omega)$ . To resolve the fast oscillations in the correlation functions, they were sampled every 10 timesteps. The correlations were robust to moderate changes in  $\chi$  and  $\Delta\tau$ , and the cumulative truncation error during the time-evolution remained small.

In Fig. D.2, we show the spin and singlet structure factors for the driven system for finite size ( $L = 40$ ) calculation, with the filling  $n = 1/2$ , fixed using a U(1) symmetric MPS. We compare this to the results obtained for the infinite system using iTEBD results computed without symmetries, and a chemical potential  $\mu = -0.2t$  result. We find essentially no difference between the results for the finite and infinite systems, thus demonstrating that the results seen for the finite system are not a finite size effect. Consequently, for simplicity and computational tractability, we use a finite system for the purposes of finite temperature calculations and for comparisons to the  $t$ - $J$  model.

For the finite temperature calculations, we obtained thermal states of a finite sized Hubbard model via imaginary-time TEBD. An initial matrix product operator (MPO) representation of the identity matrix (i.e. an infinite temperature state) was evolved in imaginary time with a timestep  $\Delta\beta = 0.01/t$  to obtain an MPO representation of the desired thermal mixed state [86], tuning the chemical potential to obtain desired

filling  $\bar{n} = 1/2$ . We then performed real-time evolution with an MPO dimension up to  $\chi = 400$  to describe the driven state.

# Appendix E

## Floquet engineering the $t$ - $J$ - $\alpha$ model in an optical lattice

In this appendix, we consider the Hubbard model as implemented by ultracold fermionic atoms trapped in a one-dimensional optical lattice. We show that by oscillating the equilibrium position of the lattice back and forth, we implement a driving term which allows us to Floquet engineer the  $t$ - $J$ - $\alpha$  model where both  $J/t$  and  $\alpha$  can be varied.

### E.1 The driving term

Here we derive the driving term for the system. Various implementations of periodic driving are possible. The one we consider here is that the entire optical lattice is oscillated back and forth at a frequency  $\Omega$  and an amplitude  $\Delta$ . The lab frame Hamiltonian is therefore

$$\hat{H}^{\text{lab}} = \frac{\hat{p}^2}{2m} + V_0 \cos^2(k(x - \Delta \cos(\Omega\tau))). \quad (\text{E.1})$$

We then apply a unitary transformation which moves us into the frame that is co-moving with respect to the lattice. We first recall that the operator  $e^{-i\hat{p}l}$  translates the position operator as

$$e^{i\hat{p}l} \hat{x} e^{-i\hat{p}l} = \hat{x} + i l [\hat{p}, \hat{x}] \quad (\text{E.2})$$

$$= \hat{x} + l, \quad (\text{E.3})$$

where we have used the Baker-Campbell-Hausdorff transformation, along with the canonical commutation relation  $[\hat{p}, \hat{x}] = i$ . Setting  $l = \Delta \cos(\Omega\tau)$ , we therefore have that the operator which brings us into the comoving frame is

$$\hat{R}(\tau) = e^{i\Delta \cos(\Omega\tau) \hat{p}}. \quad (\text{E.4})$$

We apply this to the Hamiltonian via

$$\hat{H}^{\text{cm}} = i(\partial_\tau \hat{R}) \hat{R}^\dagger + \hat{R} \hat{H} \hat{R}^\dagger. \quad (\text{E.5})$$

The first term gives  $-\Delta\Omega \sin(\Omega\tau) \hat{p}$ . In the second term, the kinetic energy is unchanged since  $[\hat{R}, \hat{p}] = 0$ , and the second term is shifted  $x \rightarrow x + \Delta \cos \Omega\tau$ , yielding

$$\hat{H}^{\text{cm}} = \frac{\hat{p}^2}{2m} - \Delta\Omega \sin(\Omega\tau) \hat{p} + V_0 \cos^2(kx). \quad (\text{E.6})$$

Completing the square of the momentum terms gives

$$\begin{aligned} \hat{H}^{\text{cm}} &= \frac{(\hat{p} - \Delta\Omega m \sin(\Omega\tau))^2}{2m} - \frac{(\Delta\Omega)^2 m}{2} \sin^2(\Omega\tau) + V_0 \cos^2(kx) \\ &= \frac{(\hat{p} - \Delta\Omega m \sin(\Omega\tau))^2}{2m} - \frac{(\Delta\Omega)^2 m}{4} (1 - 2 \cos(2\Omega\tau)) + V_0 \cos^2(kx). \end{aligned}$$

The second term consists of a constant part, which doesn't affect the dynamics, and a spatially uniform time-periodic part, which we may gauge away with another periodic unitary transformation. This leaves us with

$$\hat{H}^{\text{cm}} = \frac{(\hat{p} - \Delta\Omega m \sin(\Omega\tau))^2}{2m} + V_0 \cos^2(kx).$$

Recalling the minimal coupling form of the Hamiltonian, we see that this Hamiltonian has the form of a charged particle in a spatially uniform electric field which oscillates in time [211]. Therefore in the Coulomb gauge, this gives

$$\hat{H}^{\text{cm}} = \frac{\hat{p}^2}{2m} + \Delta\Omega m \cos(\Omega\tau) \hat{x} + V_0 \cos^2(kx).$$

Once we expand this in the Wannier basis of the lowest Bloch band (see Sec. 2.2.2), the driving term becomes

$$\hat{H}_V(\tau) = V \cos(\Omega\tau) \sum_j j \hat{n}_j. \quad (\text{E.7})$$

Recall that we used this term in Sec. 5.2.1 when discussing the tight-binding model in a shaken optical lattice.

## E.2 Engineering the $t$ - $J$ - $\alpha$ model

The full Hamiltonian we consider is

$$\hat{H}(\tau) = \hat{H}_t + \hat{H}_U + \hat{H}_V(\tau), \quad (\text{E.8})$$

where

$$\begin{aligned}\hat{H}_t &= -t \sum_j \left( \hat{c}_{j,\sigma}^\dagger \hat{c}_{j+1,\sigma} + \text{H.c.} \right) \\ \hat{H}_U &= U \sum_j \hat{n}_{j,\uparrow} \hat{n}_{j,\downarrow}.\end{aligned}\tag{E.9}$$

Using the procedure discussed in Sec. 5.2.1, we transform  $\hat{H}(\tau)$  and expand it in the Floquet basis  $|\alpha\rangle e^{im\Omega\tau}$  to obtain the block form of the quasienergy operator,

$$\hat{H}_Q = \sum_{m,m'} \hat{H}_{m,m'} \otimes |m\rangle \langle m'|,\tag{E.10}$$

with

$$\begin{aligned}\hat{H}_{m,m'} &= -t \sum_{j,\sigma} \left( \mathcal{J}_{m'-m}(\nu) \hat{c}_{j,\sigma}^\dagger \hat{c}_{j+1,\sigma} + \mathcal{J}_{m-m'}(\nu) \hat{c}_{j+1,\sigma}^\dagger \hat{c}_{j,\sigma} \right) + (\hat{H}_U + m\Omega) \delta_{m,m'} \\ &= -t \hat{T}_{m,m'} + (\hat{H}_U + m\Omega) \delta_{m,m'}.\end{aligned}\tag{E.11}$$

Note that this differs from the form of the quasienergy operator blocks in Eq. (6.19). Namely, since the driving takes the form of an oscillating tilted potential rather than sublattice-dependent driving, we do not have a sign factor  $s_j$  which depends on which sublattice the hopping process starts from. Rather the sign of the process flips depending on the direction of the hopping process.

As in Sec. 6.3.1, we consider the limit  $t \ll U, \Omega$ , and perform degenerate perturbation theory to compute the approximate Floquet Hamiltonian inside the  $m = 0$  photon block containing zero doublons. We again obtain the Hamiltonian

$$\hat{H}_{\text{eff}} \approx \hat{H}_{\text{eff}}^{(1)} + \hat{H}_{\text{eff}}^{(2)},\tag{E.12}$$

where

$$\begin{aligned}\hat{H}_{\text{eff}}^{(1)} &= -t \mathbb{P}_{0,0} \left( \sum_{m,m'} \hat{T}_{m,m'} \otimes |m\rangle \langle m'| \right) \mathbb{P}_{0,0}, \\ \hat{H}_{\text{eff}}^{(2)} &= -t^2 \sum_{p,p'} \sum_{q,q'} \sum_{n_d > 0} \sum_m \frac{\mathbb{P}_{0,0}(\hat{T}_{p,p'} \otimes |p\rangle \langle p'|) \mathbb{P}_{n_d,m}(\hat{T}_{m,m'} \otimes |q\rangle \langle q'|) \mathbb{P}_{0,0}}{n_d U + m\Omega} \\ &\quad - t^2 \sum_{p,p'} \sum_{q,q'} \sum_{m \neq 0} \frac{\mathbb{P}_{0,0}(\hat{T}_{p,p'} \otimes |p\rangle \langle p'|) \mathbb{P}_{0,m}(\hat{T}_{m,m'} \otimes |q\rangle \langle q'|) \mathbb{P}_{0,0}}{m\Omega}.\end{aligned}\tag{E.13}$$

We obtain that

$$\hat{H}_{\text{eff}}^{(1)} = \mathbb{P}_0 \left[ -t \hat{T}_{0,0} \right] \mathbb{P}_0 = \mathbb{P}_0 \left[ -t \mathcal{J}_0(\nu) \sum_j \left( \hat{c}_{j,\sigma}^\dagger \hat{c}_{j+1,\sigma} + \text{H.c.} \right) \right] \mathbb{P}_0,\tag{E.14}$$

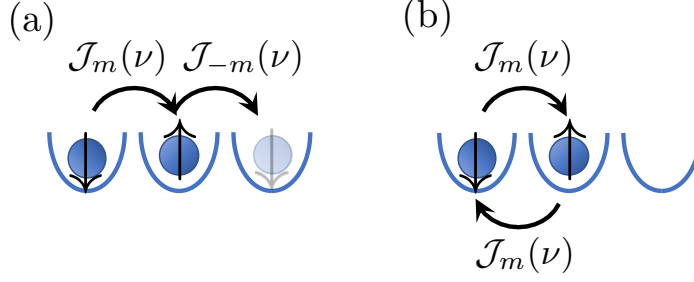


Figure E.1: We show the contributions to the pair hopping and superexchange processes for the  $m$  photon term. In (a), the two hops occur in the same direction, and so the process accumulates two Bessel function factors of opposite sign. In (b), the hops occur in opposite directions, accumulating two Bessel function factors of the same sign. Summing up these contributions over all photon numbers  $m$  results in different renormalisations for each term, breaking the fixed ratio  $\alpha$  between the superexchange and the pair hopping.

Once again finding the standard Bessel function suppression of the hopping with doublons projected out.

Looking now at the second term in Eq. (E.13), which corresponds to virtual emission/absorption of photons without creating/destroying doublons, We find that by the same arguments as in Sec. 6.3.1, this term vanishes. This leaves only the first term in Eq. (E.13). First taking care of the photon number projectors, we find that

$$\hat{H}_{\text{eff}}^{(2)} = -t^2 \sum_{n_d > 0} \sum_m \frac{\mathbb{P}_0 \hat{T}_{0,m} \mathbb{P}_{n_d} \hat{T}_{m,0} \mathbb{P}_0}{n_d U + m \Omega}. \quad (\text{E.15})$$

Just considering the numerator for a moment, we have

$$\begin{aligned} \mathbb{P}_0 \hat{T}_{0,m} \mathbb{P}_{n_d} \hat{T}_{m,0} \mathbb{P}_0 &= \sum_{j,a} \sum_{k,b} \mathbb{P}_0 \left( \mathcal{J}_m(\nu) \hat{c}_{j,a}^\dagger \hat{c}_{j+1,a} + \mathcal{J}_{-m}(\nu) \hat{c}_{j+1,a}^\dagger \hat{c}_{j,a} \right) \mathbb{P}_{n_d} \\ &\quad \times \left( \mathcal{J}_{-m}(\nu) \hat{c}_{k,b}^\dagger \hat{c}_{k+1,b} + \mathcal{J}_m(\nu) \hat{c}_{k+1,b}^\dagger \hat{c}_{k,b} \right) \mathbb{P}_0 \end{aligned} \quad (\text{E.16})$$

We see that there are four distinct nonzero processes contained within this term, which we show in Fig. E.1. First, if the virtual doublon is created by a leftward hopping process it accumulates a factor  $\mathcal{J}_{-m}(\nu)$ , while it accumulates a factor  $\mathcal{J}_m(\nu)$  if it was created by a rightward hop. Similarly the process accumulates a factor  $\mathcal{J}_m(\nu)$  the doublon is destroyed by a leftward hop, or a factor  $\mathcal{J}_{-m}(\nu)$  if it is destroyed by a rightward hop.

Next, we observe that the processes in which the hops go in opposite directions correspond to superexchange terms, and have a coefficient  $\mathcal{J}_m^2(\nu)$  or  $\mathcal{J}_{-m}^2(\nu) = \mathcal{J}_m^2(\nu)$ .

Summing up all of the contributions from different  $m$ 's, we find an effective superexchange

$$\tilde{J} = 4t^2 \sum_m \frac{\mathcal{J}_m^2(\nu)}{U + m\Omega}, \quad (\text{E.17})$$

which is the same as for the sublattice driving. As we showed in Sec. 6.3.1, this reduces to  $4t^2/U = J$  in the limit  $t \ll \Omega \ll U$ . On the other hand, processes in which the hops go in the same direction correspond to pair-hopping terms, and acquire a coefficient  $\mathcal{J}_m(\nu)\mathcal{J}_{-m}(\nu)$ . Again summing up the contributions from all  $m$ 's we find that the effective pair hopping is

$$\tilde{\alpha}\tilde{J} = 2t^2 \sum_m \frac{\mathcal{J}_m(\nu)\mathcal{J}_{-m}(\nu)}{U + m\Omega}. \quad (\text{E.18})$$

We plot  $\tilde{t}$ ,  $\tilde{J}$  and  $\tilde{\alpha}\tilde{J}$  as a function on  $\nu$  for various  $U$ 's and  $\Omega$ 's in Fig. E.2. We see that depending on the  $U$ , it is possible to engineer wide variety of  $U$ 's and  $\alpha$ s, even outside those we consider in Chapter 4. For instance, in (a), we see that we can engineer large negative values of  $\alpha$ , while in (b), we can engineer positive values of  $\alpha$ . By tuning  $\nu \approx \nu_0/2$ , we can even “switch off” the pair-hopping, thus implementing the standard one-dimensional  $t$ - $J$  model in an optical lattice. In summary, in an ultracold atom experiment, by tuning  $U$  with a Feshbach resonance, and changing the driving strength  $\nu$ , one can explore a wide range of the  $t$ - $J$ - $\alpha$  model's phase diagram, probing the superexchange physics.

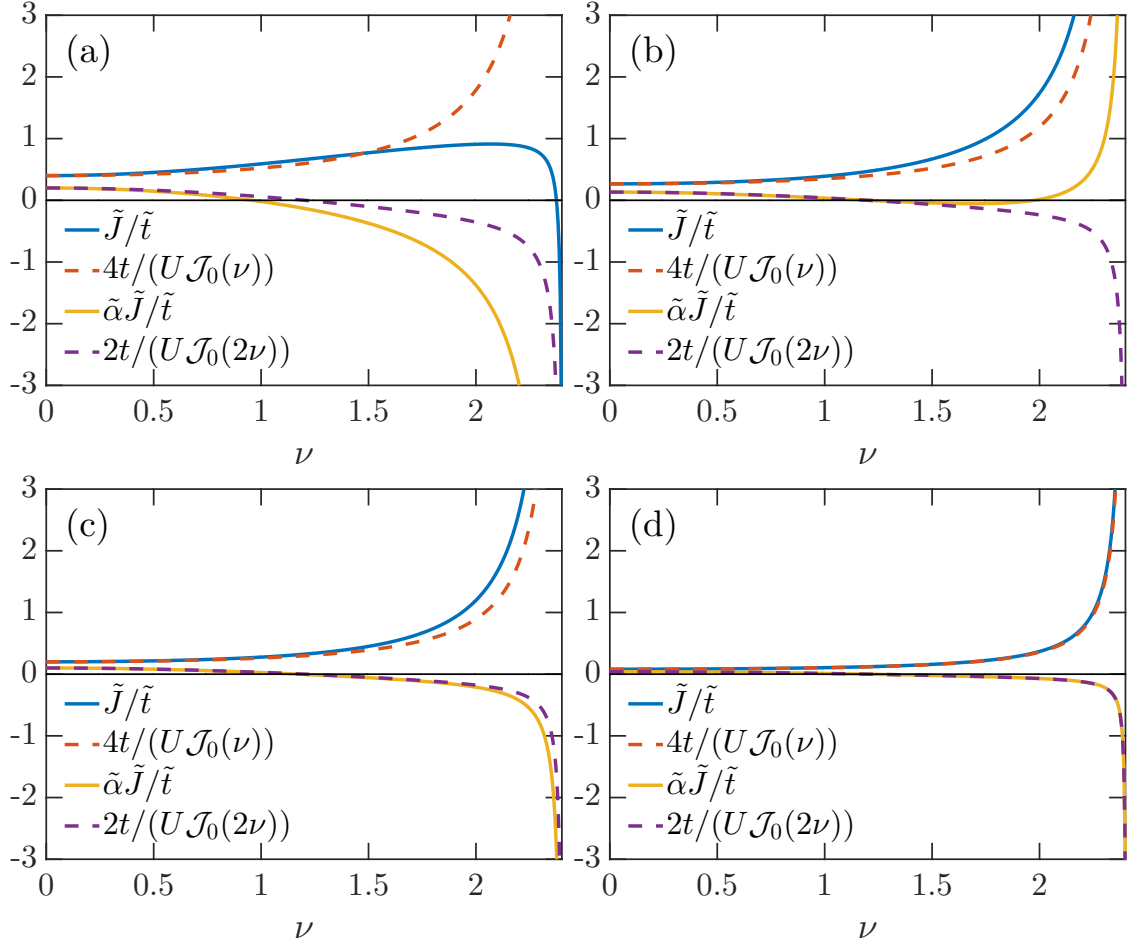


Figure E.2: We show the ratio of the effective superexchange to the effective hopping  $\tilde{J}/\tilde{t}$ , as well as the ratio of the effective pair-hopping to the effective hopping  $\tilde{\alpha}\tilde{J}/\tilde{t}$ , as a function of driving strength  $\eta$ . In all cases a driving frequency of  $\Omega = 6t$  was used. The value of the interaction strengths used were (a)  $U = 10t$ , (b)  $U = 15t$ , (c)  $U = 20t$ , (d)  $U = 50t$ .

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