

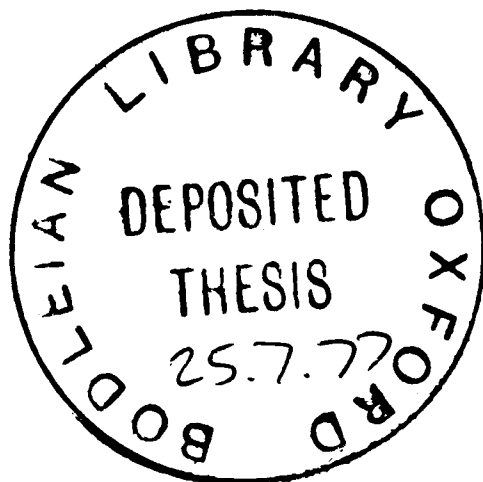
THEORY OF PROPERTIES OF SOME
ONE-DIMENSIONAL SYSTEMS

Lindberg Lima Gonçalves

A thesis submitted for the Degree of
Doctor of Philosophy at the University of Oxford

ST. JOHN'S COLLEGE

OXFORD



February, 1977

To my wife and my parents

Acknowledgements

It is a great pleasure to express my gratitude to my supervisor, Professor R. J. Elliott, for suggesting this problem and for his patience, help and encouragement at all times.

I would also like to thank Dr. A.P. Young for many enlightening discussions at the early stages of this work and Professor H. Falk for his invaluable help on many occasions.

My thanks are also due to my colleagues Drs. J. Martinez, E.J. Lage and A. Donegan, and to Dr. D.R. Taylor for many stimulating discussions, to Dr. D.F. Mayers for his help in the numerical calculations, to those from the Advisory Service of the Oxford University Computer Laboratory for having patiently helped me, and to Miss S. Reeves for so efficiently typing this thesis.

Special thanks are due to Lourdes, my wife, for drawing the graphs of this thesis and especially for her patience and understanding throughout the past three years.

The financial support from Conselho Nacional de Desenvolvimento Científico e Tecnológico (CNPq, Brazil) and Universidade Federal do Ceará (Brazil) is gratefully acknowledged.

ABSTRACT

This thesis consists in a theoretical study of some one-dimensional models. Special attention is given to simple but non-trivial soluble models.

The study starts with a resume of the Green function method which is the formalism used throughout the work. A discussion of coupled electron-phonon and spin-phonon systems is presented and a decoupling scheme introduced. The approximation gives the transition temperature for one-dimensional systems exactly, namely $T = 0$, and consequently represents a great improvement on the mean-field approximation.

The impure XY-chain in a transverse field is studied and the formal solution presented. The static and time-dependent correlations are discussed, and the effect of the boundary term reviewed in details. The one-impurity case is solved for the isotropic chain, and it is shown how to derive from it the open chain result in the thermodynamic limit. The heat-flux operator is obtained for the impure isotropic chain by solving the continuity equation for energy density.

The dynamics of the one-dimensional transverse Ising model is discussed within several approximations. The limitations of each approximation are examined in detail and the time-dependent correlations are calculated using the most successful approximation. It is also shown that this approximation is only valid in the high temperature limit in which case no critical behaviour is to be observed.

The one-impurity solution of the isotropic impure XY-chain is extended to many impurities in two different cases. In the first case the specific heat of the dilute chain is calculated in the framework of the average t-matrix approximation, and the results compared with exact numerical calculations for finite chains. In the second case the specific heat and thermal conductivity of the isotropic XY-chain in a random transverse field are calculated using the coherent-potential approximation (CPA). The results are used to explain the low temperature thermal properties of praseodymium ethyl sulphate.

Finally, two interacting systems, an electron-phonon system and a spin-phonon system, are studied after a brief discussion of the so-called Peierls instability. The first model is solved exactly in the framework of the approximation discussed at the beginning of the work. It presents a giant Kohn anomaly at zero temperature which drives a Peierls transition. The renormalized modes are discussed, and the real and imaginary parts of the phonon propagator are presented for wave vector $\frac{\pi}{a}$ and several coupling constants and temperatures.

The spin-phonon system is also studied in the framework of the approximation discussed initially in the work, and it is chosen in such a way that the relevant properties are given in terms of Green functions calculated in the transverse Ising model. The results obtained for the dynamics of this model are used, and since they are valid only in the high temperature limit, the discussion is restricted to this temperature region. Since this

region is far away from the critical one, no critical behaviour is observed, and the study is restricted to a simple discussion of modes. The real and imaginary parts of the renormalized phonon propagator are presented for the wave vector $\frac{\pi}{a}$, high temperature and various coupling constants.

Contents

	<u>Page No.</u>
Introduction	1
Chapter 1. The coupled Spin-phonon and Electron phonon systems	10
1.1 The Green Function Method	10
1.2 The Decoupling Scheme	12
Chapter 2. The Impure Anisotropic XY-chain in a Transverse Magnetic Field	26
2.1 The Hamiltonian	26
2.2 The Correlation Functions	31
2.3 The Isotropic Chain - One Impurity Case	34
2.4 Derivation of the Heat Flux Operator	38
Chapter 3. Dynamics of the Pure One-dimensional Transverse Ising Model	42
3.1 The c-cyclic Approximation	42
3.2 The Decoupling Scheme Approximation	47
3.3 The Improved c-cyclic Approximation	49
Chapter 4. Applications to One-dimensional Spin Systems	62
4.1 The Specific Heat of the Dilute XY-chain	62
4.2 The Specific Heat of the Isotropic XY- chain in a Transverse Random Field	68
4.3 The Thermal Conductivity of the Isotropic XY-chain in a Transverse Random Field	73

		<u>Page No.</u>
Chapter 5.	Peierls Instability in One-dimensional systems	80
	5.1 The One-dimensional Peierls Instability	80
	5.2 The Coupled Electron-phonon system	81
	5.3 The Coupled Spin-phonon system	92
Conclusions		96
Appendix	The Decoupling Scheme Approximation -	
	Special Cases	99
References		103

Introduction

The study of one-dimensional systems (Lieb and Mattis, 1966) has attracted in the past the interest of a great number of physicists. Naturally this interest was motivated by the possibility of obtaining exact solutions for these models, which could be used for checking the results obtained by approximate methods developed for higher dimensionalities. As far as critical behaviour is concerned the importance of the dimensionality was soon realized (Landau and Lifchitz, 1967) in this kind of phenomenon. The absence of macroscopic order at finite temperature in one dimensional systems with short range interactions, and the apparent impossibility, even approximately, of its physical realization, made these problems a part of the large collection of purely academic problems.

The discovery of quasi-one-dimensional materials (Steiner et al., 1976; Berlinsky, 1976; Hone and Richards, 1974; Zeller, 1973) has, however, renewed interest in one-dimensional problems.

The main reason for this is the possibility of getting the three dimensional behaviour from the one-dimensional solution in systems with high anisotropy (Sato, 1961; Stout and Chisholm, 1962; Stanley and Kaplan, 1967; Scalapino et al., 1975). There are of course among these materials some that, as far as critical behaviour is concerned, do not exhibit three dimensional behaviour (Folinsbee et al., 1976) at all, in which cases the one-dimension model completely describes all the properties of the system.

The main purpose of this work is to look at some one-dimensional systems and try to obtain reasonable solutions for them. Special attention is given to systems which exhibit critical behaviour.

We start the first chapter by presenting a brief discussion of the Green function method and then we study the Hamiltonian of coupled electron-phonon (spin-phonon) systems in which the interacting term, considered as linear in displacement, is written in its most general form. These types of Hamiltonian are used to describe effects like Kohn anomalies (Kohn, 1959) and related effects like Peierls transition (Peierls, 1955), and structural phase transitions (Gehring and Gehring, 1975). The solution of the problem in the framework of the mean-field approximation has been presented by many authors (Rice and Strässler, 1973; Allender et al., 1974; Horowitz et al., 1974), and as expected they have found a finite transition temperature. This very unsatisfactory answer is obtained due to the fact that fluctuations are neglected in this approach which, however, are very important in one dimensional systems. By the introduction of new operators very similar to the shifted phonon operators (Elliott et al., 1972) we are able to introduce a decoupling scheme, which involves equations of all orders, and express all the relevant properties of the system in terms of an effective electron (or spin) Green function. Provided this function is evaluated exactly we get the transition temperature correctly, namely $T = 0$, and this represents a great improvement over the known approximations which are unable to reproduce this result.

In the light of this formalism it is also shown how to eliminate the spurious terms (Elliott et al., 1972; Pytte, 1974) which are taken in account when solving the problem in the framework of the mean-field approximation. Although the effective Green function is by no means easily calculated, the problem is put in a more tractable form which contains the one-dimensional character. The discussion is restricted to the one-dimensional case. However, the results obtained are valid in any dimension.

In the second chapter we study the impure anisotropic XY-chain in a transverse field. This model without impurities has been the object of study of many authors. The static properties are known and have been considered among others by Lieb et al. (1961), Katsura (1962; 1963), McCoy (1968) and Pfeuty (1970). Although some of the dynamical properties have been evaluated (Niemeijer, 1967; McCoy et al., 1971; Abraham, 1972; Capel et al., 1974), there are, however, great difficulties in the calculation of the time-dependent correlation functions in the XY-plane. These difficulties are of course present in the impure case, and are studied in detail in a formal way.

Firstly we discuss the diagonalization of the Hamiltonian and show that even in the presence of impurities the problem reduces to the diagonalization of bilinear forms of fermion operators. The effect of the boundary is reviewed in detail following closely the work of Mazur and Siskens (1973; 1974) and Capel et al. (1974). From the discussion presented it becomes clear why the boundary term can be neglected when calculating

the static correlation functions and time-dependent transverse correlation function, but not when calculating the time-dependent correlations in the XY plane.

The one impurity case is solved when the system is isotropic and the spectrum briefly discussed. The bound states have been discussed by Vinikovetsky et al. (1973). We also study the conditions under which the open chain without impurities can be obtained from the closed chain with one impurity.

Finally we calculate the heat flux operator for the isotropic chain with many impurities by adopting the procedure developed by Hardy(1963). The calculation involves the solution of the continuity equation. The results are to be used in the calculation of the thermal conductivity in the framework of the Kubo theory (Kubo, 1957).

In the third chapter we discuss the dynamics of the pure transverse Ising model. Naturally we are concerned with the longitudinal time-dependent correlation function and we try to overcome the difficulties present in its calculations, as pointed out in the second chapter. Firstly we discuss the so-called c-cyclic approximation (Mazur and Siskens, 1973; 1974; Capel et al., 1974). Although this approximation eliminates some of the difficulties involved in the calculation it gives the wrong answer when we consider the special case where the transverse field is equal to zero. Then we present a decoupling scheme approximation which gives the solution of the problem in terms of a non-linear differential equation. The equation can be solved analytically in the special cases where transverse field or

the exchange interaction are zero and gives the exact results. These calculations are presented in the appendix. For arbitrary finite values of the exchange interaction and the transverse field the solution of the equation has to be found numerically. We have not been able to obtain stable solutions, and consequently we had to abandon this approximation as well, although it appears to be promising. Finally we discuss a new approximation that we call the improved c-cyclic approximation (Gonçalves and Elliott, 1976). This approximation seems more successful than the others. It gives the correct answer in the special cases already mentioned and the first two moments of the auto-correlation function correctly. However, the approximation becomes unsatisfactory as the temperature is lowered because translational symmetry is broken. Unfortunately the natural way to recover the translational symmetry leads to an expression very complicated to evaluate, in which case we have to restrict our approximation to the high temperature limit.

In chapter four we present two applications of the theory developed in the second chapter. The first application concerns the study of the effect of dilution in the isotropic XY-chain without field. In this application we calculate the specific heat and compare it with the exact numerical result obtained for finite chains with n (number of spins) ≤ 11 (Bartolomé et al., 1976). The one-impurity solution obtained in the second chapter is extended to a concentration x of impurities by using the so-called average t-matrix approximation (Elliott et al., 1974). The results obtained are in good agreement with the exact calculations even in high concentration where the approximation is expected to break down.

The second application concerns calculation of the specific heat and thermal conductivity of the isotropic XY-chain in presence of a transverse random field. We start by calculating the configurational average single particle Green function using the coherent-potential-approximation (Elliott et al., 1974; Yonezawa and Morigaki, 1973) and from it we calculate immediately the specific heat since we have the density of states. The results are applied for praseodymium ethyl sulphate, $\text{Pr}(\text{C}_2\text{H}_5\text{SO}_4)_3 \cdot 9\text{H}_2\text{O}$. Folinsbee et al. (1976) have studied the low-temperature thermal properties of this material and concluded that it exhibits one-dimensional behaviour which is described by the isotropic XY model. Although the specific heat measured presents a broad peak as a function of temperatures, at the same position as that of the result obtained by Katsura (1962; 1963) its value is substantially less than the value obtained from the XY model. They suggested that this decrease was due to Pr hyperfine interaction namely $AS_{i1}^Z I_{i1}^Z$, and have been able to fit the experimental results, by treating this term in a mean-field approximation, which is a very poor approximation. In fact the effect of this term in the XY Hamiltonian is equivalent to a random field and then we treat it in the framework of CPA. The result obtained when using the exact parameters for the praseodymium ethyl sulphate gives the value of C/R equal to 0.315 which is very close to Katsura's result (0.325) and far away from the experimental one which is 0.250. We also try to find parameters which could fit the experimental results, however, the minimum peak obtained was 0.303, which is very large when compared to 0.250. This last calculation rules out the possibility of the hyperfine interaction being responsible for the anomalous behaviour of the specific heat.

The thermal conductivity is attributed to phonons in which case a scattering mechanism has to be found to damp the spin excitations. Although the hyperfine interaction does not explain the anomalous behaviour of the specific heat, it provides this mechanism. This is seen by calculating the thermal conductivity of the XY-chain in presence of the hyperfine term. We start by expressing the thermal conductivity obtained in the framework of Kubo theory in terms of the configurational average single particle Green function already calculated, following the approach of Flicker and Leath (1973). The results obtained for the praseodymium ethyl sulphate as a function of temperature (apart from a small region) are at least one order of magnitude smaller than the measurements. The effectiveness of this term in damping the spin excitations is due to the fact that the system is one-dimensional and then impurities affect the mean free path much more than in three dimensions.

We begin the fifth chapter by presenting a discussion of the Peierls transition (Peierls, 1955), looking at the simplest case which is the half-filled band case. Then we study two systems, an interacting electron-phonon system and an interacting spin-phonon system. Both models are analyzed in the light of the approximation presented in the first chapter.

In the first model which is exactly soluble in the framework of our approximation, we discuss the Peierls transition which is driven by a giant Kohn anomaly. We present initially a brief discussion of the mean-field solution, including the calculation of the transition temperature which is of course finite. Then we solve the model following the new approach and we get among

the important results a zero transition temperature. We also stress the importance of the elimination of the self-energy term which constitutes a spurious contribution. As pointed out by Pytte (1974) this contribution is included in the usual mean-field approximation which constitutes a major defect of this approximation as is the neglect of fluctuations. Besides the damped renormalized phonons there is an undamped branch whose existence depends on the coupling constant and on temperature. As the coupling constant becomes weaker or the temperature increases this mode moves towards the band. This analysis is derived from the properties of the real and imaginary parts of the phonon propagator as a function of energy. Finally we mention the possibility of inclusions of weak interactions between chains in such a way that the model could be exactly solved. Although this model of course describes the behaviour of quasi-one-dimensional systems, which is the final aim of the whole study, we restrict all the calculations to the one-dimensional case.

The second model is a spin-phonon system and in this case the softening of the phonon mode corresponds to an ordered antiferromagnetic state. The system is chosen in such a way that its relevant properties are expressed in terms of the longitudinal spin Green functions calculated in the transverse Ising model. These Green functions are obviously calculated from the correlation functions discussed in the third chapter. Given the impossibility of calculating these functions at any temperature we use the high temperature result obtained. Naturally no critical behaviour is

going to be observed and the system is studied for sake of completeness and to get some information about the excitations. The real and imaginary parts of the phonon Green function are presented for various coupling constants. The results show clearly that at this temperature limit the renormalized modes are essentially the unperturbed phonon modes which are of course undamped, and in order to see any effect we had to consider lower temperatures.

Finally the main results obtained are summarized and presented in the final chapter.

Chapter 1

The Coupled Spin-phonon and Electron-phonon systems

In this chapter we present a basic approximation which allows us to decouple the equations of motion of Green Functions for spin-phonon and electron-phonon systems when the coupling is linear in displacement. These types of Hamiltonian are used in the description of several systems, and we will be interested in the so-called Peierls transitions (Peierls; 1955). We also present the Green function method which is the basic formalism that we will use throughout this work.

1.1 The Green Function Method

Although this method is very well known we will present the basic definitions in order to establish the notation. It has been discussed in detail by Zubarev (1960), and a more recent account has been given for instance by Parry (1973). Before we introduce the technique, we want to make clear that unless explicitly written $\hbar$ will be assumed equal to 1.

The time-temperature dependent Green functions most widely used are the so-called causal, retarded and advanced, which are defined as:

$$G_c^{AB}(t-t') = \langle\langle A(t); B(t') \rangle\rangle_c = \begin{cases} -i \langle A(t) B(t') \rangle & t > t' \\ -i \epsilon \langle B(t') A(t) \rangle & t' > t \end{cases} \quad (1.1)$$

$$G_r^{AB}(t-t') = \langle\langle A(t); B(t') \rangle\rangle_r = -i \theta(t-t') \langle [A(t), B(t')]_\epsilon \rangle, \quad (1.2)$$

$$G_a^A(t-t') = \langle\langle A(t); B(t') \rangle\rangle_a = i \theta(t-t') \langle [A(t), B(t')]_\epsilon \rangle \quad , \quad (1.3)$$

where A and B are arbitrary operators in the Heisenberg representation, $\langle \rangle$ denotes the thermal average in the grand-canonical ensemble, and $[A, B]_\epsilon$ is defined as:

$$[A, B]_\epsilon = AB - \epsilon BA \quad (1.4)$$

with $\epsilon = \pm 1$, depending on our choice, and $\theta(t)$ is the usual step function

$$\theta(t) = \begin{cases} 0 & t < 0 \\ 1 & t > 0 \end{cases} \quad (1.5)$$

The Green functions defined in eqs. (1.1), (1.2) and (1.3) satisfy the same equation of motion, which is given by:

$$\begin{aligned} i \frac{d}{dt} \langle\langle A(t); B(t') \rangle\rangle &= \delta(t-t') \langle [A(t), B(t')]_\epsilon \rangle \\ &+ \langle\langle [A(t), \mathcal{H}]_\epsilon; B(t') \rangle\rangle \quad , \end{aligned} \quad (1.6)$$

where

$$\mathcal{H} = H - \mu N \quad , \quad (1.7)$$

and where H is the Hamiltonian, N the total number of particle operator, and μ the chemical potential. In eq. (1.6) we have dropped the labels c, r and a for simplicity. The solution of eq. (1.6) will lead to an infinite set of coupled equations which can only be solved approximately. Introducing in eq. (1.6) the Fourier transform

$$\langle\langle A(t); B(t') \rangle\rangle = \frac{1}{2\pi} \int_{-\infty}^{\infty} \langle\langle A; B \rangle\rangle_{\omega} e^{-i\omega(t-t')} d\omega, \quad (1.8)$$

we obtain

$$\omega \langle\langle A; B \rangle\rangle_{\omega} = \langle [A, B]_{\epsilon} \rangle + \langle\langle [A, \mathcal{H}]_{+1}; B \rangle\rangle_{\omega}, \quad (1.9)$$

in which form the equation of motion method is used. The Fourier transform, $\langle\langle A; B \rangle\rangle_{\omega}$, satisfies the important property

$$\langle\langle A; B \rangle\rangle_{\omega} = \epsilon \langle\langle B; A \rangle\rangle_{-\omega}. \quad (1.10)$$

The correlation functions can be related straightforwardly to these functions, although most calculations are done using the retarded and the advanced Green functions.

The Green functions can also be calculated using diagrammatic expansions. This technique is discussed in detail by Parry (1973).

1.2 The Decoupling Scheme

We will start by considering a general type of Hamiltonian which can be used to describe systems which undergo Peierls transition (Peierls, 1955) or structural transitions (Gehring and Gehring, 1975). We will restrict the discussion to the one-dimensional case. However, as will become clear during the calculations, the result is valid to any dimensionality.

The difficulty in finding reasonable approximations to deal with one-dimensional systems is that there are large fluctuations which cannot be treated correctly in the framework of the mean field approximation. The effect of the fluctuations in one- and two-dimensional magnetic systems has been studied recently in the review by Hone and Richards (1974).

Although the solution is not known, we do know that one-dimensional systems, where the interaction between the particles is short ranged, can develop long range order only at $T = 0^{\circ}\text{K}$ (Landau and Lifchitz, 1967). This is the basic result to be achieved by the proposed approximation, which contains the one-dimensional character.

In the approximation we are going to discuss, although we do not solve the problem, we are able to express it in a more tractable form. All the Green functions are expressed in terms of an electron (or spin) Green function calculated in an effective Hamiltonian. Provided that this function is calculated exactly we can get the correct critical temperature.

We will consider initially the case where electrons interact with phonons through a linear interaction in displacement. The simplest form in which this Hamiltonian is expressed is the so-called Frölich Hamiltonian, given by:

$$H = \sum_k \epsilon_k c_k^+ c_k + \sum_q \omega_q a_q^+ a_q + \sum_{kq} V(q) c_k^+ c_{k-q} (a_q + a_{-q}^+) , \quad (1.11)$$

where c 's and a 's denote creation and annihilation operators for the electronic Bloch states, of energy ϵ_K , and the unperturbed longitudinal phonons of frequencies ω_q , respectively. The mean-field solution of Hamiltonian (1.11) has been obtained by several authors, (Rice and Strässler, 1973; Allender et al., 1974; Horowitz et al., 1974), and as expected they have found a finite transition temperature. There is associated with the transition a softening of the phonon mode of wave vector $\frac{\pi}{a}$ (a - lattice parameter).

The most general Hamiltonian where phonons are coupled to spins through a linear interaction in displacements can be written as (Madhukar, 1975):

$$H = \sum_K \epsilon_K c_K^\dagger c_K + \sum_q \omega_q a_q^\dagger a_q + \sum_{K,q} V(q,K) c_K^\dagger c_{K-q} (a_q + a_{-q}^\dagger) \quad , \quad (1.12)$$

where $V(q,K)$ satisfies the property

$$V^*(K,q) = V(-q, K-q) \quad . \quad (1.13)$$

The first step in treating Hamiltonian (1.12) is to introduce the new operators γ 's defined as:

$$\gamma_q = a_q + \frac{\beta_q}{\omega_q} \quad , \quad (1.14)$$

where

$$\beta_q = \sum_K V(K,q) c_K^\dagger c_{K+q} \quad . \quad (1.15)$$

It should be noted that the operators defined in eq. (1.14) are similar to the shifted phonon operators introduced by Elliott et al. (1972) in the study of the Jahn-Teller effect. In this more general case, where V depends on k and q , the β 's do not commute and consequently the γ 's are not boson operators.

Putting together eqs. (1.13) and (1.15) we obtain:

$$\beta_{-q}^+ = \beta_q \quad . \quad (1.16)$$

Introducing the γ -operators in Hamiltonian (1.12), and using eqs. (1.15) and (1.16) we obtain:

$$H = \sum_k \mathcal{E}_k c_k^+ c_k + \sum_q \omega_q \gamma_q^+ \gamma_q - \sum_q \frac{\beta_q \beta_q}{\omega_q} \quad . \quad (1.17)$$

The Hamiltonian as shown in the previous equation is composed of two parts, one of these being the effective electron Hamiltonian

$$H_{eff} = \sum_k \mathcal{E}_k c_k^+ c_k - \sum_q \frac{\beta_q \beta_q}{\omega_q} \quad , \quad (1.18)$$

and the other term corresponding to the boson-like excitations

$$H' = \sum_q \omega_q \gamma_q^+ \gamma_q \quad . \quad (1.19)$$

Obviously the problem is by no means solved, since these two parts of the Hamiltonian do not commute.

Let us calculate the commutator Green function defined by

$$G_q = \langle\langle \gamma_q^+ \gamma_{-q}^+ ; \gamma_q^+ + \gamma_{-q} \rangle\rangle \quad . \quad (1.20)$$

Using eq. (1.9) we get:

$$\omega G_q = \langle [\gamma_q + \gamma_q^+, \gamma_q^+ + \gamma_{-q}] \rangle + \langle\langle [\gamma_q + \gamma_q^+, H]; \gamma_q^+ + \gamma_{-q} \rangle\rangle. \quad (1.21)$$

From eq. (1.14) we have:

$$\gamma_q + \gamma_{-q}^+ = a_q + a_{-q}^+ + \frac{2\beta_q}{\omega_q}, \quad (1.22)$$

and then substituting this in eq. (1.21) we obtain:

$$\begin{aligned} \omega G_q = & \frac{2}{\omega_q} \langle [\beta_q, \gamma_q^+ + \gamma_{-q}] \rangle + \frac{2}{\omega_q} \langle\langle [\beta_q, H]; \gamma_q^+ + \gamma_{-q} \rangle\rangle \\ & + \omega_q \langle\langle \gamma_q - \gamma_{-q}^+; \gamma_q^+ + \gamma_{-q} \rangle\rangle. \end{aligned} \quad (1.23)$$

Defining

$$\bar{G}_q = \langle\langle \gamma_q - \gamma_{-q}^+; \gamma_q^+ + \gamma_{-q} \rangle\rangle, \quad (1.24)$$

and making the identification

$$\begin{aligned} \omega \langle\langle \beta_q; \gamma_q^+ + \gamma_{-q} \rangle\rangle \equiv \omega F_q = & \langle [\beta_q, \gamma_q^+ + \gamma_{-q}] \rangle \\ & + \langle\langle [\beta_q, H]; \gamma_q^+ + \gamma_{-q} \rangle\rangle, \end{aligned} \quad (1.25)$$

we can write eq. (1.23) in the form:

$$\omega G_q = \omega_q \bar{G}_q + \frac{2\omega}{\omega_q} F_q. \quad (1.26)$$

Similarly we get:

$$\omega \bar{G}_q = 2 + \omega_q G_q \quad . \quad (1.27)$$

To solve the system composed of eqs. (1.26) and (1.27) we have to consider higher order Green functions, which means we need to consider the equation of motion of F_q . Before we follow this procedure we will get other exact relations between Green functions which will be used later on. Let us consider first the Green function:

$$\bar{F}_q = \langle\langle \gamma_q^+ + \gamma_{-q} ; \beta_q \rangle\rangle \quad , \quad (1.28)$$

which satisfies the equation

$$\begin{aligned} \omega \bar{F}_q &= \frac{2}{\omega_q} \langle [\beta_{-q}, \beta_q] \rangle + \frac{2}{\omega_q} \langle\langle [\beta_{-q}, H] ; \beta_q \rangle\rangle \\ &\quad + \omega_q \langle\langle \gamma_{-q} - \gamma_q^+ ; \beta_q \rangle\rangle \quad . \end{aligned} \quad (1.29)$$

Using the result

$$\omega \langle\langle \beta_{-q} ; \beta_q \rangle\rangle = \langle [\beta_{-q}, \beta_q] \rangle + \langle\langle [\beta_{-q}, H] ; \beta_q \rangle\rangle \quad (1.30)$$

in eq. (1.29) we get:

$$\omega \bar{F}_q = \frac{2}{\omega_q} \langle\langle \beta_{-q} ; \beta_q \rangle\rangle + \omega_q \langle\langle \gamma_{-q} - \gamma_q^+ ; \beta_q \rangle\rangle \quad . \quad (1.31)$$

Similarly we obtain:

$$\omega \langle\langle \gamma_{-q} - \gamma_q^+ ; \beta_q \rangle\rangle = \omega_q \bar{F}_q \quad (1.32)$$

and from the last equations

$$\overline{F}_q(\omega) = \frac{2\omega^2}{\omega_q(\omega^2 - \omega_q^2)} \langle\langle \beta_q ; \beta_q \rangle\rangle . \quad (1.33)$$

From eq. (1.10) we have

$$\overline{F}_q(\omega) = F_q(-\omega) \quad (1.34)$$

and finally we get

$$F_q(\omega) = \frac{2\omega^2}{\omega_q(\omega^2 - \omega_q^2)} \langle\langle \beta_q ; \beta_{-q} \rangle\rangle . \quad (1.35)$$

Then using previous equation and eqs. (1.26) and (1.27), the following results are obtained:

$$G_q = \frac{2\omega_q}{\omega^2 - \omega_q^2} + \frac{2\omega^2}{\omega_q(\omega^2 - \omega_q^2)} F_q , \quad (1.36)$$

and

$$G_q = \frac{2\omega_q}{\omega^2 - \omega_q^2} + \frac{4\omega^4}{\omega_q^2(\omega^2 - \omega_q^2)^2} \langle\langle \beta_q ; \beta_{-q} \rangle\rangle . \quad (1.37)$$

Of course to solve the problem, as has been already mentioned, we have to consider the equation of motion of F_q , and then to impose some approximation in order to decouple the system. Therefore we have

$$\begin{aligned} \omega F_q = & \frac{2}{\omega_q} \langle [\beta_q, \beta_{-q}] \rangle + \langle\langle [\beta_q, H_{eff}] ; \gamma_q^+ + \gamma_{-q} \rangle\rangle \\ & + \langle\langle [\beta_q, \sum_{q'} \omega_{q'} \gamma_{q'}^+ \gamma_{q'}] ; \gamma_q^+ + \gamma_{-q} \rangle\rangle . \end{aligned} \quad (1.38)$$

To decouple this system we will use the R.P.A. only in the coupled term, which is the last term of eq. (1.38), and we will consider that the average of γ 's is equal to zero. This is an extension of the procedure adopted by Young (1975) in the study of the Jahn-Teller effect. Since part of the system is being treated exactly, certainly the result that will emerge will be better than the usual mean-field result. Introducing this procedure in eq. (1.38) we obtain:

$$\omega F_q = \langle [\beta_q, \beta_{-q}] \rangle \left(\frac{2}{\omega_q} + G_q \right) + \langle \langle [\beta_q, H_{\text{eff}}]; \gamma_q^+ + \gamma_{-q} \rangle \rangle, \quad (1.39)$$

where we have used

$$\langle [\beta_q, \beta_{-q}] \rangle = \delta_{q,-q} \langle [\beta_q, \beta_{-q}] \rangle. \quad (1.40)$$

Continuing the process by writing the equation of motion of the $\langle \langle [\beta_q, H_{\text{eff}}]; \gamma_q^+ + \gamma_{-q} \rangle \rangle$, and applying the same decoupling scheme we get:

$$\begin{aligned} \omega \langle \langle [\beta_q, H_{\text{eff}}]; \gamma_q^+ + \gamma_{-q} \rangle \rangle &= \langle [\beta_q, H_{\text{eff}}], \beta_{-q} \rangle \left(\frac{2}{\omega_q} + G_q \right) \\ &+ \langle \langle [\beta_q, H_{\text{eff}}], H_{\text{eff}} \rangle \rangle; \gamma_q^+ + \gamma_{-q} \rangle \rangle. \end{aligned} \quad (1.41)$$

The eqs. (1.39) and (1.41) are identical to the equations obtained for the Green function $\langle \langle \beta_q; \beta_{-q} \rangle \rangle_{\text{eff}}$, which is calculated considering only the effective Hamiltonian H_{eff} , apart from the inhomogeneous term which is multiplied by the constant $\frac{2}{\omega_q} + G_q$. Since the systems are both linear we can then write:

$$F_q = \langle \langle \beta_q; \beta_{-q} \rangle \rangle_{\text{eff}} \left(\frac{2}{\omega_q} + G_q \right). \quad (1.42)$$

Strictly speaking this result is only true if all the equations of the infinite set obtained after eq. (1.41) have the inhomogeneous term multiplied by $\frac{2}{\omega_q} + G_q$. In order to prove this result let us consider the operator O_q defined as:

$$O_q = [[\beta_q, H_{eff}] \dots] H_{eff}] \quad . \quad (1.43)$$

The equation of motion of $\langle\langle O_q; \gamma_q^+ + \gamma_{-q} \rangle\rangle$ is

$$\begin{aligned} \omega \langle\langle O_q; \gamma_q^+ + \gamma_{-q} \rangle\rangle &= \langle [O_q, \beta_q] \rangle \frac{2}{\omega_q} + \langle\langle [O_q, H_{eff}]; \gamma_q^+ + \gamma_{-q} \rangle\rangle \\ &+ \sum_{q'} \langle\langle [O_q, \omega_{q'} \gamma_{q'}^+ \gamma_{q'}]; \gamma_q^+ + \gamma_{-q} \rangle\rangle \quad . \end{aligned} \quad (1.44)$$

Using the decoupling scheme in the last term we get:

$$\begin{aligned} \sum_{q'} \langle\langle [O_q, \omega_{q'} \gamma_{q'}^+ \gamma_{q'}]; \gamma_q^+ + \gamma_{-q} \rangle\rangle &\cong \\ \langle\langle \sum_{q'} \langle [O_q, \beta_{q'}] \rangle \gamma_{q'}^+ + \sum_{q'} \langle [O_q, \beta_{q'}] \rangle \gamma_{q'}; \gamma_q^+ + \gamma_{-q} \rangle\rangle \quad , \end{aligned} \quad (1.45)$$

which can be written as

$$\sum_{q'} \langle\langle [O_q, \omega_{q'} \gamma_{q'}^+ \gamma_{q'}]; \gamma_q^+ + \gamma_{-q} \rangle\rangle \cong \langle [O_q, \beta_q] \rangle G_q \quad , \quad (1.46)$$

where we have used the result

$$\langle [O_q, \beta_{q'}] \rangle = \langle [O_q, \beta_q] \rangle \delta_{q',q} \quad , \quad (1.47)$$

which is obtained using translational symmetry. Therefore we have

$$\omega \langle\langle O_q ; \gamma_q^+ + \gamma_{-q} \rangle\rangle = \langle [O_q, \beta_q] \rangle \left(\frac{2}{\omega_q} + G_q \right) + \langle\langle [O_q, H_{eff}] ; \gamma_q^+ + \gamma_{-q} \rangle\rangle , \quad (1.48)$$

and obviously this proves that eq. (1.42) is exact in our approximation.

From eqs. (1.42) and (1.36) we get:

$$G_q = \frac{G_q^o \left[1 + \frac{2\omega^2}{\omega_q^3} \langle\langle \beta_q ; \beta_{-q} \rangle\rangle_{eff} \right]}{1 - G_q^o \frac{\omega^2}{\omega_q^2} \langle\langle \beta_q ; \beta_{-q} \rangle\rangle_{eff}} , \quad (1.49)$$

where

$$G_q^o = \frac{2\omega_q}{\omega^2 - \omega_q^2} , \quad (1.50)$$

and using this result we obtain from eq. (1.37)

$$\langle\langle \beta_{-q} ; \beta_q \rangle\rangle = \frac{\langle\langle \beta_q ; \beta_{-q} \rangle\rangle_{eff}}{1 - G_q^o \frac{\omega^2}{\omega_q^2} \langle\langle \beta_q ; \beta_{-q} \rangle\rangle_{eff}} . \quad (1.51)$$

The real displacement-displacement Green function, namely

$$\tilde{G}_q = \langle\langle a_{-q}^+ + a_q ; a_q^+ + a_{-q} \rangle\rangle , \quad (1.52)$$

is then obtained by using eqs. (1.22), (1.42), (1.49) and (1.51):

$$\tilde{G}_q = \frac{G_q^0 \left(1 - \frac{2}{\omega_q} \langle\langle \beta_q; \beta_{-q} \rangle\rangle_{\text{eff}}\right)}{1 - G_q^0 \frac{\omega_q^2}{\omega_q^2} \langle\langle \beta_q; \beta_{-q} \rangle\rangle_{\text{eff}}} . \quad (1.53)$$

The poles of this Green function give the excitations of the system, which are

$$\omega^2 = \frac{\omega_q^2}{1 - \frac{2}{\omega_q} \langle\langle \beta_q; \beta_{-q} \rangle\rangle_{\text{eff}}} . \quad (1.54)$$

It is clear from eq. (1.54) that a phonon mode will become soft only when $\langle\langle \beta_q; \beta_{-q} \rangle\rangle_{\text{eff}}$ diverges, and provided this function is calculated exactly this will happen only at $T = 0^\circ\text{K}$. This is indeed a very interesting result, which allows us to decouple the electrons from the phonons and gives the correct answer. Naturally it is not at all easy to calculate $\langle\langle \beta_q; \beta_{-q} \rangle\rangle_{\text{eff}}$, however, as pointed out at the beginning, the problem has been put in a more tractable form.

If we consider the mean-field result for $\langle\langle \beta_q; \beta_{-q} \rangle\rangle_{\text{eff}}$, namely

$$\langle\langle \beta_q; \beta_{-q} \rangle\rangle_{\text{eff}} = \frac{g_q}{1 + \frac{2g_q}{\omega_q}} \quad (1.55)$$

where

$$g_q = \sum_k \frac{(n_k - n_{k-q}) V(k-q, q) V(k, -q)}{\omega + \epsilon_k - \epsilon_{k-q}} , \quad (1.56)$$

we get:

$$\tilde{G}_q = \frac{2\omega_q}{\omega^2 - \omega_q^2 - 2g_q \omega_q} , \quad (1.57)$$

which is equal to the R.P.A. result obtained using the full Hamiltonian (1.12).

Provided $\ll \beta_q; \beta_{-q} \gg_{\text{eff}}$ is calculated exactly, the Green function $\ll \beta_q; \beta_{-q} \gg$, eq. (1.51), will diverge at $T = 0^\circ\text{K}$ and this means that our approximation predicts the formation of a charge-density wave (CDW). Although the denominator of eq. (1.49) goes to zero, the Green function G_q does not diverge. This is not surprising, since it is the displacement response function which should diverge. This is clear in the case solved exactly (Pytte, 1974), where the G_q is equal to the unperturbed Green function G_q^0 .

The results obtained up to now can be used in the case where we have the simpler Hamiltonian (1.11), as well as when we consider the spin-phonon Hamiltonian

$$H = H_s + \sum_q V_q (a_q + a_{-q}^+) S_q^x + \sum_q \omega_q a_q^+ a_q, \quad (1.58)$$

where H_s is the spin-dependent part of the Hamiltonian. In the electron-phonon case the operator γ 's are defined as:

$$\gamma_q = a_q + \frac{V_{-q}}{\omega_q} \rho_q, \quad (1.59)$$

where ρ_q is usual density operator

$$\rho_q = \sum_k c_k^+ c_{k+q}, \quad (1.60)$$

and in the spin-phonon case

$$\gamma_q = a_q + \frac{V_{-q}}{\omega_q} S_{-q}^x, \quad (1.61)$$

where in both cases the γ 's are the so-called shifted phonon operator, since they are boson operators. In order to get the Green functions in these cases we have only to consider in the previous expressions the substitution

$$\langle\langle \beta_q ; \beta_{-q} \rangle\rangle_{\text{eff}} \longrightarrow V_q V_{-q} \langle\langle \rho_q ; \rho_{-q} \rangle\rangle_{\text{eff}} \quad (1.62)$$

in the first case, and

$$\langle\langle \beta_q ; \beta_{-q} \rangle\rangle_{\text{eff}} \longrightarrow V_q V_{-q} \langle\langle S_{-q}^x ; S_q^x \rangle\rangle \quad (1.63)$$

in the second case. Therefore $\tilde{G}_q$ is given respectively by

$$\tilde{G}_q = \frac{G_q^0 \left(1 - \frac{2V_q V_{-q}}{\omega_q} \langle\langle \rho_q ; \rho_{-q} \rangle\rangle_{\text{eff}} \right)}{1 - G_q^0 \frac{\omega^2}{\omega_q^2} V_q V_{-q} \langle\langle \rho_q ; \rho_{-q} \rangle\rangle_{\text{eff}}} , \quad (1.64)$$

and

$$\tilde{G}_q = \frac{G_q^0 \left(1 - \frac{2V_q V_{-q}}{\omega_q} \langle\langle S_{-q}^x ; S_q^x \rangle\rangle_{\text{eff}} \right)}{1 - G_q^0 \frac{\omega^2}{\omega_q^2} V_q V_{-q} \langle\langle S_q^x ; S_{-q}^x \rangle\rangle_{\text{eff}}} , \quad (1.65)$$

where the effective Hamiltonians are given respectively by

$$H_{\text{eff}} = \sum_k \mathcal{E}_k c_k^+ c_k - \sum_q \frac{V_q V_{-q}}{\omega_q} \rho_q \rho_{-q} , \quad (1.66)$$

and

$$H_{\text{eff}} = H_S - \sum_q \frac{V_q V_{-q}}{\omega_q} S_q^x S_{-q}^x . \quad (1.67)$$

As pointed out by Elliott et al. (1972), when considering the interaction between electrons (or spins) generated by transformation (1.59) [or (1.61)], namely $\frac{V_q V_{-q}}{\omega_q}$, we have to subtract the self-energy, so the effective interaction is

$$v_q = \frac{V_q V_{-q}}{\omega_q} - \frac{1}{N} \sum_q \frac{V_q V_{-q}}{\omega_q} . \quad (1.68)$$

As we stressed at the beginning, we have been able to express all relevant properties of the interacting electron-phonon (or spin-phonon) system in terms of an electronic Green function and/or spin Green function. A rather similar result has been obtained by Pytte (1974), when considering an exactly soluble model.

Chapter 2

The Impure Anisotropic XY-chain in a Transverse Magnetic Field

In this chapter we present formal results concerning diagonalization of the Hamiltonian, as well as calculation of the time-dependent correlation functions. The one-impurity case is solved when the system is isotropic. Finally we present a calculation of the thermal flux operator in the isotropic case which will be used later in the calculation of thermal conductivity within the framework of Kubo theory.

2.1 The Hamiltonian

We start by writing the Hamiltonian in its more general form:

$$H = \sum_{j=1}^N J_j \left\{ (1+\gamma) S_j^x S_{j+1}^x + (1-\gamma) S_j^y S_{j+1}^y \right\} - \sum_{j=1}^N h_j S_j^z, \quad (2.1)$$

where

$$S_{-1}^v \equiv S_{N+1}^v, \quad v = x, y, z, \quad (2.2)$$

and S_i^v are $1/2$ the Pauli spin matrices.

Introducing the lowering and raising operators (Lieb, Schultz and Mattis, 1961)

$$a_j^+ = S_j^x + i S_j^y, \quad a_j = S_j^x - i S_j^y \quad (2.3)$$

in terms of which the Pauli spin operators are

$$S_j^x = \frac{a_j^+ + a_j}{2}, \quad S_j^y = \frac{a_j^+ - a_j}{2i}, \quad S_j^z = a_j^+ a_j - \frac{1}{2}, \quad (2.4)$$

we get

$$H = \frac{1}{2} \sum_{j=1}^N J_j [a_j^+ a_{j+1} + a_{j+1}^+ a_j + \gamma (a_j^+ a_{j+1}^+ + a_{j+1} a_j)] - \sum_{j=1}^N h_j (a_j^+ a_j - \frac{1}{2}). \quad (2.5)$$

Then, if we introduce the Jordan-Wigner transformation

(Jordan and Wigner, 1928) defined by:

$$a_j^+ = e^{i\pi \sum_{l=1}^{j-1} c_l^+ c_l} c_j^+, \quad a_1^+ = c_1^+, \quad (2.6)$$

$$a_j = e^{-i\pi \sum_{l=1}^{j-1} c_l^+ c_l} c_j, \quad a_1 = c_1, \quad (2.7)$$

where c 's are fermion operators, the Hamiltonian (2.5) is written as:

$$H = H^+ P^+ + H^- P^-, \quad (2.8)$$

where P^+ and P^- are given by:

$$P^\pm = \frac{1}{2} (1 \pm P) = \frac{1}{2} \left(1 \pm e^{i\pi \sum_{l=1}^N c_l^+ c_l} \right), \quad (2.9)$$

and H^+ and H^- are:

$$H^\pm = \frac{1}{2} \sum_{j=1}^{N-1} J_j (c_j^+ c_{j+1} + \gamma c_j^+ c_{j+1}^+ + h.c.) - \sum_{j=1}^N h_j (c_j^+ c_j - \frac{1}{2}) \mp \frac{J_N}{2} (c_N^+ c_1 + \gamma c_N^+ c_1^+ + h.c.). \quad (2.10)$$

As we see the Hamiltonian H^- and H^+ differ by a boundary term

$$H^- - H^+ \equiv B = \sum_N (c_N^+ c_1 + \gamma c_N^+ c_1^+ + h.c.) . \quad (2.11)$$

The above result reduces to that of McCoy et al. (1971) when all J 's and h 's are equal.

The operator P defined in eq. (2.9) satisfies the relations

$$[P, H] = [P, H^+] = 0 , \quad (2.12)$$

$$\{P, c_j\} = \{P, c_j^+\} = 0 , \quad (2.13)$$

$$P^2 = I , \quad (2.14)$$

where the notations $[]$ and $\{ \}$ stand for commutator and anti-commutator, respectively.

Using eqs. (2.9), (2.12), (2.13) and (2.14) we get immediately (Capel et al., 1974) the results:

$$[P^\pm, H] = [P^\pm, H^\pm] = 0 , \quad (2.15)$$

$$(P^\pm)^2 = P^\pm , \quad P^+ P^- = P^- P^+ = 0 , \quad (2.16)$$

$$f(H) = f(H^+) P^+ + f(H^-) P^- , \quad (2.17)$$

where $f(z)$ is an analytic function of z .

Since the parity operator P commutes with the total Hamiltonian as well as with H^+ and H^- , the eigenstates of these Hamiltonians have definite parity. On the other hand, by definition, P^+ and P^- are projection operators for states of positive and negative parity respectively. Therefore, putting these results together with eq. (2.8) we conclude that the eigenstates of the total Hamiltonian are the eigenstates of H^+ with positive parity, and the eigenstates of H^- with negative parity. The Hamiltonians H^+ and H^- do not commute, and consequently they have to be diagonalized separately. This is possible due to the decomposition shown in eq. (2.8) which allows us to use two different canonical transformations.

As we can see, even in the presence of impurities the solution of the spin 1/2 XY-model in a transverse field is reduced, as in the pure case, to a diagonalization of bilinear forms of creation and annihilation fermion operators. This diagonalization has been discussed in great detail by Tyablikov (1967).

We will consider first of all very briefly the diagonalization of the pure case, which has been treated in detail by McCoy et al. (1971) and Abraham (1972), and recently by Jha and Valatin (1973) using an algebraic approach. The main purpose of this procedure is to clarify notation. The important step is the imposition of boundary conditions on c operators, which should be anticyclic when diagonalizing H^+ and cyclic when diagonalizing H^- .

Defining the Fourier transform of c_j^+ as

$$c_j^+ = \frac{1}{\sqrt{N}} \sum_k e^{ik a_j} c_k^+ \quad , \quad (2.18)$$

where a is the lattice parameter, the boundary conditions imply that the allowed values of k are given by

$$k = \pm \frac{2\pi(n + 1/2)}{Na} , \quad (2.19)$$

in the anticyclic case, and by

$$k = \pm \frac{2\pi n}{Na} , \quad (2.20)$$

in the cyclic case, where n runs over integers from 0 to $N/2$ (N is assumed even for convenience). By introducing the Fourier transform in eq.(2.10), and the Bogoliubov-Valatin transformation (Bogoliubov, 1959; Valatin, 1961)

$$\beta_k = x_k c_k + y_k c_{k-k}^+ , \quad (2.21)$$

the inverse of which is given by

$$c_k = x_k^* \beta_k + y_k \beta_{-k}^+ , \quad (2.22)$$

we get

$$H^\pm = \sum_k E_k \left(\beta_k^\pm \beta_k - \frac{1}{2} \right) , \quad (2.23)$$

where

$$E_k = \sqrt{(J \cos ka - h)^2 + J^2 \gamma^2 \sin^2 ka} , \quad (2.24)$$

and the signs $+$ and $-$ in (2.23) hold for k 's given by eqs. (2.19) and (2.20), respectively. The x 's and y 's in eqs. (2.21) and (2.22) are given by:

$$x_k = \frac{i\gamma J \sin ka}{[2E_k(\bar{E}_k - E_k)]^{1/2}} \quad , \quad (2.25)$$

$$y_k = \left[\frac{E_k - \bar{E}_k}{2E_k} \right]^{1/2} \quad , \quad (2.26)$$

with

$$\bar{E}_k = J \cos ka - h \quad . \quad (2.27)$$

In the limiting isotropic case, namely $\gamma = 0$, we will consider E_k as:

$$E_k = J \cos ka - h \quad . \quad (2.28)$$

This means that we have abandoned in this case the particle-hole picture. The Fermi energy is assumed to be zero.

2.2 The Correlation Functions

From eqs. (2.4), (2.6), (2.7) and (2.13) we conclude immediately that

$$[P, S_j^z] = 0 \quad , \quad (2.29)$$

$$\{P, S_j^x\} = \{P, S_j^y\} = 0 \quad . \quad (2.30)$$

These results together with eq. (2.9) give

$$P^\pm S_j^x = S_j^x P^\mp \quad , \quad (2.31)$$

$$P^\pm S_j^y = S_j^y P^\mp \quad , \quad (2.32)$$

$$P^{\pm} S_j^z = S_j^z P^{\pm} \quad (2.33)$$

The results shown above are extremely important, and we will see that they are responsible for the fact that in some cases the boundary term B cannot be neglected in calculations of the correlation functions. This has been discussed recently by Capel et al. (1974), and it had been pointed out by McCoy et al. (1971).

In order to see this let us consider the time-dependent correlation function:

$$\langle S_j^z(t) S_l^z(0) \rangle = \frac{\text{Tr} \left(e^{-\beta H} e^{iHt} S_j^z e^{-iHt} S_l^z \right)}{\text{Tr} \left(e^{-\beta H} \right)} \quad (2.34)$$

where the notation Tr stands for trace, and H is the total Hamiltonian (eq. (2.8)).

Using eqs. (2.15), (2.16), (2.17) and (2.33) we get:

$$\langle S_j^z(t) S_l^z(0) \rangle = \frac{\text{Tr} \left(P^+ e^{-\beta H^+} e^{iH^+ t} S_j^z e^{-iH^+ t} S_l^z \right) + \text{Tr} \left(P^- e^{-\beta H^-} e^{iH^- t} S_j^z e^{-iH^- t} S_l^z \right)}{\text{Tr} \left(P^+ e^{-\beta H^+} \right) + \text{Tr} \left(P^- e^{-\beta H^-} \right)} \quad (2.35)$$

In the limit $N \rightarrow \infty$, Capel et al. (1974) have shown that the previous expression can be written as

$$\langle S_j^z(t) S_l^z(0) \rangle = \frac{\text{Tr} \left(e^{-\beta H} e^{iHt} S_j^z e^{-iHt} S_l^z \right)}{\text{Tr} \left(e^{-\beta H} \right)} \quad (2.36)$$

where the trace is calculated over the eigenstates of H^- . The above result is identical to the one obtained if we had neglected in the total Hamiltonian the boundary term B.

Let us consider now the time-dependent correlation:

$$\langle S_j^x(t) S_l^x(0) \rangle = \frac{\text{Tr} \left(e^{-\beta H^-} e^{iH^- t} S_j^x e^{-iH^- t} S_l^x \right)}{\text{Tr} \left(e^{-\beta H^-} \right)} . \quad (2.37)$$

Then using eqs. (2.15), (2.16), (2.17) and (2.31) we get

$$\langle S_j^x(t) S_l^x(0) \rangle = \frac{\text{Tr} \left(P^- e^{-\beta H^-} e^{iH^- t} S_j^x e^{-iH^- t} S_l^x \right) + \text{Tr} \left(P^+ e^{-\beta H^+} e^{iH^+ t} S_j^x e^{-iH^+ t} S_l^x \right)}{\text{Tr} \left(P^+ e^{-\beta H^+} \right) + \text{Tr} \left(P^- e^{-\beta H^-} \right)} \quad (2.38)$$

which in the thermodynamic limit can be written as (Capel et al., 1974):

$$\langle S_j^x(t) S_l^x(0) \rangle = \frac{\text{Tr} \left(e^{-\beta H^-} e^{iH^- t} S_j^x e^{-iH^- t} S_l^x \right)}{\text{Tr} \left(e^{-\beta H^-} \right)} , \quad (2.39)$$

where the trace is calculated over the eigenstates of H^- . Since the time evolution of S_j^x is given by H^- and H^+ , we cannot neglect the boundary term in the total Hamiltonian. As we will see in the next chapter, to neglect the boundary corresponds in fact to a very bad approximation. However, it should be noted that for the $t = 0$ case in eq. (2.39) we get the correct result, even when we neglect the boundary term.

2.3 The Isotropic Chain-One Impurity Case

The diagonalization of the Hamiltonian (2.10) in its more general form cannot be obtained in closed form. There are, however, approximate methods (Elliott et al. 1974; Yonezawa and Morigaki 1973) based on the one-impurity case which give very good results. Therefore we will consider the one-impurity problem, in particular the isotropic case, although the case with general anisotropy could be treated as well. We will make use of this result in chapter 4 when studying the thermal properties of some materials which exhibit one-dimensional behaviour in some range of temperature.

In order to define the problem we will consider that the second spin in the chain couples to its neighbours with an exchange constant J' , and to the magnetic field with a strength h' . Then the Hamiltonian H^- , eq. (2.10), is written as:

$$H = \frac{J}{2} \sum_{j=1}^N (c_j^+ c_{j+1} + h.c.) - h \sum_{j=1}^N (c_j^+ c_j - \frac{1}{2})$$

$$+ \frac{\Delta J}{2} (c_1^+ c_2 + c_2^+ c_3 + h.c.) - \Delta h (c_2^+ c_2 - \frac{1}{2}) \quad , \quad (2.40)$$

where

$$\Delta J = J' - J \quad , \quad \Delta h = h' - h \quad (2.41)$$

and we have considered $\gamma = 0$, and dropped the symbol $-$ for sake of simplicity. As we have already pointed out the only difference in the diagonalization of H^- and H^+ is the selection of different k 's. Considering the Fourier transform defined in eq. (2.18) we get:

$$H = \sum_k \epsilon_k c_k^\dagger c_k + \frac{\Delta J}{2N} \sum_{k,k'} (f_{k'}^* g_k + f_k g_{k'}^*) c_k^\dagger c_{k'} - \frac{\Delta h}{N} \sum_{k,k'} g_k g_{k'}^* c_k^\dagger c_{k'} + \frac{Nh}{2} + \frac{\Delta h}{2} \quad , \quad (2.42)$$

where

$$f_k = e^{2ika} \quad , \quad g_k = e^{ika} + e^{i3ka} \quad , \quad (2.43)$$

and ϵ_k defined as in eq. (2.27).

Although there are different methods for treating Hamiltonian (2.42) we will use the Green function technique discussed in chapter 1. This method has the advantage of giving the solution in a form suitable for extension to the many impurity case. A rather different approach has been adopted by Tjon (1970) in the study of the open isotropic chain with one impurity. Defining the anticommutator Green function

$$G_{kk'}(\omega) = \langle\langle c_k ; c_{k'}^\dagger \rangle\rangle \quad , \quad (2.44)$$

and using the equations of motion method we get after some algebraic manipulations the result:

$$G_{kk'}(\omega) = \frac{\delta_{kk'}}{\omega - \epsilon_k} + \frac{\frac{\Delta J}{2} (1 - \frac{\Delta J}{2} B) (\gamma_k \lambda_{k'}^* + \lambda_k \gamma_{k'}^*) + \left(\frac{\Delta J}{2}\right)^2 A \gamma_k \gamma_{k'}^* - \lambda_k \lambda_{k'}^* [\Delta h - \left(\frac{\Delta J}{2}\right)^2 C]}{N(\omega - \epsilon_k)(\omega - \epsilon_{k'}) \left[\left(1 - \frac{\Delta J}{2} B + \Delta h A\right) \left(1 - \frac{\Delta J}{2} B\right) - \left(\frac{\Delta J}{2} C - \Delta h B\right) \frac{\Delta J A}{2} \right]} \quad , \quad (2.45)$$

where

$$A = \frac{1}{N} \sum_k \frac{1}{\omega - \epsilon_k} \quad , \quad (2.46)$$

$$B = \frac{2}{N} \sum_k \frac{\cos Ka}{\omega - \varepsilon_k} \quad , \quad (2.47)$$

$$C = \frac{2}{N} \sum_k \frac{1 + \cos 2ka}{\omega - \varepsilon_k} \quad . \quad (2.48)$$

Eqs. (2.47) and (2.48) can be written in terms of A as:

$$B = -\frac{2}{J} + \frac{2(h+\omega)}{J} A \quad (2.49)$$

$$C = -\frac{4(\omega+J)}{J^2} + \frac{4(\omega+h)^2}{J^2} A \quad (2.50)$$

Using these results in eq. (2.45) we get

$$\begin{aligned} G_{kk'}(\omega) = & \frac{\delta_{kk'}}{\omega - \varepsilon_k} - \frac{1}{N(\omega - \varepsilon_k)(\omega - \varepsilon_{k'})D} \left\{ \left[\frac{\Delta J}{2} \left(1 + \frac{\Delta J}{J} \right) - \frac{(\Delta J)^2(h+\omega)}{2J} A \right] (\gamma_k \lambda_{k'}^* + \lambda_k \gamma_{k'}^*) + \right. \\ & \left. + \left(\frac{\Delta J}{2} \right)^2 A \gamma_k \gamma_{k'}^* - \lambda_k \lambda_{k'}^* \left[\Delta h + \left(\frac{\Delta J}{J} \right)^2 (\omega+h) - (\omega+h)^2 \left(\frac{\Delta J}{J} \right)^2 A \right] \right\} \quad (2.51) \end{aligned}$$

where

$$D = 1 + 2 \frac{\Delta J}{J} \left(1 + \frac{\Delta J}{2J} \right) + \left[\Delta h - 2 \frac{\Delta J}{J} \left(1 + \frac{\Delta J}{2J} \right) (h+\omega) \right] A \quad . \quad (2.52)$$

From this equation we obtain immediately that the T-matrix (Elliott et al. 1974) is given by:

$$\begin{aligned} T(k, k') = & \frac{1}{ND} \left\{ \left[\frac{\Delta J}{2} \left(1 + \frac{\Delta J}{J} \right) - \frac{(\Delta J)^2(h+\omega)}{2J} A \right] (\gamma_k \lambda_{k'}^* + \lambda_k \gamma_{k'}^*) + \right. \\ & \left. + \left(\frac{\Delta J}{2} \right)^2 A \gamma_k \gamma_{k'}^* - \lambda_k \lambda_{k'}^* \left[\Delta h + \left(\frac{\Delta J}{J} \right)^2 (\omega+h)^2 \left(\frac{\Delta J}{J} \right)^2 A \right] \right\} \quad (2.53) \end{aligned}$$

The poles of the T-matrix give the excitations of the system. The spectrum consists of a band plus a bound state. The bound states have been discussed recently by Vinikovetsky et al. (1973). This discussion is straightforward and we will not repeat. In the case of $\Delta J = 0$ this problem is almost identical to that of vibrations in a lattice when there is a mass defect, discussed by Elliott and Dawber (1963). However, the bound state in the spin case is always present.

One interesting limit is when $J' = 0$, which means that we have broken the chain. In this case the T-matrix reduces to

$$T(k, k') = \frac{-\frac{J}{2}(h+\omega)A(\gamma_k \lambda_{k'}^* + \lambda_k \gamma_{k'}^*) + \frac{J^2}{4}A\gamma_k \gamma_{k'}^* + (\omega+h)^2A\lambda_k \lambda_{k'}^* - (\omega+h')\lambda_k \lambda_{k'}^*}{N(h'+\omega)A} \quad (2.54)$$

This can be written as a sum of two terms, the first having a pole at $\omega = -h'$, and the second having poles at the ω 's which satisfy the equation $A = 0$. Since after breaking the chain we have to remove the boundary site, the pole $\omega = -h'$ is spurious as well as the first part of the T-matrix. Then the T-matrix in the case of an open chain is given by

$$T(k, k') = - \frac{\lambda_k \lambda_{k'}^*}{NA} \quad (2.55)$$

It should be noticed that the solution of the equation $A = 0$ consists simply of a band, and this coincides with that obtained by Lieb et al. (1961) for the case $h = 0$, and large N .

From all this we conclude that it is possible to study an open chain starting from a closed chain with one impurity, with the advantage of getting the results more easily, since they are expressed in terms of sums over k which become integrals in the limit $N \rightarrow \infty$.

2.4 Derivation of the Heat Flux Operator

The thermal conductivity in the framework of linear response theory developed by Kubo (1957), in the one-dimensional case can be written as (Flicker and Leath, 1973):

$$K = \lim_{\eta \rightarrow 0} \frac{1}{LT} \int_0^\infty dt e^{-\eta t} e^{i\omega t} \int_0^\infty d\lambda \langle Q(q=0) Q(q=0, t+i\lambda) \rangle , \quad (2.56)$$

where L is the size of the chain, and Q is the heat flux operator which is related to the energy-density operator $\mathcal{H}(x)$ through the continuity equation

$$\dot{\mathcal{H}}(x) + \frac{dQ(x)}{dx} = 0 , \quad (2.57)$$

which can also be written as

$$\frac{dQ(x)}{dx} = i [\mathcal{H}(x), H] . \quad (2.58)$$

Obviously the first step in calculating the thermal conductivity is to obtain the operator Q by solving eq. (2.57). When impurities are not present in the system this equation is easily solved by introducing the Fourier transforms:

$$Q(x) = \sum_q e^{iqx} Q_q \quad , \quad (2.59)$$

$$\mathcal{H}(x) = \sum_q e^{iqx} H_q \quad . \quad (2.60)$$

Substituting these transforms in eq. (2.57) we get (Kawasaki, 1963)

$$q Q_q = [H_q, H] \quad . \quad (2.61)$$

From this equation we immediately obtain $Q(q = 0)$ by taking the limit $q \rightarrow 0$ after having calculated the commutator on the right hand side. Unfortunately when impurities are present we can no more follow this procedure, which depends on the existence of translational symmetry. However, it is still possible to solve eq. (2.57) by using an approach introduced by Hardy (1963). The basic point consists in the definition of the energy-density operator as:

$$\mathcal{H}(x) = \sum_j H_j \Delta(x - x_j) \quad (2.62)$$

where $\Delta(x - x_j)$ is a well behaved function which has a peak at the point x_j and satisfies the relation

$$\int \Delta(x - x_j) dx = 1 \quad , \quad (2.63)$$

and H_j in the isotropic chain is given by:

$$H_j = J_j (S_j^x S_{j+1}^x + S_j^y S_{j+1}^y) - h_j S_j^z. \quad (2.64)$$

Substituting eqs. (2.62) and (2.64) in eq. (2.58) we get:

$$\begin{aligned} \frac{dQ(x)}{dx} = & \sum_j J_j J_{j-1} [\Delta(x-x_j) - \Delta(x-x_j+a)] S_{j+1}^x S_{j-1}^y S_j^z + \\ & + \sum_j J_j J_{j+1} [\Delta(x-x_j) - \Delta(x-x_j-a)] S_j^x S_{j+2}^y S_{j+1}^z + \\ & + \sum_j J_j h_{j+1} [\Delta(x-x_j) - \Delta(x-x_j-a)] S_j^x S_{j+1}^y + \\ & + \sum_j J_{j-1} h_j [\Delta(x-x_j) - \Delta(x-x_j+a)] S_j^x S_{j-1}^y \end{aligned} \quad (2.65)$$

Expanding $\Delta(x - x_j + a)$ and $\Delta(x - x_j - a)$ about the point $x - x_j$ and keeping only the linear term we get

$$\begin{aligned} \frac{dQ(x)}{dx} \cong & \sum_j [J_j J_{j+1} S_j^x S_{j+2}^y S_j^z - J_j J_{j-1} S_{j+1}^x S_{j-1}^y S_j^z + J_j h_{j+1} S_j^x S_{j+1}^y - \\ & - J_{j-1} h_j S_j^x S_{j-1}^y] a \frac{\partial}{\partial x} \Delta(x-x_j), \end{aligned} \quad (2.66)$$

and from this

$$\begin{aligned} Q = \int Q(x) dx = & \sum_j [J_j J_{j+1} S_j^x S_{j+2}^y S_j^z - J_j J_{j-1} S_{j+1}^x S_{j-1}^y S_j^z + \\ & + J_j h_{j+1} S_j^x S_{j+1}^y - J_{j-1} h_j S_j^x S_{j-1}^y] a. \end{aligned} \quad (2.67)$$

From the discussion presented in section 2.2 we conclude that in the calculation of the time-dependent correlation function $\langle Q(0) Q(t) \rangle$, the time evolution of Q is given by H^+ and H^- separately. This means that in its calculation the boundary term can be neglected in the thermodynamic limit. Finally using the Jordan-Wigner transformation we get

$$Q = \sum_j \frac{J_j J_{j+1}}{4i} a (c_j^+ c_{j+2} - c_{j+2}^+ c_j) + \sum_j \frac{J_j h_{j+1}}{4i} a (c_{j+1}^+ c_j - c_j^+ c_{j+1}).$$

(2.68)

Chapter 3

Dynamics of the Pure One-dimensional

Transverse Ising Model

In this chapter we propose an approximation to calculate the time-dependent longitudinal correlation function which overcomes the difficulties mentioned in the previous chapter. Although the result can be applied to the pure general case (any γ), we will look in detail only at the pure transverse Ising model ($\gamma = 1$), whose Hamiltonian obtained from eq. (2.1) is written as:

$$H = \sum_{j=1}^N 2J S_j^x S_{j+1}^x - \sum_{j=1}^N h S_j^z, \quad (3.1)$$

because in this case the approximation is better understood, and the result will be used afterwards in the study of coupled spin-phonon system. We also discuss some unsuccessful attempts to sort out the difficulties already mentioned.

3.1 The c-cyclic Approximation

As we have discussed, the calculation of the longitudinal time-dependent correlation function, namely $\langle S_j^x(t) S_\ell^x(0) \rangle$ presents great difficulties: These are of two different natures. The first one comes from the phase factor that appears when we express the spin operators in terms of fermion operators. It should be noticed that this difficulty is present even when calculating the static correlation functions. The second one, which is the most important, comes from the fact that the time evolution in the fermion representation is given by two different Hamiltonians.

Explicitly, $\langle S_j^x(t) S_\ell^x(0) \rangle$, as obtained in eq. (2.39), is given in the thermodynamic limit by:

$$\langle S_j^x(t) S_\ell^x(0) \rangle = \langle e^{iH\bar{t}} S_j^x e^{-iH^+t} S_\ell^x \rangle . \quad (3.2)$$

Given the impossibility of calculating the right hand side of the above equation exactly, the most natural approximation consists in substituting H^- for H^+ . This is the so called c-cyclic approximation (Mazur and Siskens, 1973; 1974) in which we write eq. (3.1) explicitly as:

$$\langle S_j^x(t) S_\ell^x(0) \rangle \cong \langle e^{iH\bar{t}} S_j^x e^{-iH^-t} S_\ell^x \rangle . \quad (3.3)$$

When we substitute H^- by H^+ , we then have the so called c-anti-cyclic approximation which of course gives the same result in the thermodynamic limit as the c-cyclic.

The calculation of the right hand side of eq. (3.3) will be performed by using the Green Function method discussed in the first chapter. Therefore, let us consider the anti-commutator Green function, $\langle\langle S_1^x; S_{1+n}^x \rangle\rangle$, which using eqs. (2.3), (2.6), (2.7), (2.18) and (2.22) can be written as:

$$\langle\langle S_1^x; S_{1+n}^x \rangle\rangle = \frac{1}{2\sqrt{N}} \sum_k e^{ik\alpha} (x_k + y_k) \langle\langle \beta_k^+ \beta_{-k}^+; S_{1+n}^x \rangle\rangle , \quad (3.4)$$

where x_k and y_k are given by eqs. (2.25) and (2.26), considering $\gamma = 1$. Using the equation of motion method, eq. (1.9), with H equal to H^- , given by eq. (2.23), we get:

$$\begin{aligned} \langle\langle S_1^x, S_{1+n}^x \rangle\rangle = & \frac{1}{2\sqrt{N}} \sum_k e^{ika} (x_k + y_k) \left[\frac{\omega \langle \{ \beta_k^+ + \beta_{-k}, S_{1+n}^x \} \rangle}{\omega^2 - E_k^2} + \right. \\ & \left. + \frac{E_k \langle \{ \beta_k - \beta_{-k}, S_{1+n}^x \} \rangle}{\omega^2 - E_k^2} \right] , \end{aligned} \quad (3.5)$$

which can be written as

$$\begin{aligned} \langle\langle S_1^x, S_{1+n}^x \rangle\rangle = & \frac{1}{2N} \sum_k \sum_{j=1}^N \frac{e^{ika} e^{-ika}}{\omega^2 - E_k^2} \left[\omega (x_k + y_k) (x_k^* + y_k) \langle \{ c_j^+ + c_j, S_{1+n}^x \} \rangle \right. \\ & \left. - E_k (x_k + y_k) (x_k^* - y_k) \langle \{ c_j^+ - c_j, S_{1+n}^x \} \rangle \right] , \end{aligned} \quad (3.6)$$

where we have used eq. (2.22) and the inverse of eq. (2.18). In order to calculate the averages in the previous equation we use the technique developed by Lieb et al. (1961), in which we use the operators

$$A_j = c_j^+ + c_j \quad (3.7)$$

and

$$B_j = c_j^+ - c_j . \quad (3.8)$$

These operators satisfy the relations

$$\{A_j, B_l\} = 0 \quad (3.9)$$

$$A_j^2 = I , \quad B_j^2 = -I , \quad (3.10)$$

$$\{A_j, A_l\} = \{B_j, B_l\} = 0 \quad \text{if } j \neq l . \quad (3.11)$$

Using eqs. (2.18) and (2.22) we immediately get the results

$$\langle A_j A_l \rangle = \delta_{j,l} \quad , \quad (3.12)$$

$$\langle B_j B_l \rangle = -\delta_{j,l} \quad , \quad (3.13)$$

$$G(n) \equiv \langle B_j A_l \rangle = \frac{1}{N} \sum_k \tanh \frac{\beta E_k}{2} \frac{\hbar \cos nka - J \cos(n+1)ka}{E_k} \quad (3.14)$$

where

$$n = j - l \quad . \quad (3.15)$$

Since S_{1+n}^x is written in terms of c operators as

$$S_{1+n}^x = e^{i\pi \sum_{\ell=1}^n c_{\ell}^+ c_{\ell}} \frac{(c_{1+n}^+ + c_{1+n})}{2} \quad , \quad (3.16)$$

it is easy to see that in terms of A's and B's this expression can be written as

$$S_{1+n}^x = \left(\prod_{\ell=1}^n A_{\ell} B_{\ell} \right) \frac{A_{n+1}}{2} \quad . \quad (3.17)$$

Then by using eq. (3.9) to (3.16) we get:

$$\langle \{ B_j, S_{1+n}^x \} \rangle = 0 \quad , \quad \text{for any } j \quad , \quad (3.18)$$

$$\langle \{ A_j, S_{1+n}^x \} \rangle = 0 \quad , \quad \text{if } j > n+1 \quad , \quad (3.19)$$

and

$$\langle \{ A_j, S_{1+n}^x \} \rangle = \langle A_{\ell} A_1 B_1 A_2 B_2 \dots A_n B_n A_{n+1} \rangle, \text{ if } j \leq n+1 \quad (3.20)$$

which can be written as:

$$\langle \{ A_j, S_{1+n}^x \} \rangle = (-1)^{j-1} M_{n+1}^j, \quad (3.21)$$

where M_{n+1}^j is the minor of the normal Toeplitz determinant (Hartwig and Fisher, 1969):

$$M = \begin{pmatrix} G(0) & G(-1) & . & . & . & G(-n) \\ G(1) & G(0) & . & . & . & . \\ . & . & . & . & . & . \\ . & . & . & . & . & . \\ G(n) & . & . & . & . & G(0) \end{pmatrix} \quad (3.22)$$

calculated with respect to the $(n+1)$ th row, j th column. Therefore by using eq. (3.18), (3.19) and (3.21), eq. (3.6) is written as:

$$\langle \langle S_1^x, S_{1+n}^x \rangle \rangle = \frac{1}{2N} \sum_k \sum_{j=1}^N \frac{e^{-ika(j-1)} \omega (-1)^{j-1} M_{n+1}^j}{\omega^2 - E_k^2}, \quad (3.23)$$

where we have also used the explicit expressions for x_K and y_K .

From previous equation we get after straightforward algebraic manipulations the final result:

$$\langle S_1^z(t) S_{1+n}^z(0) \rangle = \frac{1}{4N} \sum_k \sum_{j=1}^{n+1} \cos(j-1)Ka (-1)^{j-1} M_{n+1}^j \left[\cos E_k t - i \sin E_k t \tanh \beta \frac{E_k}{2} \right]. \quad (3.24)$$

The Toeplitz determinants appear in different contexts (Fischer and Hartwig, 1969) and have been used extensively in calculations of the correlation functions of the two-dimensional Ising model (McCoy and Wu, 1973), and of course in the calculation of the correlation functions of the XY-model in a transverse field

(Barouch and McCoy, 1971; Johnson and McCoy, 1971; McCoy et al., 1971). In fact, there is an equivalence between the static properties of XY-chain in a transverse field at $T = 0$, and the two-dimensional Ising model at finite T without field, as first pointed out by Pfeuty (1970) for the $\gamma = 1$ case, and later by Suzuki (1971) for any γ .

If in eq. (3.24) we consider the limit $h = 0$, we get:

$$\langle S_1^x(t) S_{1+n}^x(0) \rangle = \frac{(-1)^n}{4} \left(\tanh \frac{\beta J}{2} \right)^n (\cos Jt - i \sin Jt \tanh \frac{\beta J}{2}) \quad , \quad (3.25)$$

whereas the correct result is (McCoy and Wu, 1973)

$$\langle S_1^x(t) S_{1+n}^x(0) \rangle = \frac{(-1)^n}{4} \left(\tanh \frac{\beta J}{2} \right)^n \quad . \quad (3.26)$$

This has also been pointed out by Capel and Siskens (1975).

It is a very clear example, in a simple case of the importance of the boundary term B . Therefore, this approximation is very unsatisfactory and cannot be used to describe the dynamics of the real system.

3.2 The Decoupling Scheme Approximation

In this second attempt to overcome the already mentioned difficulties we propose a decoupling scheme that is more like the RPA type approximation. The basic idea consists in considering the correlation function $\langle S_j^Z(t) S_l^Z(0) \rangle$ (Tommet and Huber, 1975; Niemeijer, 1967), which can be calculated exactly and writing it down in the following form:

$$\langle S_j^z(t) S_\ell^z(0) \rangle = -4 \langle S_j^x(t) S_j^y(t) S_\ell^x(0) S_\ell^y(0) \rangle, \quad (3.27)$$

which is an exact result. Then we use the generalized Wick's theorem to decouple the right hand side of the above equation, which would be an exact calculation if the spins were fermions. This gives the result:

$$\begin{aligned} \langle S_j^z(t) S_\ell^z(0) \rangle &\cong \langle S_j^z \rangle^2 + 4 \langle S_j^x(t) S_\ell^x(0) \rangle \langle S_j^y(t) S_\ell^y(0) \rangle \\ &\quad - 4 \langle S_j^x(t) S_\ell^y(0) \rangle \langle S_j^y(t) S_\ell^x(0) \rangle, \end{aligned} \quad (3.28)$$

and is the basic and unique approximation. This equation can be transformed into a differential equation by using the equation of motion of S_j^x :

$$\dot{S}_j^x = h S_j^y, \quad (3.29)$$

which substituted in eq. (3.28) leads to the differential equation:

$$\ddot{f}_{j\ell}^{xx} - \left(\dot{f}_{j\ell}^{xx} \right)^2 = - \frac{h^2}{4} \left(- \langle S_j^z \rangle + f_{j\ell}^{zz} \right), \quad (3.30)$$

where

$$f_{j\ell}^{\alpha\alpha} = \langle S_j^\alpha(t) S_\ell^\alpha(0) \rangle, \quad \alpha = x, y, z. \quad (3.31)$$

This approximation gives exact results in the cases where the exchange interaction or the transverse field is zero, and consequently is a good improvement on the c-cyclic approximation. These results are calculated in detail in appendix. Unfortunately we have not been able to get stable solutions for the eq. (3.31) for general values of J and h . The difficulties in the numerical

calculations appear when $|f_{j\ell}^{xx}|$ is very small or zero, in which case it is clear from eq. (3.30) that an analytical treatment is necessary. If $|f_{j\ell}^{xx}|$ is very small in a large interval compared with the step length used in the numerical solution, then the problem is not tractable, since we do not know an analytical approximate solution in this interval. On the other hand if $|f_{j\ell}^{xx}|$ is zero at some point t , and $|f_{j\ell}^{xx}|$ is very small only in a small interval about this point, then it is possible to work out an expansion for $f_{j\ell}^{xx}$ provided the root of $f_{j\ell}^{xx}$ is known to good accuracy. Unfortunately we cannot get the third derivative of $f_{j\ell}^{xx}$ at this point, and consequently we have to limit the expansion to second order which is not sufficient to accurately obtain the value of $f_{j\ell}^{xx}$ in a point distant a step length from t . Naturally the convergence of the solution is by no means certain under these conditions, and in principle is very difficult to achieve. These difficulties have obliged us to abandon this approximation as well.

3.3 The Improved c-cyclic Approximation

This approximation is the most successful one (Gonçalves and Elliott, 1976) and we believe that under certain conditions it gives a good answer to the problem. It is an improvement over the c-cyclic approximation that gives the Ising case ($h = 0$) correctly. As the first step we start with the eq. (3.2), which is exact in the thermodynamic limit and is given by:

$$\langle S_1^x(t) S_{1+n}^x(0) \rangle = \langle e^{iHt} S_1^x e^{-iH^*t} S_{1+n}^x \rangle, \quad (3.32)$$

where we have made explicit use of the translational symmetry.

The above equation can also be written as:

$$\langle S_1^x(t) S_{1+n}^x(0) \rangle = \langle e^{iH^-t} S_1^x e^{-iH^-t} e^{iH^-t} e^{-iH^+t} S_{1+n}^x \rangle, \quad (3.33)$$

where the approximation is easily introduced. Although it is simple to calculate

$$S_1^x(\tilde{t}) = e^{iH^-t} S_1^x e^{-iH^-t}, \quad (3.34)$$

it is very difficult to evaluate the operator $O(t)$ given by

$$O(t) = e^{iH^-t} e^{-iH^+t}. \quad (3.35)$$

Capel et al. (1974) have expanded this operator in powers of t and consequently eq. (3.33) can be written as a power series. They have proved that the series converges although it is very difficult to sum. This approach is very useful when we are interested in short time behaviour. On the other hand McCoy et al. (1971) have avoided these expansions and evaluated (3.13) by calculating the four spin correlation and using the cluster property

$$\lim_{N \rightarrow \infty} \langle S_{1+\frac{N}{2}}^x(t) S_{1-R+N}^x(t) S_1^x(0) S_{1-R+\frac{N}{2}}^x(0) \rangle = \langle S_1^x(t) S_{1+R}^x(0) \rangle^2. \quad (3.36)$$

Within this approach they have been able to calculate (3.17) only for large R and $T = 0$.

Although H^+ and H^- do not commute we will approximate $O(t)$ by the expression

$$O(t) \cong e^{i(H^- - H^+)t}, \quad (3.37)$$

and then

$$\langle S_1^x(t) S_{1+N}^x(0) \rangle \cong \langle e^{iH\bar{t}} S_1^x e^{-iH\bar{t}} e^{iBt} S_{1+N}^x \rangle \quad (3.38)$$

where

$$B = J (c_N^+ c_1 + c_N^+ c_1^+ + h.c.) \quad , \quad (3.39)$$

is the boundary term defined in eq. (2.11). If we compare eqs. (3.14) and (3.2) we realize that the c-cyclic approximation corresponds to $O(t)$ equal to the identity, which is the lowest order term in the series expansion developed by Capel et al. (1974). This new approximation is indeed an improvement over the mentioned one, although apparently in a rather arbitrary way.

Eq. (3.39) can be written as

$$B = -J A_1 B_N \quad , \quad (3.40)$$

thus from eq. (3.9), (3.10) and (3.11) we obtain:

$$B^2 = J^2 \quad , \quad (3.41)$$

and then we get:

$$O(t) \cong \cos Jt - i \sin Jt A_1 B_N \quad , \quad (3.42)$$

and from this:

$$\langle S_1^x(t) S_{1+n}^x(0) \rangle \cong \langle e^{iH\bar{t}} S_1^x e^{-iH\bar{t}} (\cos Jt - \sin Jt A_1 B_N) S_{1+n}^x \rangle \quad . \quad (3.43)$$

The first term in this expression is the c-cyclic result multiplied by $\cos Jt$. In order to get the second one we will again use the Green function method which is the most appropriate. Then we start by considering the anti-commutator Green function, $\langle\langle S_1^x; A_1 B_N S_{1+n}^x \rangle\rangle$, which using eqs. (2.3), (2.6), (2.7), (2.18) and (2.19) can be written as:

$$\langle\langle S_1^x; A_1 B_N S_{1+n}^x \rangle\rangle = \frac{1}{2\sqrt{N}} \sum_k e^{ika} (x_k + y_k) \langle\langle \beta_k^+ + \beta_{-k}; A_1 B_N S_{1+n}^x \rangle\rangle. \quad (3.44)$$

Using the equation of motion method, eq. (1.9) and considering as before H equal to H^- , we get:

$$\begin{aligned} \langle\langle S_1^x; S_{1+n}^x \rangle\rangle = \frac{1}{2\sqrt{N}} \sum_k e^{ika} (x_k + y_k) & \left[\frac{\omega(\{\beta_k^+ + \beta_{-k}, A_1 B_N S_{1+n}^x\})}{\omega^2 - E_k^2} \right. \\ & \left. + \frac{E_k(\{\beta_{-k} - \beta_k^+, A_1 B_N S_{1+n}^x\})}{\omega^2 - E_k^2} \right], \end{aligned} \quad (3.45)$$

and from this, by using eq. (2.22) and the inverse of eq. (2.18) we obtain:

$$\begin{aligned} \langle\langle S_1^x; S_{1+n}^x \rangle\rangle = \frac{1}{2N} \sum_k \sum_{j=1}^N \frac{-ika(j-1)}{\omega^2 - E_k^2} & \left[\omega(x_k + y_k)(x_k^+ + y_k) \langle\{A_j, A_1 B_N S_{1+n}^x\}\rangle - \right. \\ & \left. - E_k(x_k + y_k)(x_k^* - y_k) \langle\{B_j, A_1 B_N S_{1+n}^x\}\rangle \right]. \end{aligned} \quad (3.46)$$

The averages in previous equation are obtained by using eqs. (3.12), (3.13), (3.14), and (3.17), and we get the following results:

$$\langle\{A_j, A_1 B_N S_{1+n}^x\}\rangle = 0, \text{ for any } j, \quad (3.47)$$

$$\langle\{B_j, A_1 B_N S_{1+n}^x\}\rangle = 0, \text{ if } n+1 \leq j \leq N, \quad (3.48)$$

and

$$\langle \{B_j, A_1 B_N S_{1+n}^x\} \rangle = - \langle B_j B_N B_1 A_2 B_2 \dots A_n B_n A_{n+1} \rangle, \quad (3.49)$$

if $j < n + 1$ and $j = N$.

It should be noted that the label N which appears in previous equation is formally identical to zero, and provided this substitution is made, we have to consider j from zero to n . However, we can consider j varying from 1 to $n + 1$, in which case eq. (3.49) is written as

$$\langle \{B_j, A_1 B_N S_{1+n}^x\} \rangle = - \langle B_j B_1 B_2 A_3 B_3 \dots A_{n+1} B_{n+1} A_{n+2} \rangle. \quad (3.50)$$

Then eq. (3.46) is written as:

$$\langle\langle S_1^x, A_1 B_N S_{1+n}^x \rangle\rangle = \frac{1}{2N} \sum_k \sum_{j=1}^{n+1} \frac{e^{-ika(j-2)} E_k}{\omega^2 - E_k^2} \langle B_j B_1 B_2 A_3 B_3 \dots A_{n+1} B_{n+1} A_{n+2} \rangle, \quad (3.51)$$

which can be put into the form:

$$\langle\langle S_1^x, A_1 B_N S_{1+n}^x \rangle\rangle = \frac{1}{2N} \sum_k \sum_{j=1}^{n+1} \frac{e^{-ika(j-2)} E_k (x_k + y_k) (x_k^+ - y_k^+) (-1)^j N_{n+1}^j}{\omega^2 - E_k^2} \quad (3.52)$$

where N_{n+1}^j is the minor of the shifted Toeplitz determinant

$$N = \begin{pmatrix} G(-1) & G(-2) & . & . & . & G(-n-1) \\ G(0) & G(-1) & . & . & . & . \\ . & . & . & . & . & . \\ . & . & . & . & . & . \\ G(n-1) & . & . & . & . & G(-1) \end{pmatrix} \quad (3.53)$$

calculated with respect to the first column, j th row. From eq. (3.52) by using the Green function properties after some algebraic manipulations we obtain:

$$\begin{aligned} \langle S_1^x(t) A_1 B_N S_{1+n}^x(0) \rangle &= \frac{1}{4N} \sum_k \sum_{j=1}^{n+1} (-1)^j N_{n+1}^j \left(\tanh \frac{\beta E_k}{2} \cos E_k t - i \sin E_k t \right), \\ &\times \left[\frac{h \cos(j-2)ka - J \cos(j-1)ka}{E_k} \right] \end{aligned} \quad (3.54)$$

Therefore by using eq. (3.24), (3.43) and the previous equation we get the final result:

$$\begin{aligned} \langle S_1^x(t) S_{1+n}^x(0) \rangle &= \frac{1}{4N} \sum_k \sum_{j=1}^{n+1} \left\{ \cos(j-1)ka \cos Jt (-1)^{j-1} M_{n+1}^j \left[\cos E_k t - \right. \right. \\ &- i \sin E_k t \tanh \frac{\beta E_k}{2} \left. \right] + i \sin Jt (-1)^j N_{n+1}^j \left(\tanh \frac{\beta E_k}{2} \cos E_k t - \right. \\ &\left. \left. - i \sin E_k t \right) \left[\frac{h \cos(j-2)ka - J \cos(j-1)ka}{E_k} \right] \right\}. \end{aligned} \quad (3.55)$$

Considering in eq. (3.55) the limit $h = 0$ we get

$$\langle S_1^x(t) S_{1+n}^x(0) \rangle = \frac{(-1)^n}{4} \left(\tanh \frac{\beta J}{2} \right)^n, \quad (3.56)$$

which is the correct result.

The introduction of the approximation shown in eq. (3.38) implies the loss of translational symmetry. As we will see later on, the variation of $\langle S_j^x(t) S_{j+n}^x(0) \rangle$ with j is only negligible in the high temperature limit. There is, however, a way to recover the translational symmetry, which is to define the time-dependent correlation function $C_n(t)$ as

$$C_n(t) = \frac{1}{N} \sum_{j=1}^N \langle S_j^x(t) S_{j+n}^x(0) \rangle \quad (3.57)$$

Unfortunately this expression cannot be easily evaluated even in the proposed approximation. Despite the loss of translational symmetry we will look in detail at the function $\langle S_1^x(t) S_{1+n}^x(0) \rangle$ and compare some of the results with the known exact ones.

Considering $n = 0$ in eq. (3.55) we get the first two moments exactly, at any temperature. We also conclude from eq. (3.55) that at $T = \infty$ only the auto-correlation is different from zero, which is exact (Brandt and Jacoby, 1976).

If figs. (3.1), (3.2) and (3.3) we show the auto-correlation and in figs. (3.4) and (3.5), the nearest neighbour correlation for different temperatures ($\beta = \frac{2J}{K_B T}$) and $\lambda = \frac{J}{h}$. The real part is symmetric and the imaginary is anti-symmetric. It should be noticed that as we increase λ we approach the Ising case and consequently the real part of the correlation falls off less rapidly, and the imaginary part decreases as expected. For λ greater than 100 the systems behave essentially as the Ising case, independently of temperature. Naturally the real part becomes constant and the imaginary part goes to zero. As we increase the temperature the imaginary part decreases, and at $T = \infty$ the auto-correlation is real.

The auto-correlation function when the field is equal to the critical field ($h = J$) is written in a simple form, namely

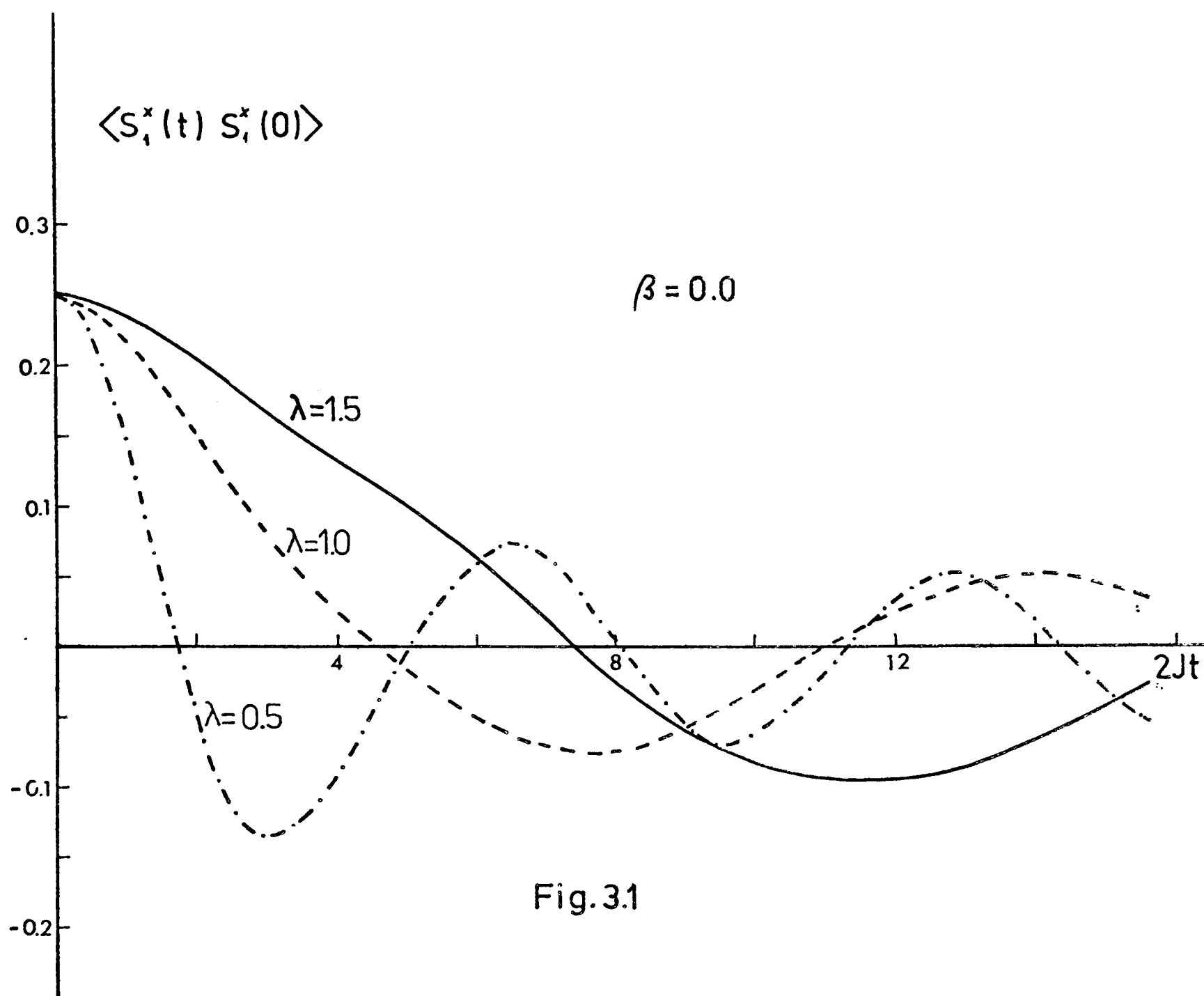
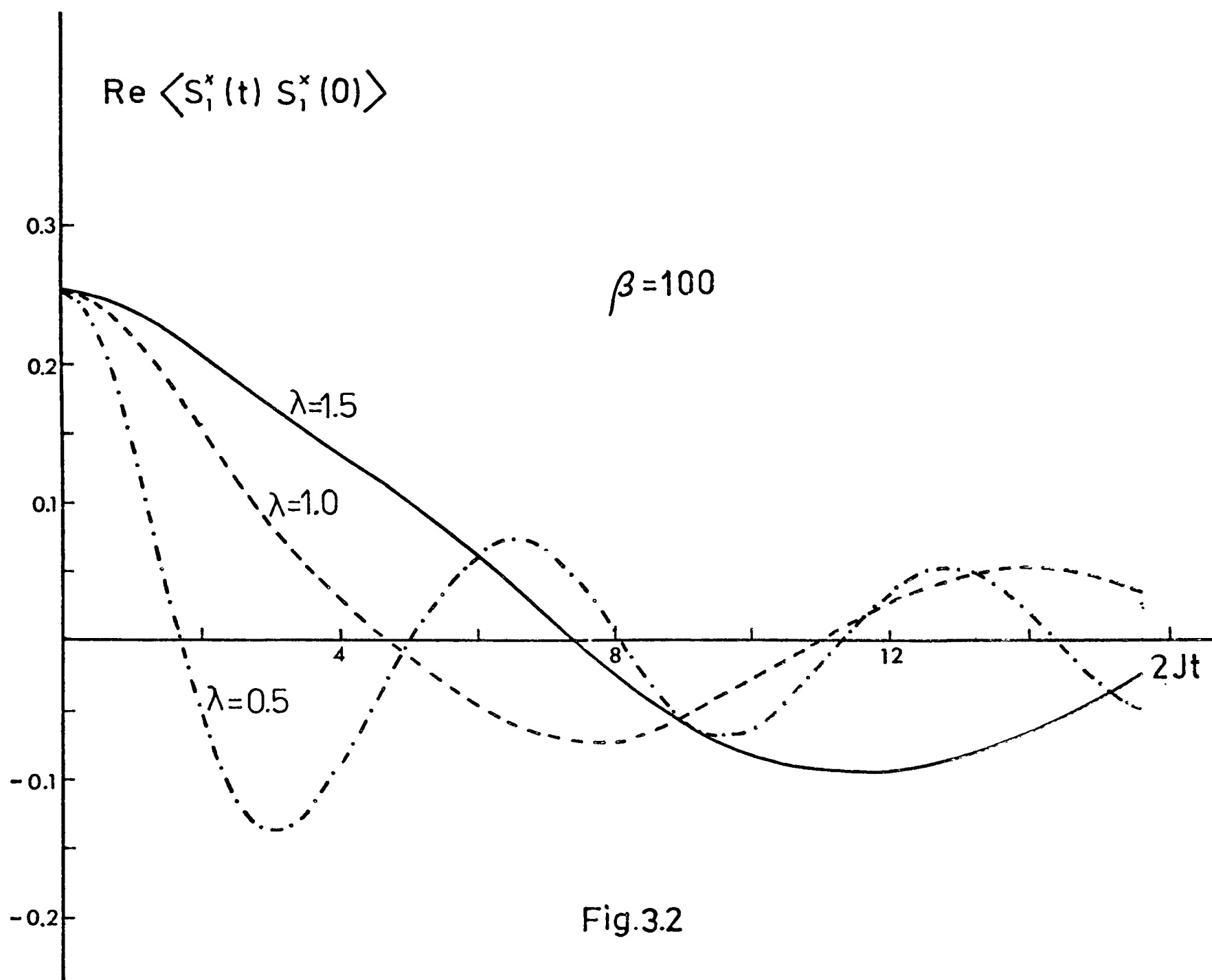


Fig.3.1



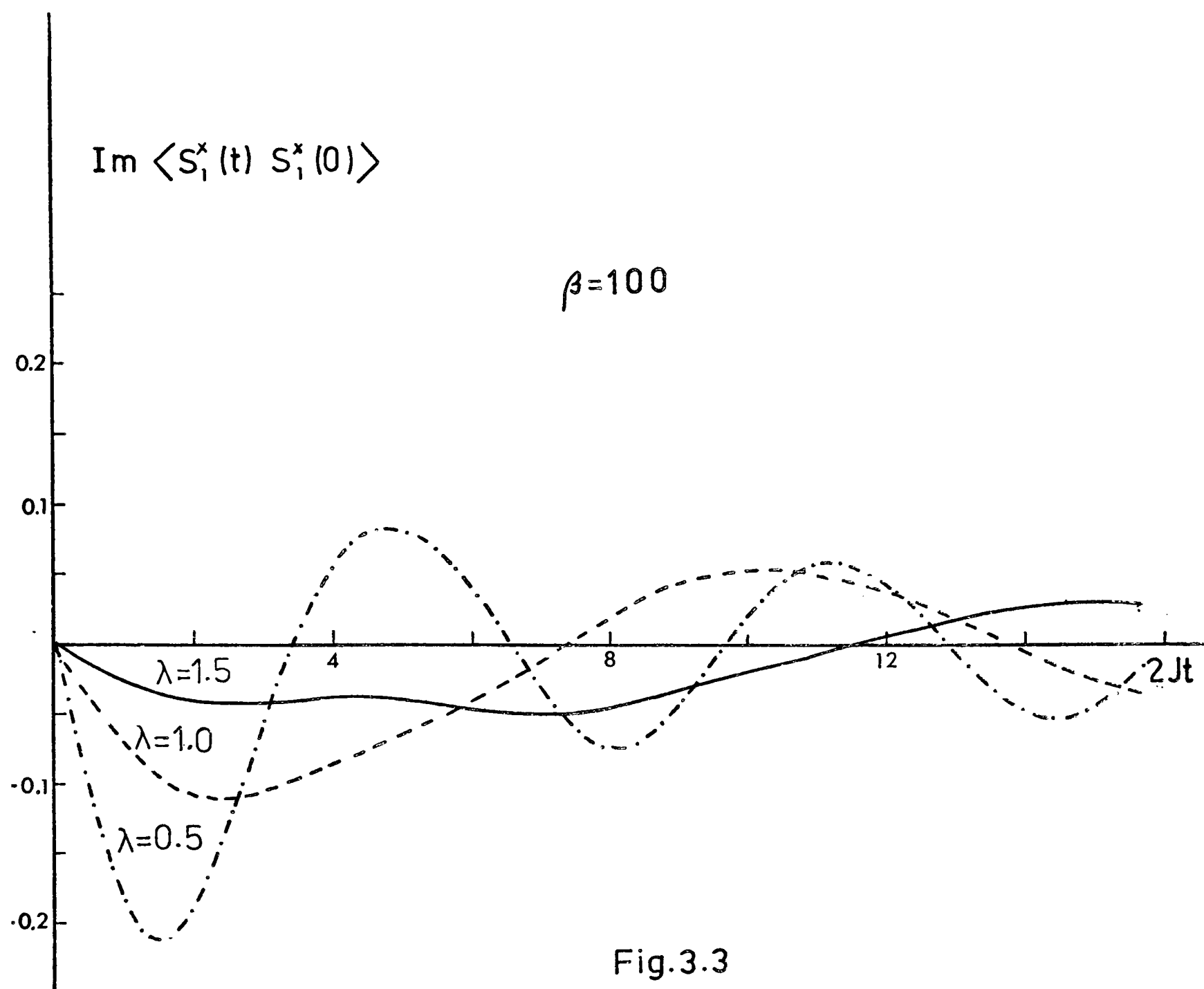


Fig.3.3

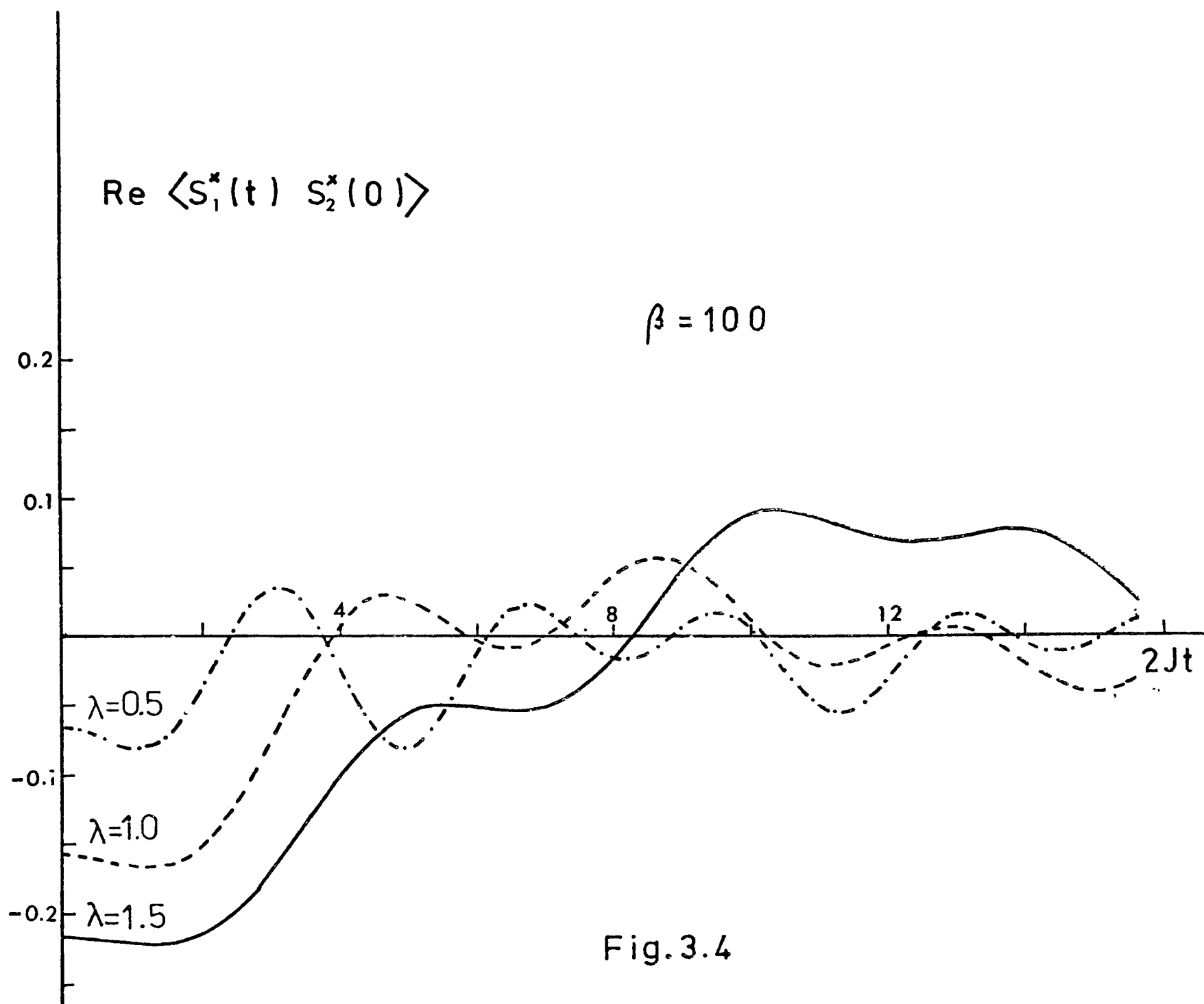


Fig.3.4

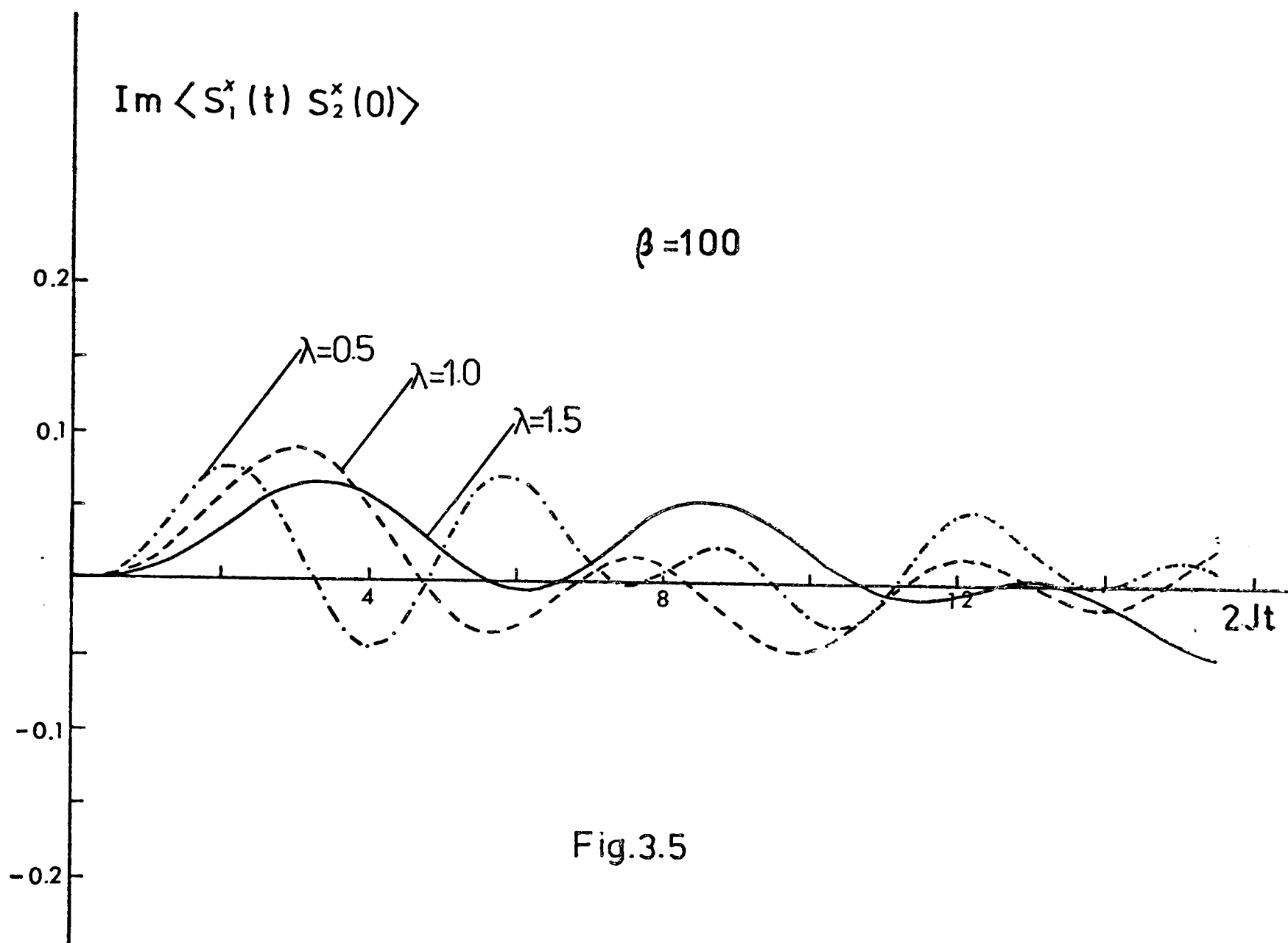


Fig.3.5

$$\begin{aligned} \langle S_1^x(t) S_1^x(0) \rangle = & \frac{1}{4N} \sum_k \left[\cos E_k t - i \sin E_k t \tanh \frac{\beta E_k}{2} \right] \cos Jt \\ & + \frac{i}{4N} \sum_k \sin \frac{Ka}{2} \left[\tanh \frac{\beta E_k}{2} \cos E_k t - i \sin E_k t \right] \sin Jt \end{aligned} \quad (3.58)$$

where

$$E_k = 2J \sin \frac{Ka}{2}. \quad (3.59)$$

If $\beta = 0$ the integrals over k in (3.58) can be performed and the result takes the form (Gradshteyn and Ryzhik, 1965)

$$\langle S_1^x(t) S_1^x(0) \rangle = \frac{1}{4} \left[J_0(2Jt) \cos Jt + J_1(2Jt) \sin Jt \right], \quad (3.60)$$

where J_0 and J_1 are Bessel functions of the first kind of order 0 and 1 respectively. This does not agree with the exact result (Capel and Perk, 1977):

$$\langle S_1^x(t) S_1^x(0) \rangle = \frac{1}{4} e^{-\frac{1}{2} J^2 t^2} \quad (3.61)$$

If $\beta = \infty$ we get

$$\begin{aligned} \langle S_1^x(t) S_1^x(0) \rangle = & \frac{1}{4} \left[J_0(2Jt) \cos Jt + J_1(2Jt) \sin Jt \right. \\ & \left. - 2i E_0(2Jt) \cos Jt + (i E_1(2Jt) - i E_{-1}(2Jt)) \sin Jt \right], \end{aligned} \quad (3.62)$$

where E_0 , E_1 and E_{-1} are Weber's functions.

The asymptotic behaviour of this correlation is given by (Watson, 1966)

$$\langle S_1^x(t) S_1^x(0) \rangle \sim \frac{\alpha}{t^{1/2}}. \quad (3.63)$$

which disagrees with the exact result obtained by Lajzerowicz and Pfeuty (1975), which is

$$\langle S_1^x(t) S_1^x(0) \rangle \sim \frac{\alpha'}{t^{1/4}} \quad (3.64)$$

Some difference was to be anticipated, since our approximation gives only two correct moments. In fact the agreement is better than might have been expected for the asymptotic form.

The frequency transform of the time-dependent correlation function defined as

$$c_n(\omega) = \int_{-\infty}^{\infty} e^{i\omega t} \langle S_1^x(t) S_{1+n}^x(0) \rangle dt \quad , \quad (3.65)$$

is easily obtained from eq. (3.55) and the result is:

$$\begin{aligned} c_n(\omega) = & \frac{\mathcal{H}}{8N} \left\{ \sum_k (1 - \tanh \frac{\beta E_k}{2}) \delta(\omega + E_k + J) \left[\sum_j (F_n^j - G_n^j) \right] \right. \\ & + \sum_k (1 - \tanh \frac{\beta E_k}{2}) \delta(\omega + E_k - J) \left[\sum_j (F_n^j + G_n^j) \right] + \sum_k (1 + \tanh \frac{\beta E_k}{2}) \times \\ & \times \delta(\omega - E_k + J) \left[\sum_j (F_n^j + G_n^j) \right] + \sum_k (1 + \tanh \frac{\beta E_k}{2}) \delta(\omega - E_k - J) \left[\sum_j (F_n^j - G_n^j) \right] \left. \right\} \quad , \end{aligned} \quad (3.66)$$

where

$$F_n^j = \cos(j-1)ka (-1)^{j-1} M_{n+1}^j \quad , \quad (3.67)$$

$$G_n^j = \frac{(h \cos(j-1)ka - J \cos j ka) (-1)^j N_{n+1}^j}{E_k} \quad . \quad (3.68)$$

The auto-correlation function and near neighbour correlation function are shown in figs. (3.6), (3.7) and (3.8) for various λ and β . In these graphs the full line represents the self-correlation at high temperature ($\beta = 0$), and the dashed line

and dot-dash line represent the self-correlation and the near neighbour correlation respectively at low temperature ($\beta = 100$). The non-zero values of the transforms are restricted to intervals limited by the values $\pm h$, $\pm h \pm 2J$ which are obtained by adding the energy necessary to flip a spin in presence of an Ising interaction, under the action of an external field. If $\lambda > 1$ this implies that there is a gap in the response which for positive frequency is limited by h and $2J - h$. This is shown in fig. (3.8) for $\lambda = 1.5$.

If figs. (3.9) to (3.16) we present the spatial Fourier transform of the time-dependent correlation function

$$C_q(t) = \langle S_1^x(t) S_1^x(0) \rangle + 2 \sum_{n=1}^{N-1} \cos qna \langle S_1^x(t) S_{1+n}^x(0) \rangle, \quad (3.69)$$

for various β and λ , and for the wave-vectors $0, \frac{\pi}{2a}$. As expected at high temperatures (figs. (3.9) to (3.12)) the important contribution to the spatial Fourier transform is the auto-correlation function and consequently the results are essentially the same for the wave-vector 0 and $\frac{\pi}{2a}$. Besides this the imaginary part of the correlations are very small and tend to zero as $\beta \rightarrow 0$. At $\beta = 1$ (figs. (3.13) to (3.16)) besides the auto-correlation function we have also the contribution of other correlations to the spatial Fourier transform and then, since we are considering the anti-ferromagnetic case, the correlation increases as we increase the wave-vector.

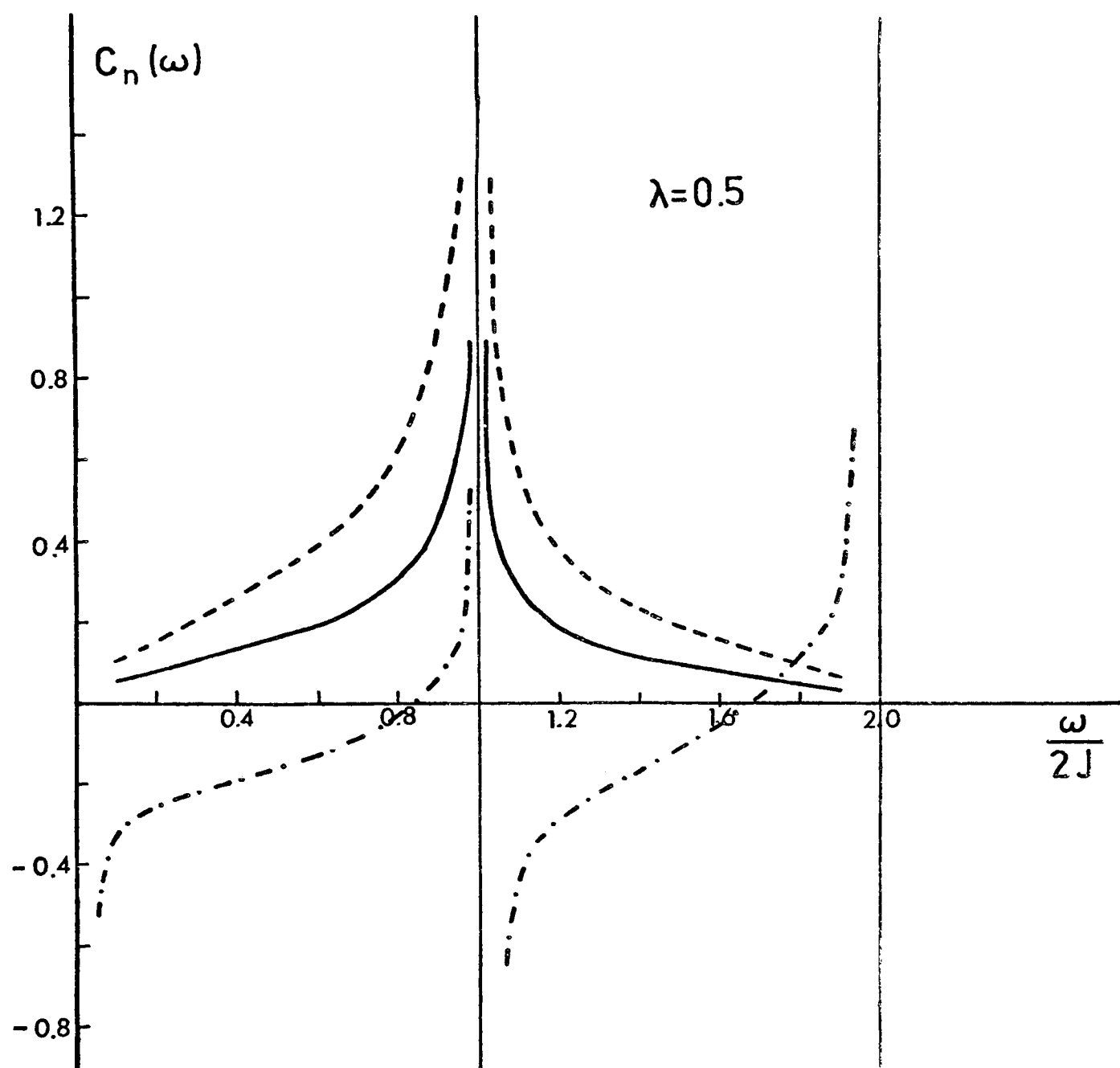


Fig.3.6

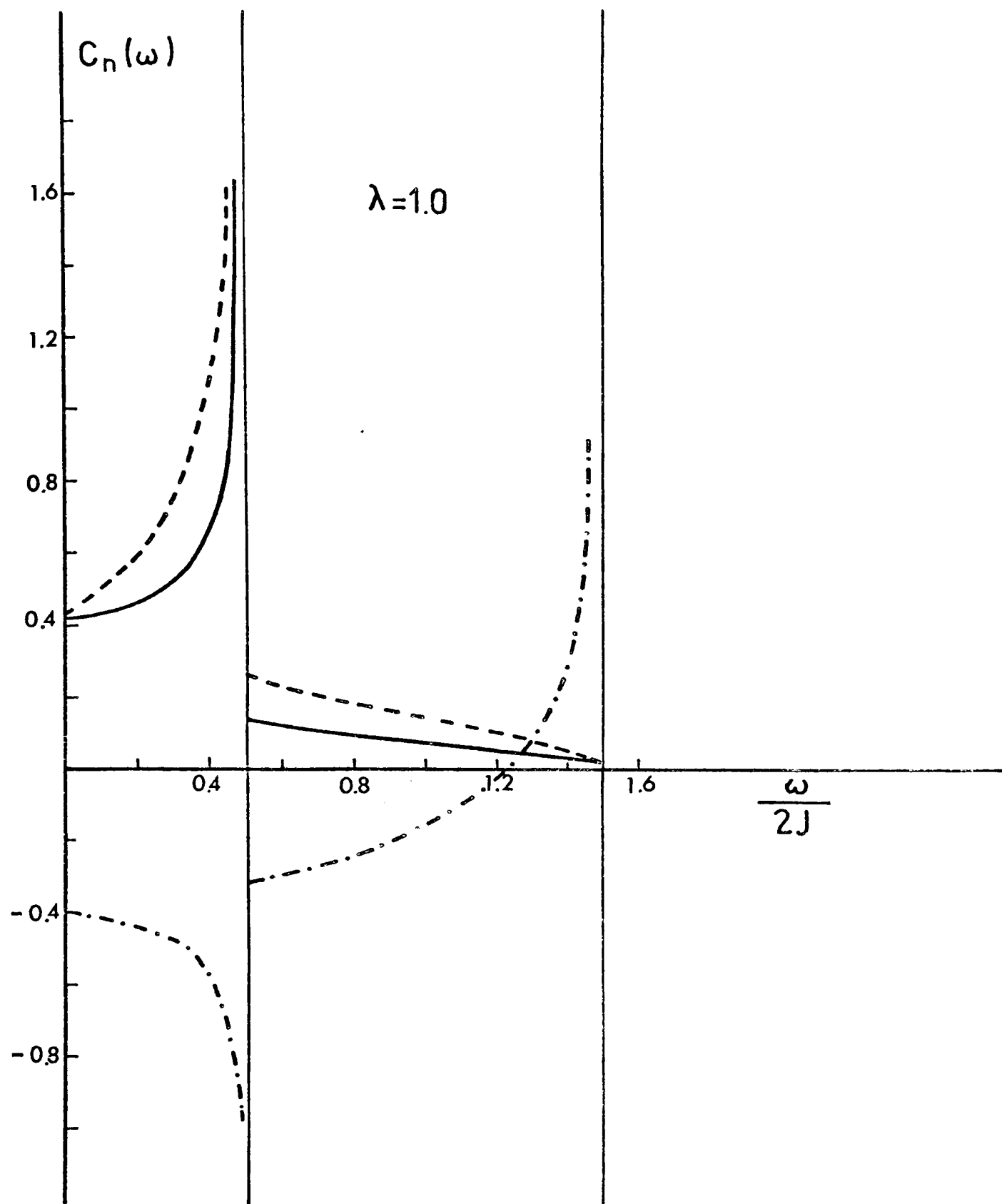


Fig. 3.7

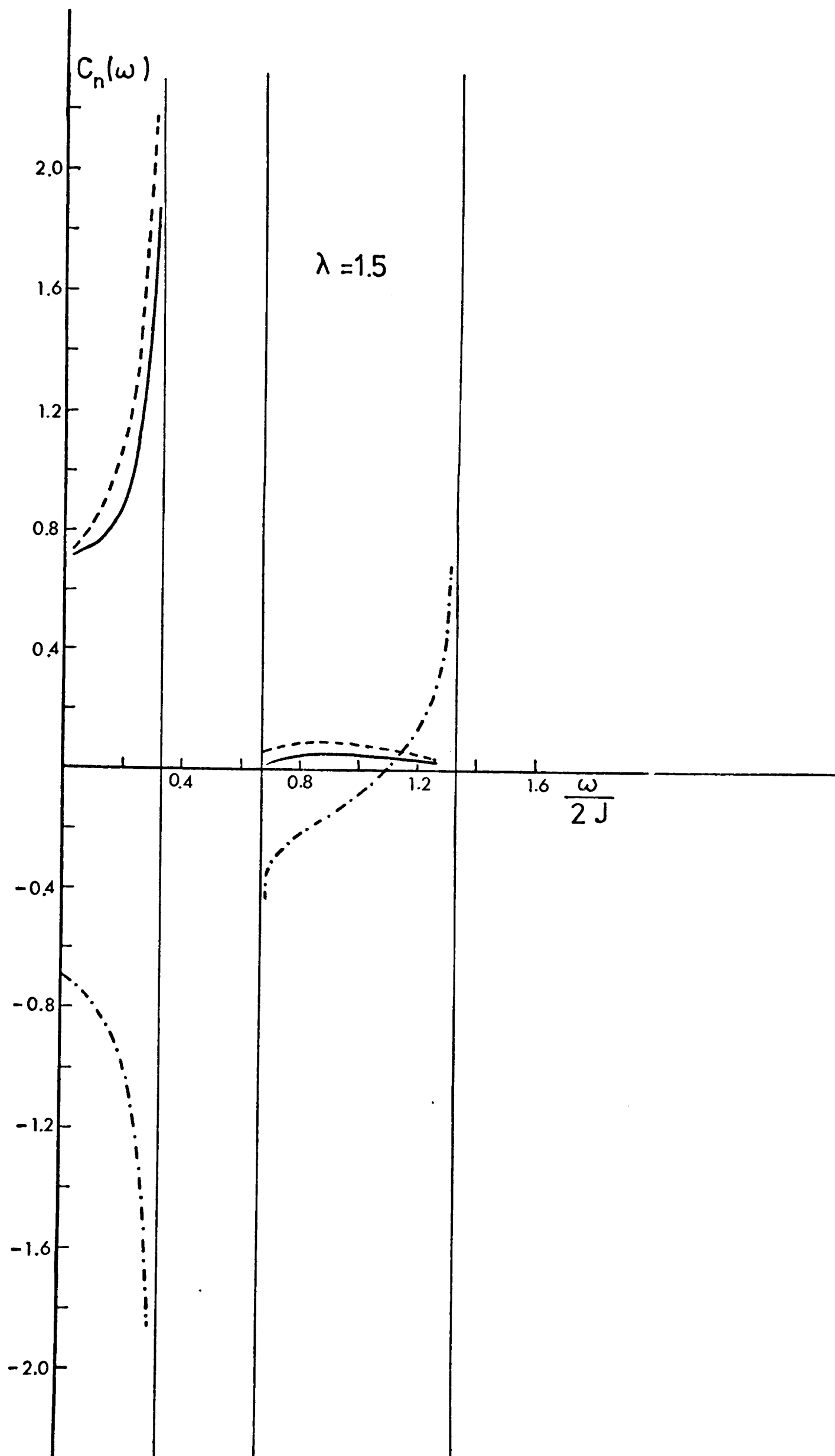


Fig.3.8

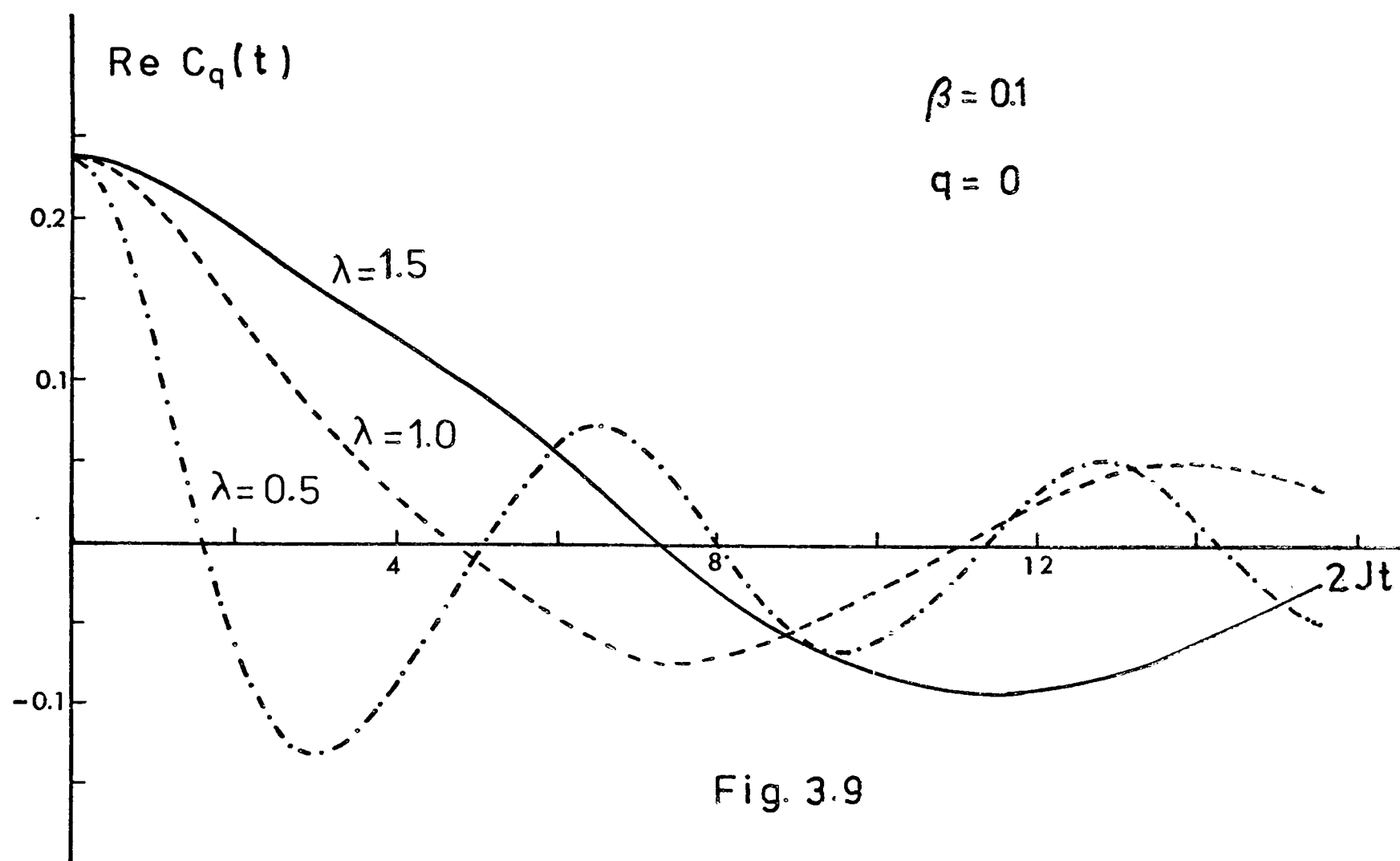


Fig. 3.9

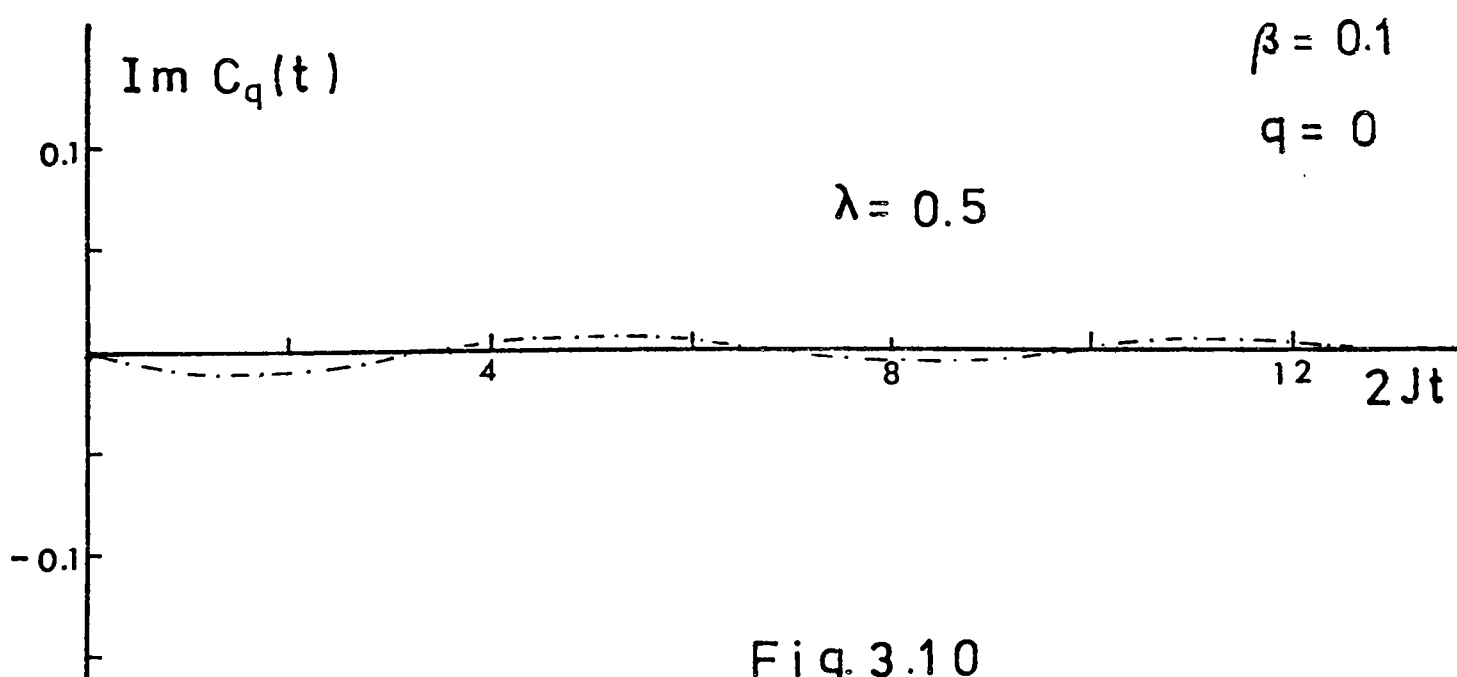
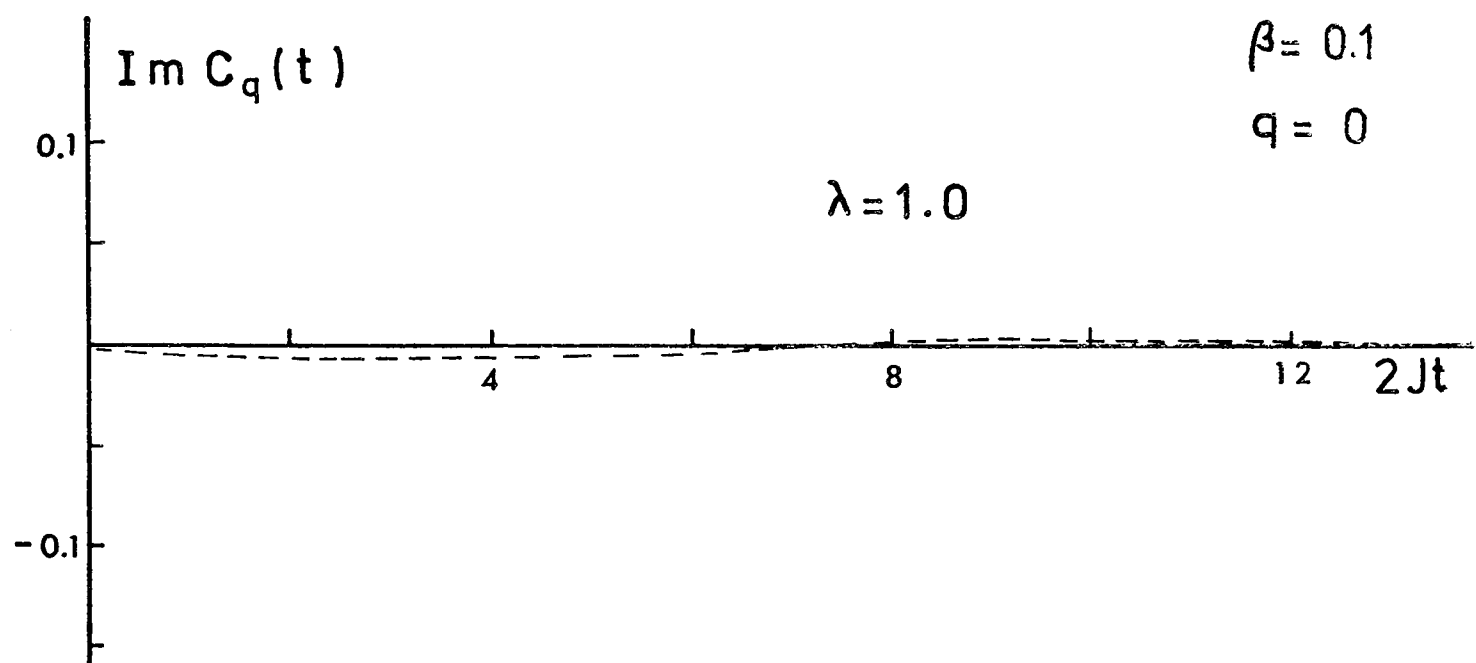
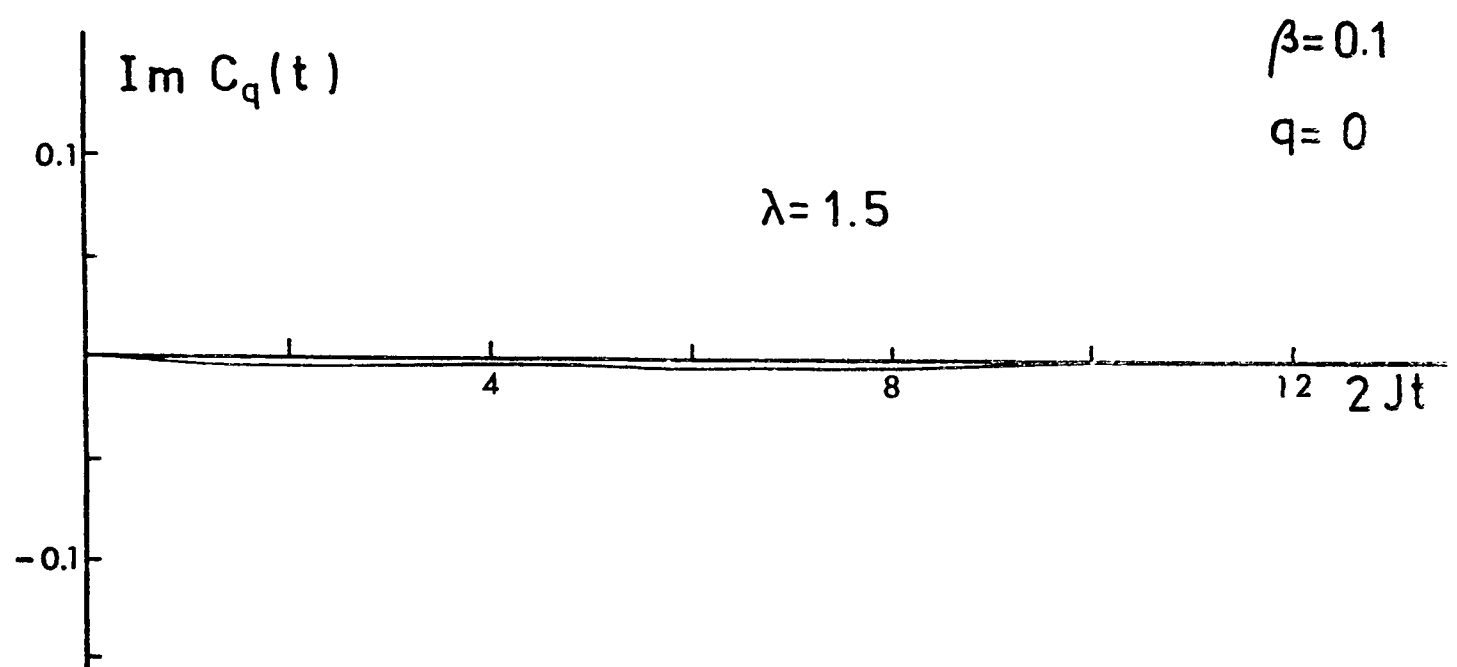
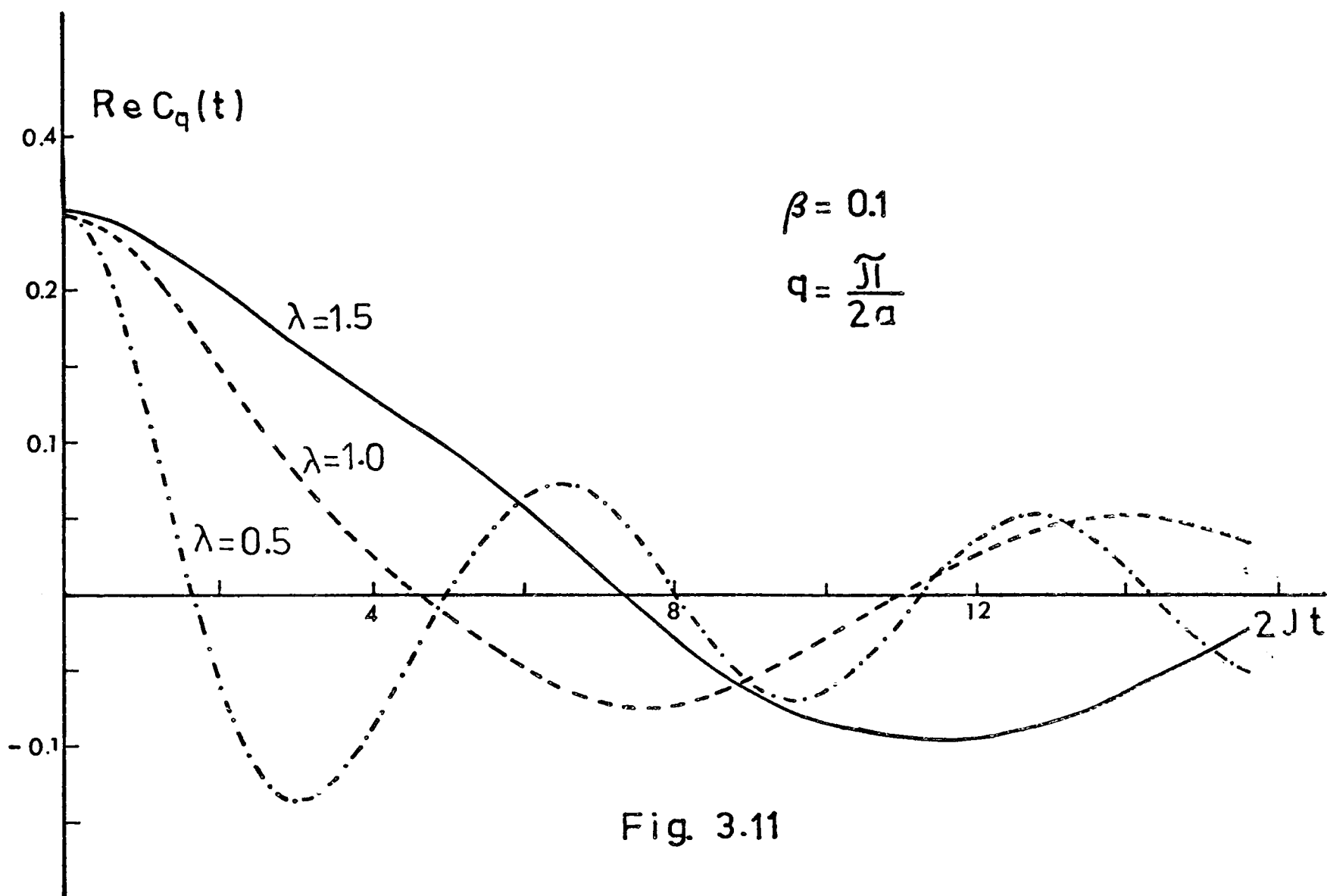


Fig. 3.10



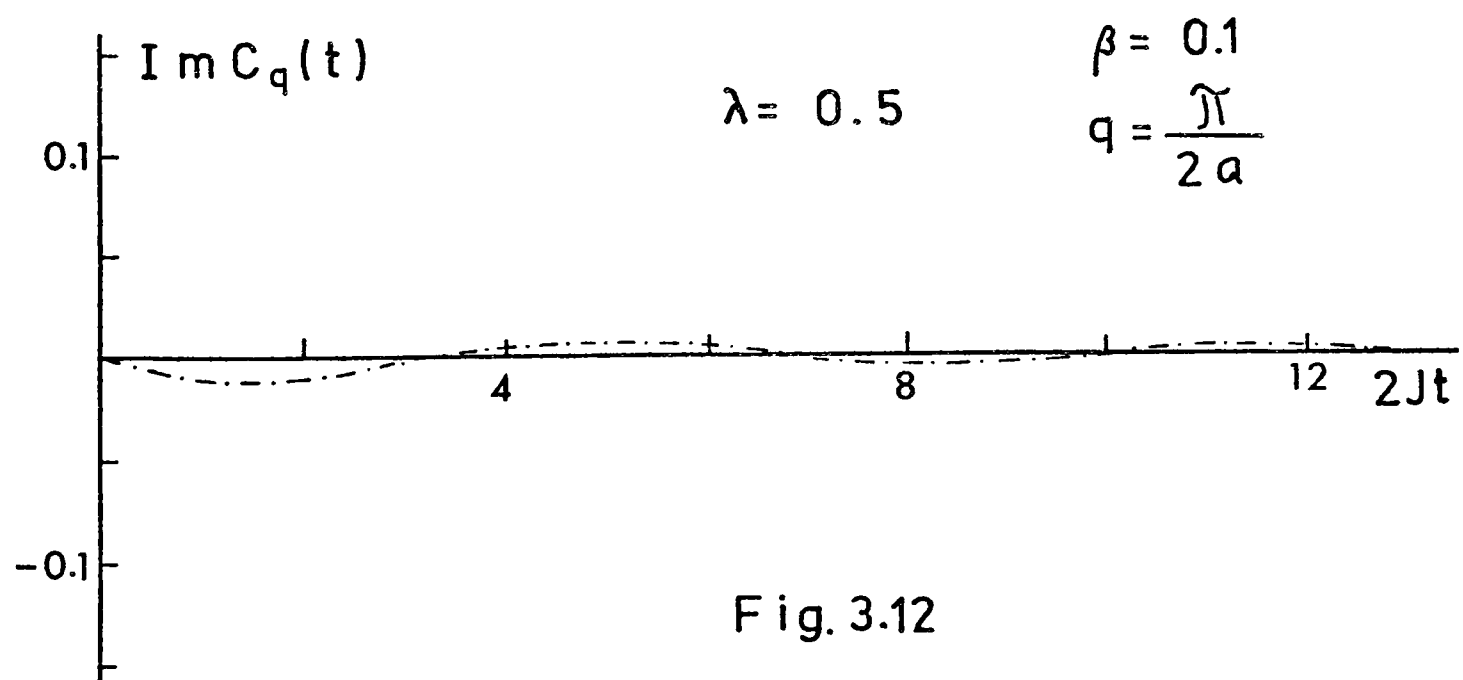
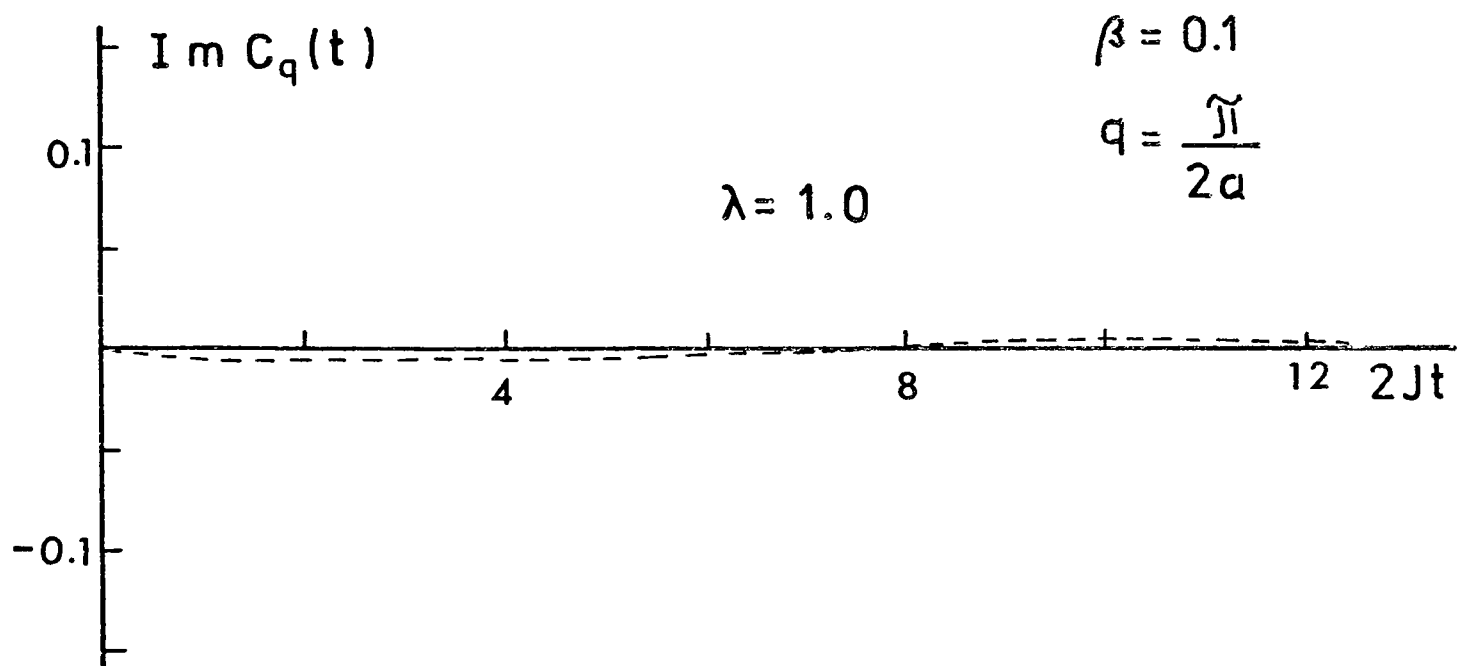
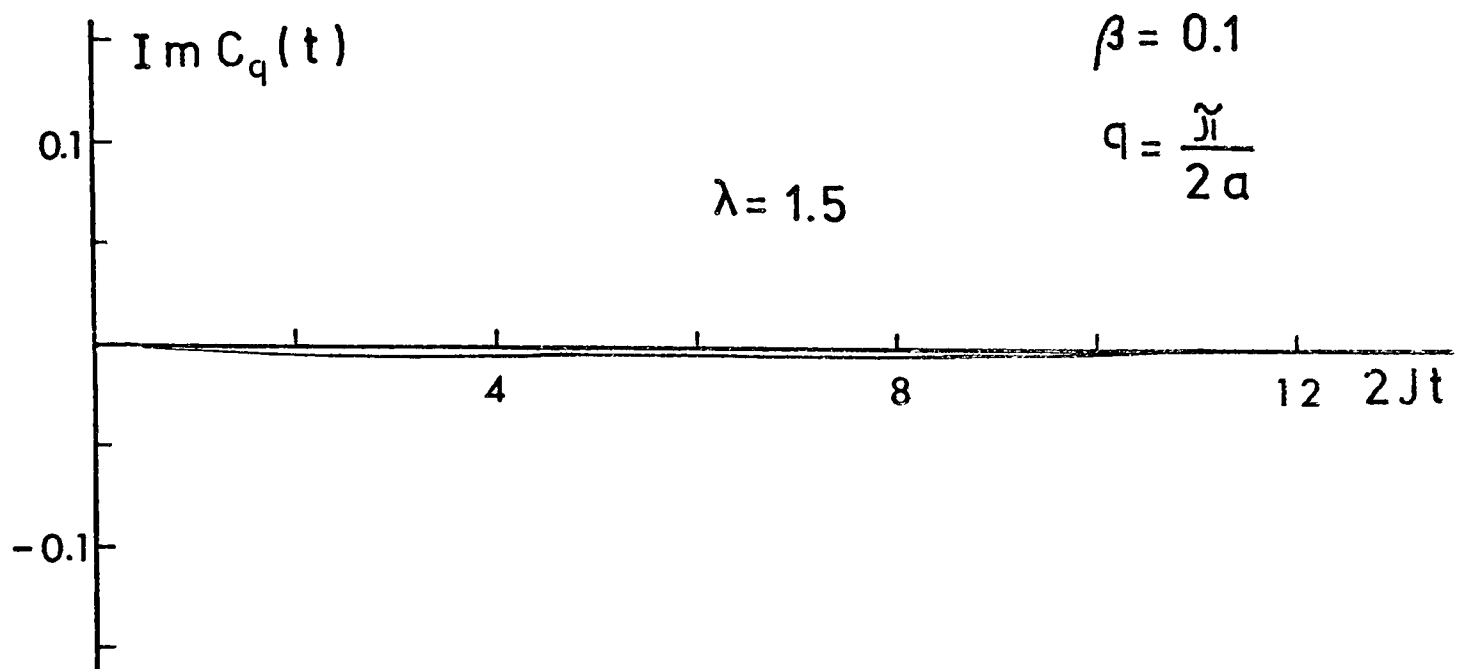
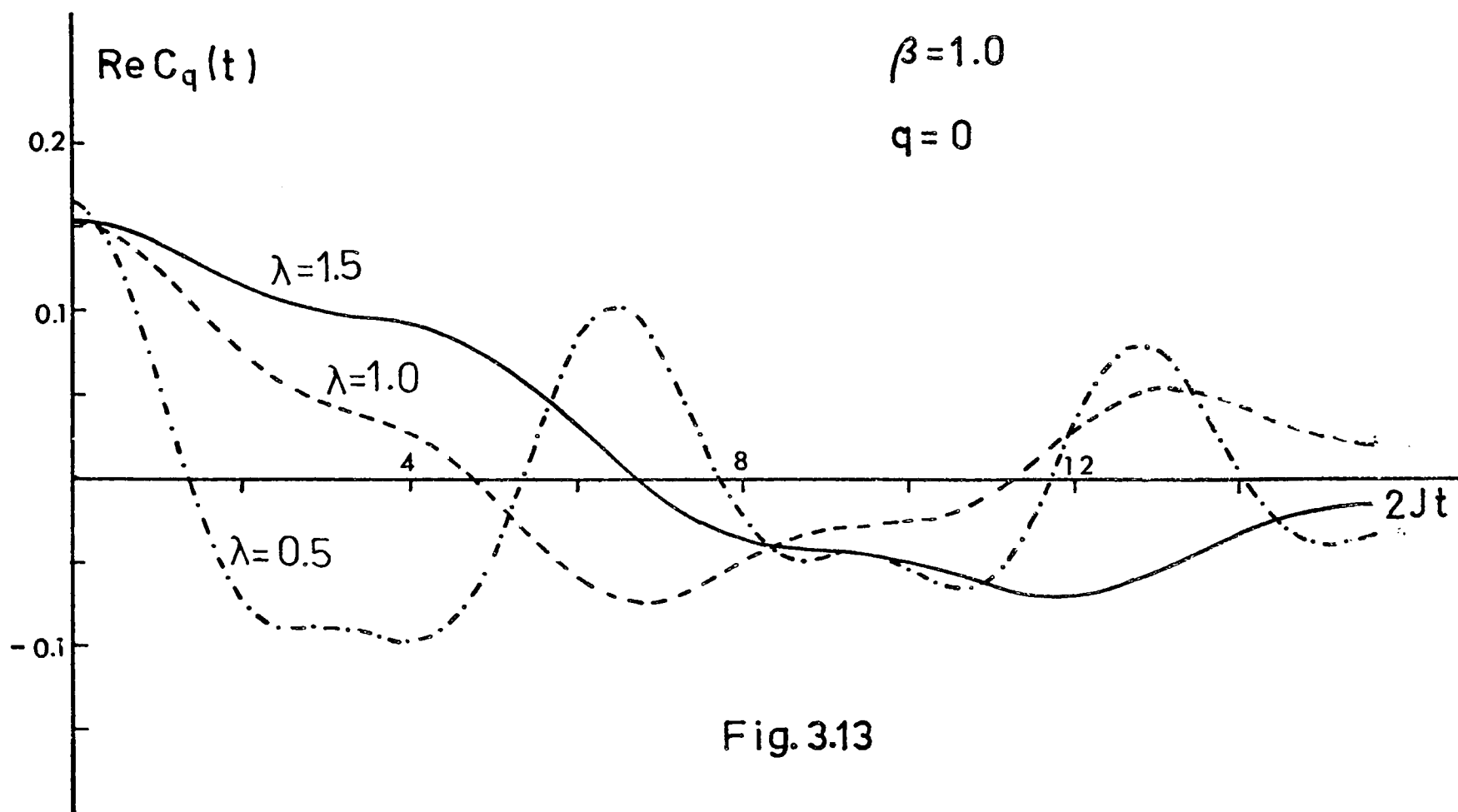
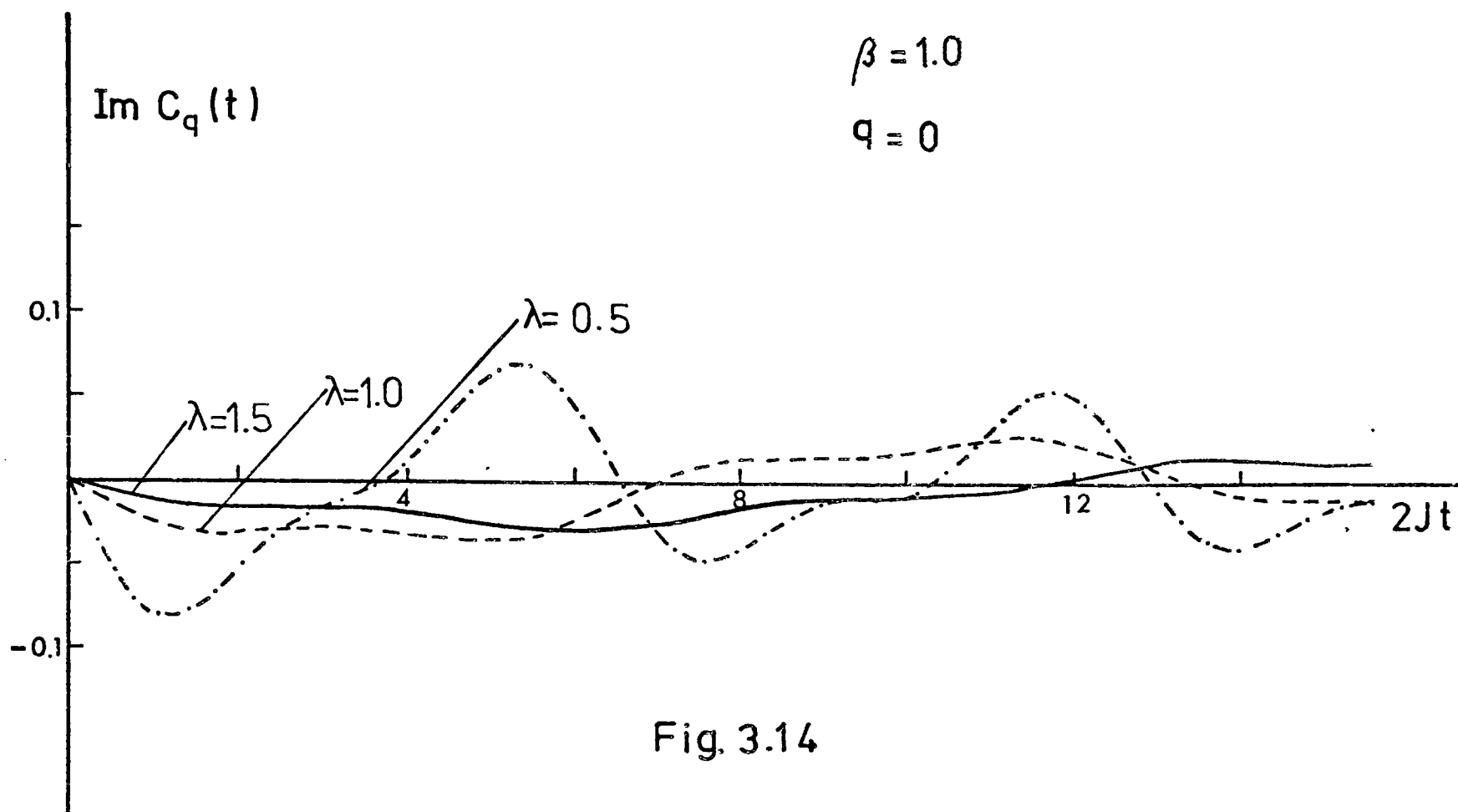
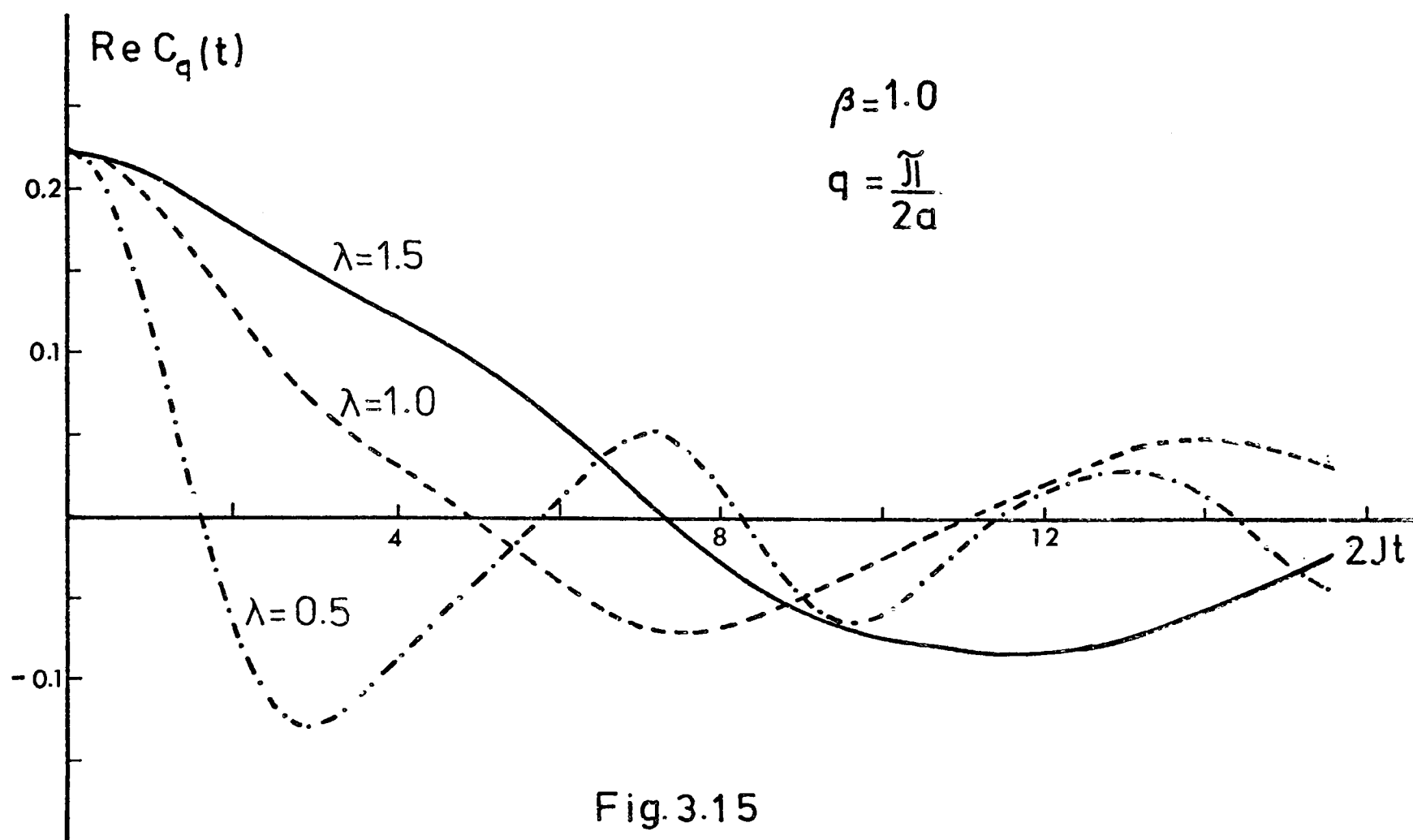


Fig. 3.12







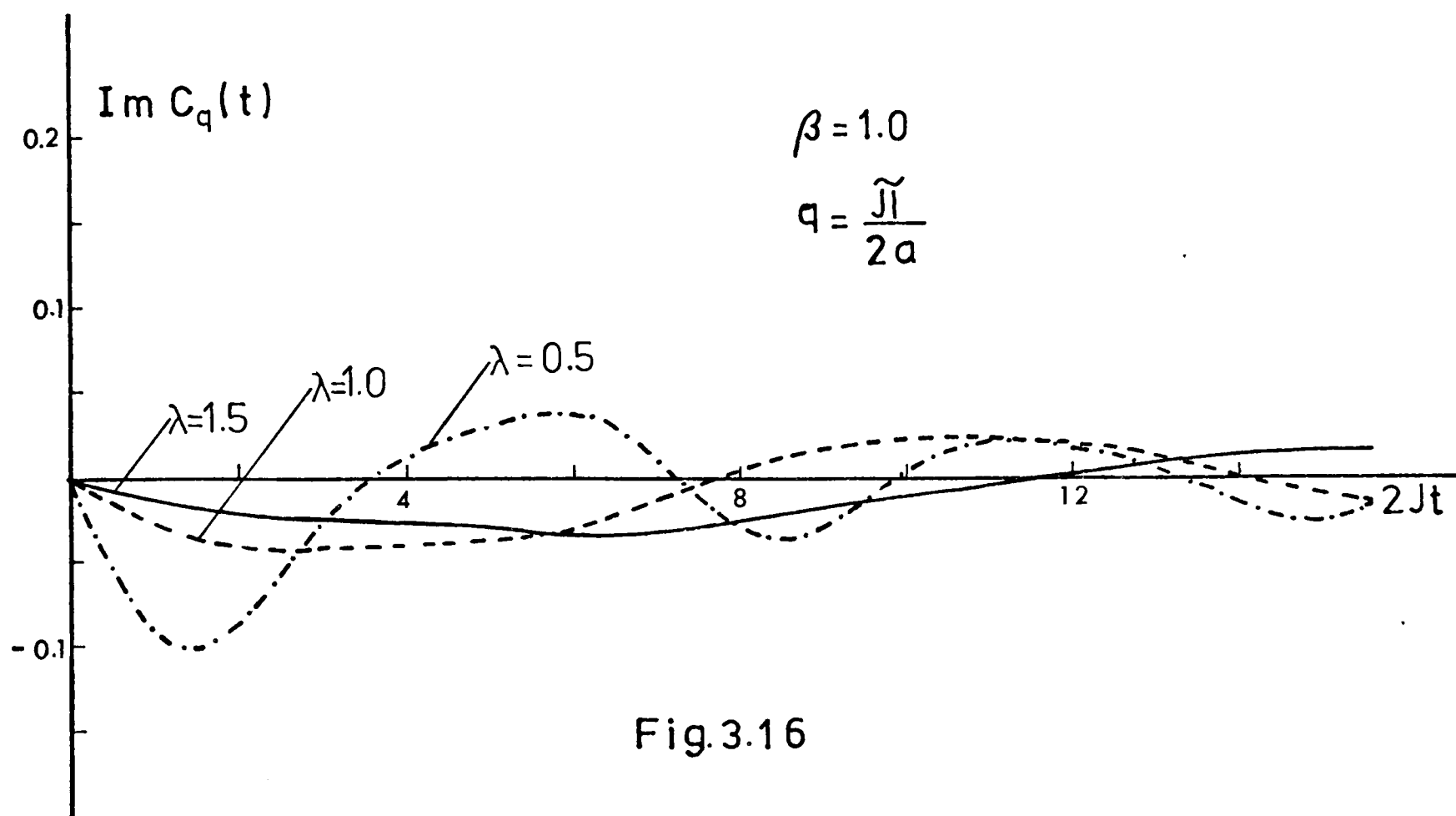


Fig.3.16

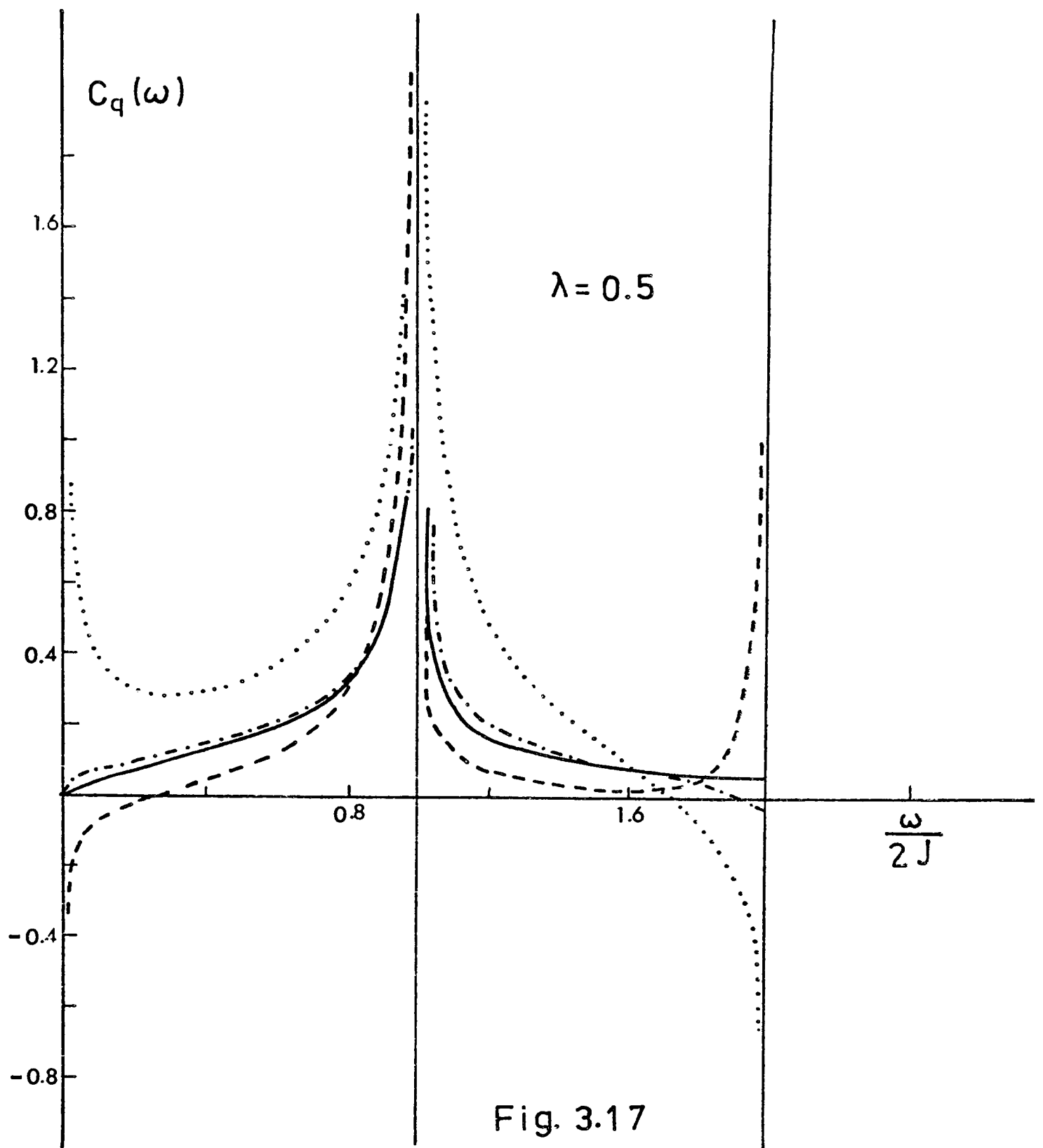
Obviously as we increase λ , the real part tends to a constant and the imaginary tends to zero. Unfortunately we have been unable to get the asymptotic behaviour of the $\langle S_1^X(t) S_{1+n}^X(0) \rangle$ (large n), and consequently we cannot obtain the spatial Fourier transform at very low temperature. However, it is possible numerically to get results as low as $\beta = 5$, which is lower than the critical temperature obtained using mean field theory (for $\lambda = 1.5$, $\beta_c \sim 2$).

Finally in figs. (3.17), (3.18) and (3.19) we present the transform of the spatial Fourier transform

$$C_q(\omega) = \int_{-\infty}^{\infty} e^{i\omega t} C_q(t) dt, \quad (3.70)$$

for various λ and β , and wave-vectors $0, \frac{\pi}{a}$. The full line and dashed line represent the transforms of wave-vector 0 at β 's given respectively by 0.1 and 1.0. The dot-dash line and dotted line represent the transforms of wave-vector $\frac{\pi}{a}$ at β 's given respectively by 0.1 and 1.0. As discussed previously the non-zero values are restricted to intervals limited by the values $\pm h, \pm h \pm 2J$, therefore for $\lambda > 1$ there is a gap in the response which for positive frequency is shown in fig. (3.19). These results as expected do not depend on wave-vector at high temperature ($\beta = 0.1$), and increase with the wave-vector as we lower the temperature ($\beta = 1.0$).

Although most of the results presented up to now seem reasonable, we have naturally to discuss the problem of the translational symmetry. This can be more easily seen by calculating the commutator Green function $\langle\langle S_{-q}^X; S_q^X \rangle\rangle$ which is given by (Parry, 1973)



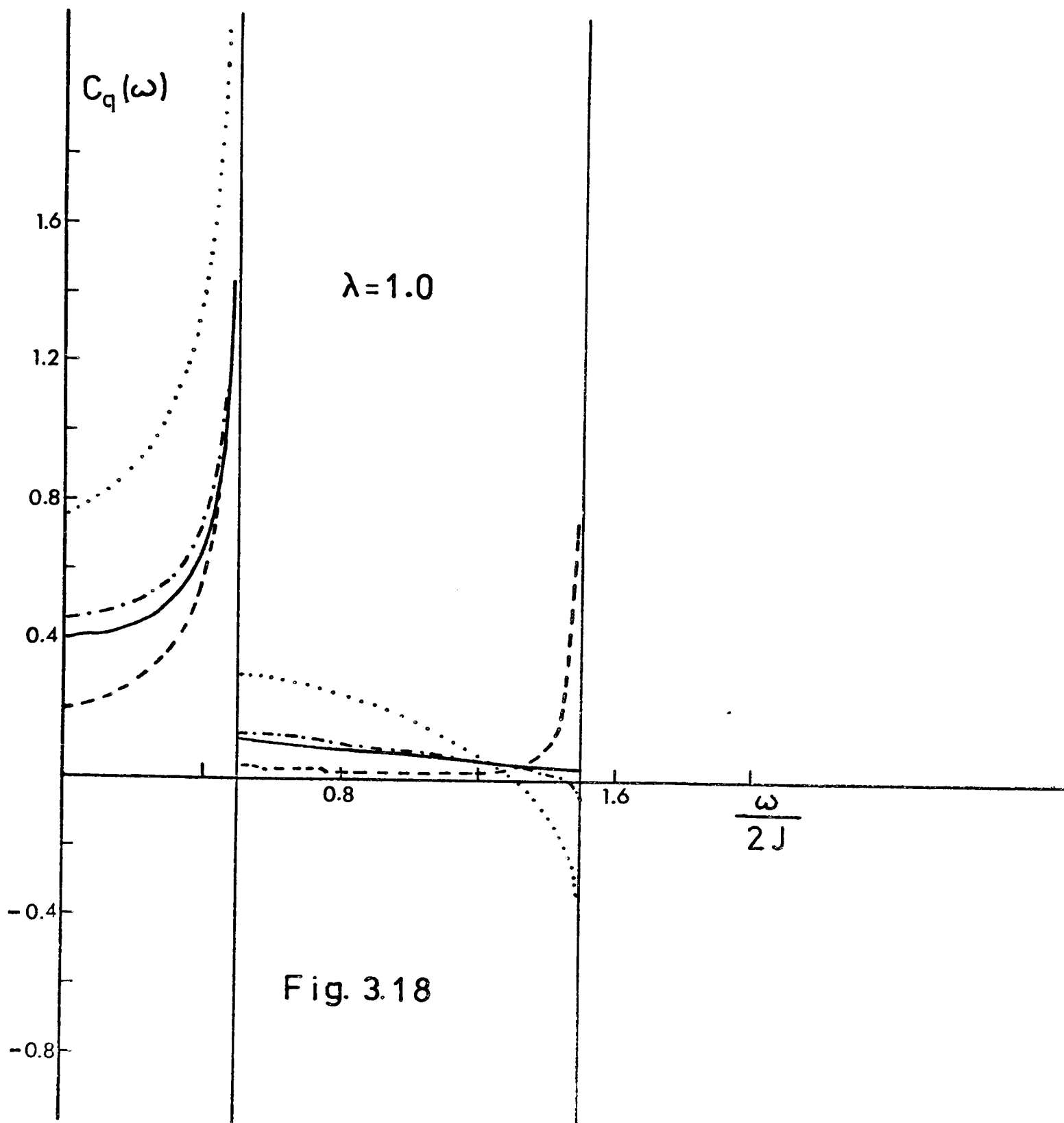


Fig. 3.18

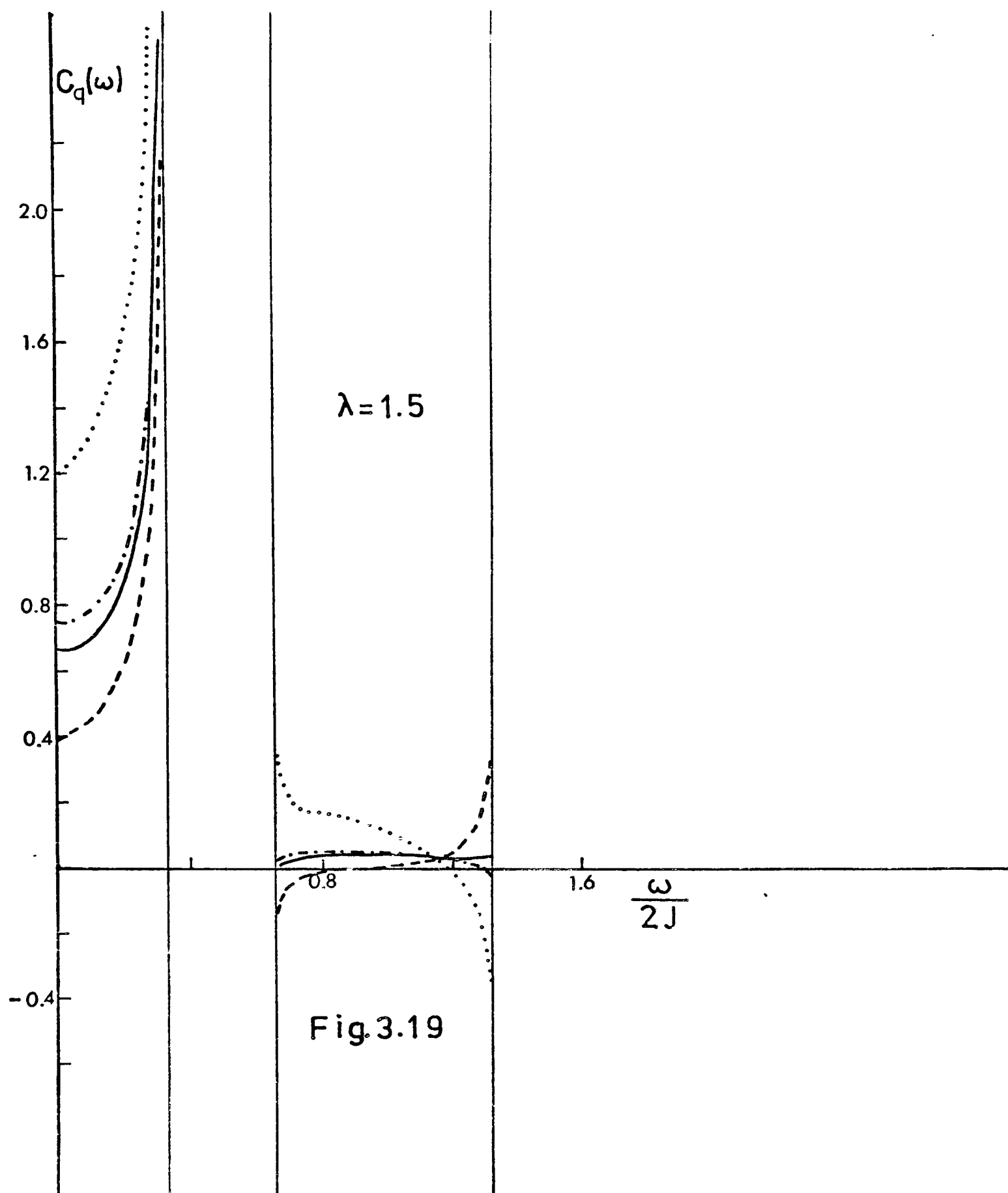


Fig.3.19

$$\frac{1}{N} \langle\langle S_{-q}^x; S_q^x \rangle\rangle = \frac{1}{2\pi} \int_{-\infty}^{\infty} d\omega' \frac{e^{-\beta\omega'} (e^{\beta\omega'} - 1)}{\omega - \omega'} C_q(\omega') . \quad (3.71)$$

Due to translational symmetry we have

$$\langle\langle S_{-q}^x; S_q^x \rangle\rangle = \langle\langle S_q^x; S_{-q}^x \rangle\rangle , \quad (3.72)$$

and this result together with eq. (1.10) implies that $\langle\langle S_{-q}^x; S_q^x \rangle\rangle$ must be a symmetric function of ω . In order to satisfy this condition we see immediately from eq. (3.71) that $C_q(\omega)$ should satisfy the equation

$$C_q(\omega) = e^{\beta\omega} C_q(-\omega) . \quad (3.73)$$

Unfortunately this equation is only satisfied at $\beta = 0$. We can, however, make it exact at any temperature by defining a new $C_q(\omega)$ as

$$\tilde{C}_q(\omega) = \frac{1}{2} [C_q(\omega) + e^{\beta\omega} C_q(-\omega)] . \quad (3.74)$$

The parameter ϵ , defined as

$$\epsilon = \left| \frac{\tilde{C}_q - C_q}{C_q} \right| , \quad (3.75)$$

has of course to be small in order to $C_q(\omega)$ be accepted as a good approximation. At $\beta = 0.1$, ϵ is less than 10^{-3} , which means that C_q is a good approximation. However, at $\beta = 1.0$, ϵ becomes of the order of 1, which shows clearly that we have to restrict the use of the approximation for $\beta \ll 0.1$.

Finally it should be noted that we cannot at this stage of the calculation restore the translational symmetry by simply considering C_q defined at in eq. (3.74). The redefinition of C_q implies for instance that the new static correlation functions obtained from it are no longer correct.

Chapter 4

Applications to One-dimensional Spin Systems

In this chapter we discuss two applications of the theory developed in the second chapter. In the first application we study the specific heat of a dilute isotropic XY-chain in a simple approximation, and compare it with the exact results obtained for finite chains. The second application is a study of the specific heat and thermal conductivity of the isotropic XY-chain in the presence of a multi-component random transverse field, in the framework of the coherent potential approximation. These results will be used to explain the thermal properties of $\text{Pr}(\text{C}_2\text{H}_5\text{SO}_4)_3 \cdot 9\text{H}_2\text{O}$, where one-dimensional behaviour has been suggested.

4.1 The Specific Heat of the Dilute XY-chain

The effect of non-magnetic impurities is to divide the chain into smaller open chains. As pointed out in chapter 2, provided the number of spins in any of these smaller chains is sufficiently large, this effect can be studied by considering the closed chain with one impurity and taking the limit $J' = 0$, eliminating at the same time the spurious contribution introduced by the limiting process.

The one-impurity solution will be extended to a concentration x of defects using the so-called average T-matrix approximation (Elliott et al., 1974). Our basic purpose is to treat an assembly of open chains of various lengths by using one of the

established methods of the study of disordered systems. Following the prescription above we have from eq. (2.55) that the T-matrix for the one impurity case is

$$T(k, k') = - \frac{\lambda_k \lambda_{k'}^*}{N A} , \quad (4.1)$$

where

$$A = \frac{1}{N} \sum_k \frac{1}{\omega - \epsilon_k} , \quad (4.2)$$

with

$$\epsilon_k = J \cos k a , \quad (4.3)$$

and where we have taken the external field equal to zero. From the above equation we get immediately

$$T(\ell, \ell') = - \frac{\delta_{\ell,2} \delta_{\ell',2}}{A} . \quad (4.4)$$

The lowest order average T-matrix approximation (ATA) consists in writing the self-energy as

$$\Sigma = \langle T(\ell, \ell') \rangle_{av} = \frac{-C}{A} , \quad (4.5)$$

where $\langle \rangle_{av}$ stands for configurational average. The averaged one-particle Green function $\langle G(k) \rangle_{av}$ is then written as

$$\langle G(k) \rangle_{av} = \frac{1}{\omega - \epsilon_k - \Sigma} , \quad (4.6)$$

and of course $\langle G(k) \rangle_{av}$ is by definition translationally invariant.

The density of states normalized to π is given by (Elliott et al., 1974)

$$\rho(\omega) = \frac{1}{2i} \lim_{\epsilon \rightarrow 0} [G(\omega - i\epsilon) - G(\omega + i\epsilon)] \quad , \quad (4.7)$$

where

$$G(\omega) = \frac{1}{N} \sum_k \langle G(k) \rangle_{av} \quad . \quad (4.8)$$

The internal energy is given by:

$$E = \frac{1}{\pi} \int_{-\infty}^{\infty} \frac{\omega \rho(\omega) d\omega}{e^{\beta\omega} + 1} \quad (4.9)$$

and the specific heat (Stanley, 1971) is

$$C_v = \frac{1}{\pi} \int_{-\infty}^{\infty} \frac{e^{\beta\omega} \omega^2 \rho(\omega) d\omega}{(e^{\beta\omega} + 1)^2} \quad (4.10)$$

Bartolomé et al. (1976) have considered the effect of dilution in Cs_2CoCl_4 . The magnetic behaviour of this material approximates that of the isotropic XY-chain ($S = \frac{1}{2}$) (Algra et al., 1975). The ratio $|\bar{J}/J|$ of inter-to intra-chain interaction is smaller than 10^{-2} , which ensures a good one-dimensional behaviour. However, the material develops three dimensional ordering at $T = 0.222^\circ\text{K}$. As has been shown by Imry et al. (1975), impurities have a drastic effect on the three dimensional ordering of quasi-one-dimensional systems. In the case of non-magnetic impurities this is mainly due to the

limitation of the correlation length following the division of the chain into smaller chains. Although Bartolomé et al. (1976) were particularly interested in the effect impurities on three dimensional ordering, they compared their measurements in the one-dimensional phase with numerical calculations performed by Blöte (see Bartolomé et al., 1976). These results were obtained by averaging the contributions of different chains and considering $n(\text{number of spins}) \leq 11$ (Blöte, 1975): we here obtain these results by a new approach. The system is only approximately an isotropic XY-chain and its Hamiltonian is written as:

$$H = - \sum [J(S_j^x S_{j+1}^x + S_j^y S_{j+1}^y) + J_{//} S_j^z S_{j+1}^z] , \quad (4.11)$$

where

$$\frac{J_{//}}{J} \cong \frac{1}{4} . \quad (4.12)$$

In our calculations we will neglect the last term in the Hamiltonian (4.11). This procedure seems justifiable since the specific heat of a single XY-chain does not change very much when the Ising term is added (Blöte, 1975), in particular when the parameters satisfy the relation (4.12).

Then the calculation of the specific heat is performed immediately by using eqs. (4.5) to (4.10). Since $A(\omega - i\epsilon)$ can be calculated exactly, and it does not depend on k , we can also calculate the density of states exactly. From eq. (4.2), for $|\omega| \leq J$, we have

$$\lim_{\epsilon \rightarrow 0} A(\omega - i\epsilon) = \frac{\mathcal{P}}{N} \sum_k \frac{1}{\omega - \varepsilon_k} + i \tilde{\Pi} \frac{1}{N} \sum_k \delta(\omega - \varepsilon_k) , \quad (4.13)$$

by using the well known identity (Parry, 1973)

$$\lim_{\epsilon \rightarrow 0} \frac{1}{x - i\epsilon} = \frac{\mathcal{P}}{X} + i \tilde{\Pi} \delta(x) , \quad (4.14)$$

where $\mathcal{P}$ stands for Cauchy principal value. Then we get immediately

$$\Im A(\omega) = \frac{1}{\sqrt{J^2 - \omega^2}} . \quad (4.15)$$

The real part of $A(\omega)$ is calculated by transforming the sum over k into an integral, and then evaluating it in the complex plane. Although the procedure is well known we will briefly summarize it here because this result will be used on several occasions. Thus, we have

$$\Re A(\omega) = \mathcal{P} \frac{1}{N} \sum_k \frac{1}{\omega - \varepsilon_k} = \frac{\mathcal{P}}{2\tilde{\Pi}} \int_{-\tilde{\Pi}}^{\tilde{\Pi}} \frac{d\theta}{\omega - J \cos \theta} , \quad (4.16)$$

and from this equation we get

$$\Re A(\omega) = \frac{\mathcal{P}}{J\tilde{\Pi}i} \oint \frac{dz}{(2z\bar{\omega} - z^2 - 1)} , \quad (4.17)$$

where

$$\bar{\omega} = \frac{\omega}{J} \quad (4.18)$$

and the contour is the unit circle in the complex plane centred on the origin. The poles of the integrand are at

$$z = \bar{\omega} \pm \sqrt{\bar{\omega}^2 - 1} , \quad (4.19)$$

and since $-1 \leq \omega \leq 1$ both are on the integration contour.

Although the integral does not exist in this case, the principal value does and is calculated by deforming the contour and using the residue theorem (Whittaker and Watson, 1973). This procedure is straightforward and gives

$$\text{Re } A(\omega) = 0 . \quad (4.20)$$

then for $|\omega| \leq J$

$$\lim_{\epsilon \rightarrow 0} \sum (\omega - i\epsilon) = i\epsilon \sqrt{J^2 - \omega^2} . \quad (4.21)$$

Using eqs. (4.15) and (4.21) in eq. (4.8), and following the procedure already discussed we get

$$\lim_{\epsilon \rightarrow 0} G(\omega - i\epsilon) = - \frac{2}{(z_1 - z_2)} , \quad (4.22)$$

where z_1 is the smaller (in absolute value) and z_2 the larger of the z 's defined as

$$z = \omega - \sum \pm \sqrt{(\omega - \sum)^2 - J} . \quad (4.23)$$

Of course from eq. (4.7) $\rho(\omega)$ is the imaginary part of eq. (4.22).

If $|\omega| > J$ we obtain $A(\omega)$ immediately, as

$$A(\omega) = \begin{cases} \frac{1}{\sqrt{\omega^2 - J^2}} & \omega > J \\ -\frac{1}{\sqrt{\omega^2 - J^2}} & \omega < J \end{cases} \quad (4.24)$$

It is easy to verify that $\langle G(k) \rangle_{av}$ has no poles, and consequently $\rho(\omega)$ is zero for those frequencies which are outside the band, i.e. $|\omega| > J$. The calculation of the specific heat, eq. (4.10), is performed numerically using eqs. (4.21), (4.22) and (4.23). The results obtained are shown in figs. (4.1), (4.2), and (4.3), where we compare them with Blöte's numerical calculations (dashed line). They are in good agreement with the others already mentioned, even at high concentration. In fact, our calculations are in better agreement with the experimental results presented by Bartolomé et al. (1976), than those by Blöte. It should be remembered, however, that we have neglected the Ising term in eq. (4.11). Even considering that the specific heat is not particularly sensitive to the approximations, apart from the critical region, the results are better than one should expect from a simple approximation.

4.2 The Specific Heat of the Isotropic XY-Chain in a Transverse Random Field

In the application that we are going to present, we will consider only site diagonal disorder and the Green function G , defined in eqs.(4.7) and (4.8), will be calculated by using the coherent potential approximation which was developed

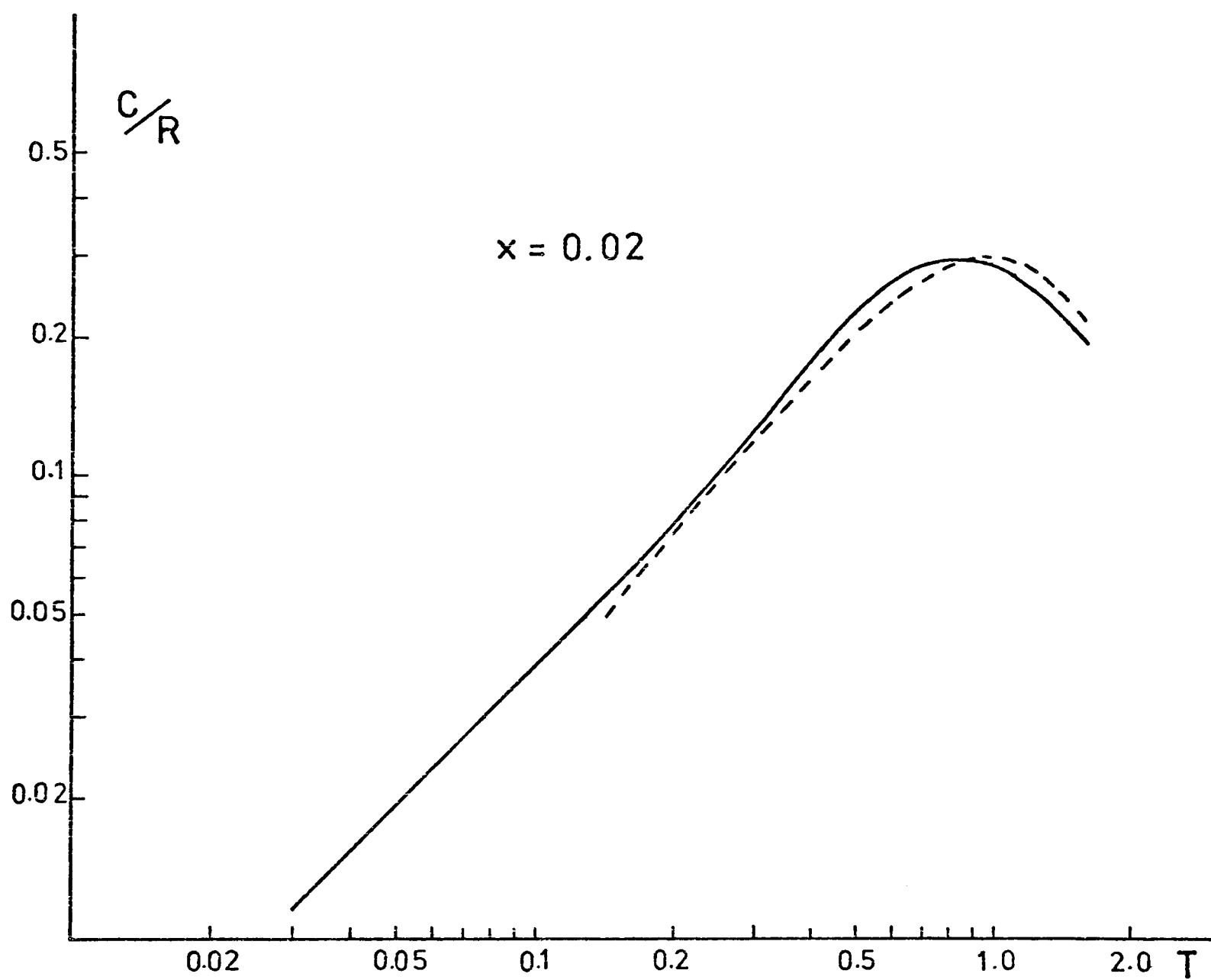


Fig. 4.1

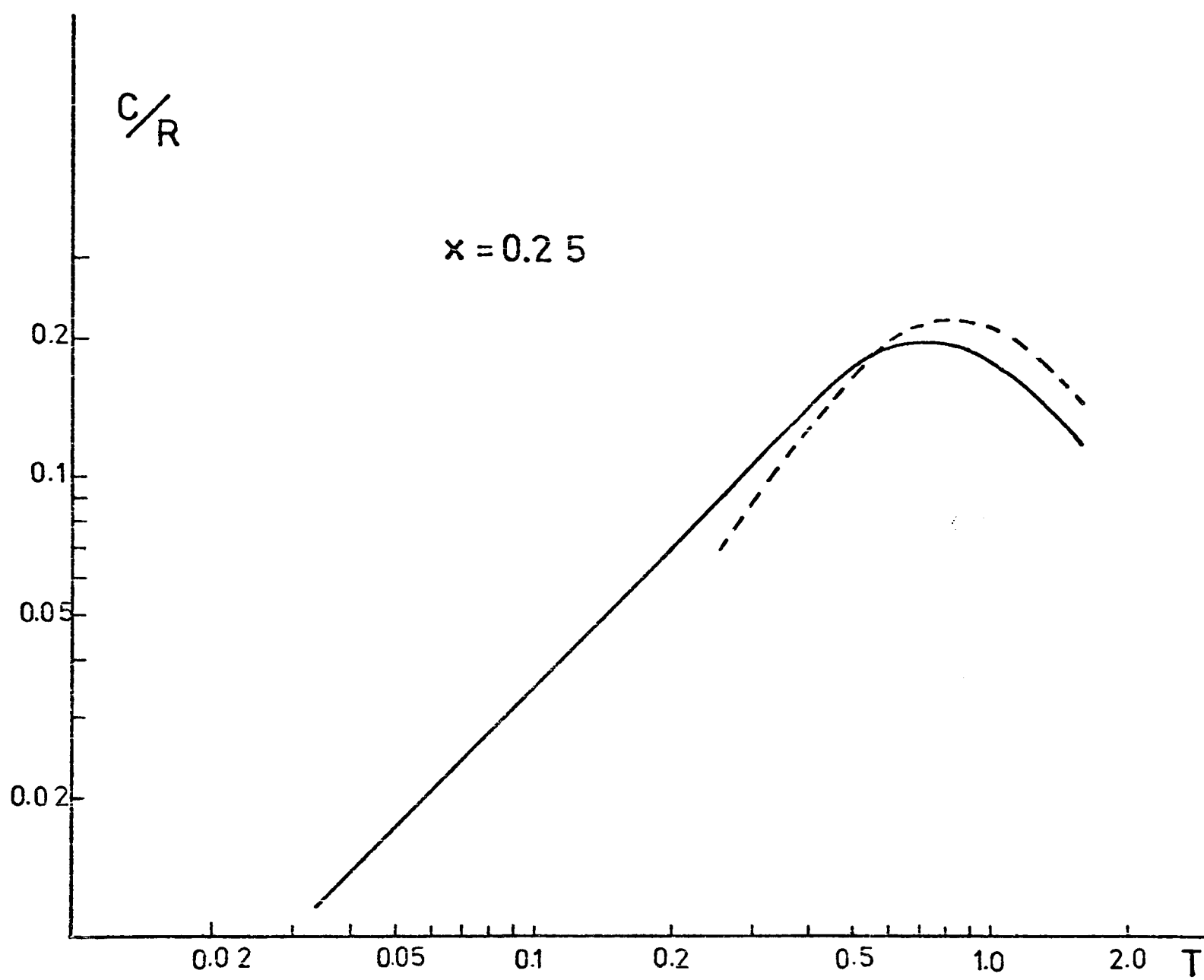


Fig. 4.2

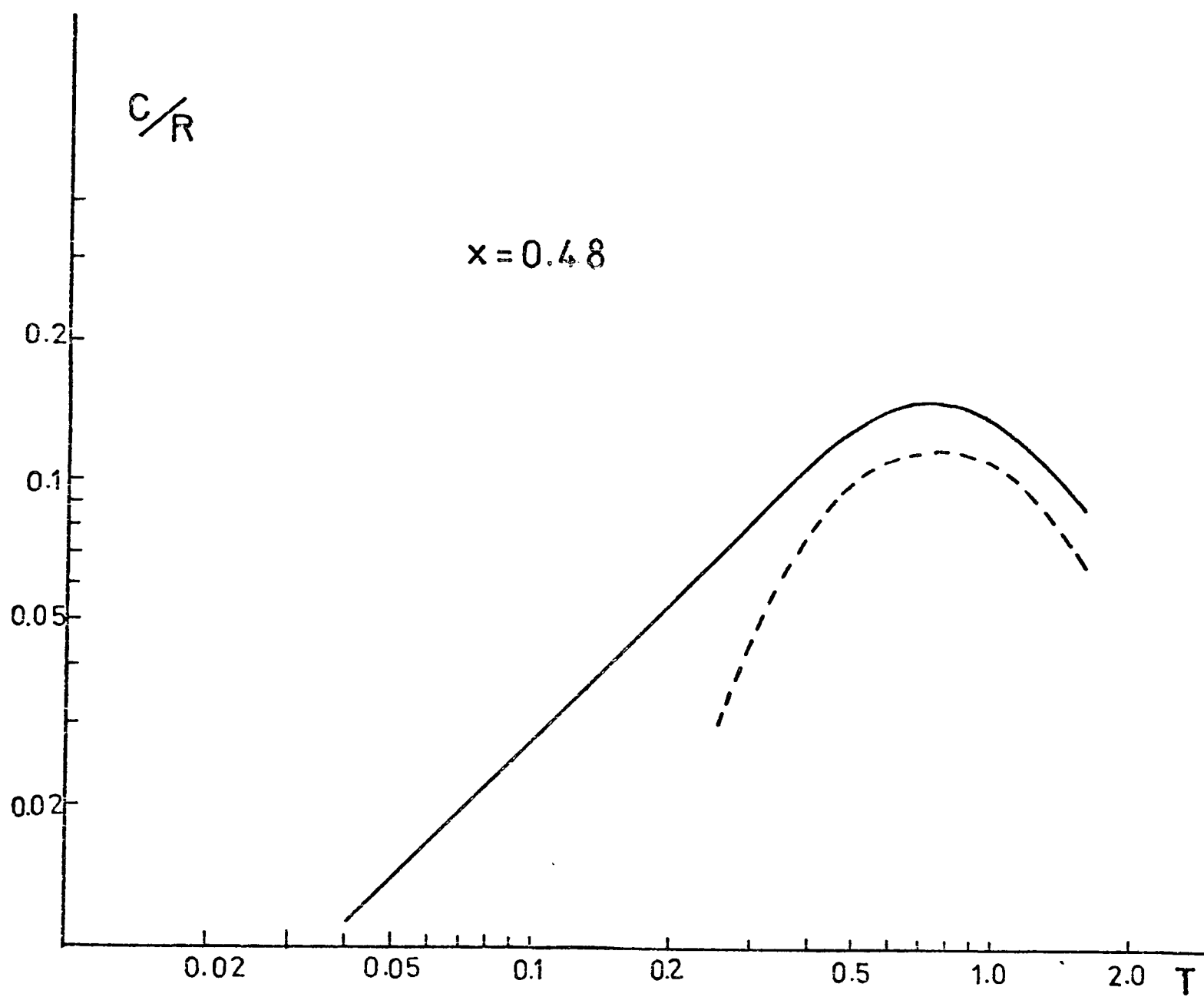


Fig. 4.3

simultaneously by Taylor (1967) and Soven (1967). This approximation is well established and discussed in detail in the reviews by Elliott et al. (1974), and Yonezawa and Morigaki (1973). It is based on the assumption that the average of the exact T-matrix is zero, and since we do not know how to obtain it we approximate this condition by

$$\langle t \rangle_{av} = 0, \quad (4.25)$$

where t is the single-site t -matrix with internal propagator G . This of course leads to a self consistent theory which is solved numerically. G is an effective medium Green function which is assumed to be equal to the configurational average Green function.

As has already been pointed out, G can be obtained analytically in terms of Σ through the eqs. (4.22) and (4.23).

Folinsbee et al. (1976) have studied the low-temperature properties of praseodymium ethyl sulphate, $\text{Pr}(\text{C}_2\text{H}_5\text{SO}_4)_3 \cdot 9\text{H}_2\text{O}$, and concluded that the material exhibits one-dimensional behaviour which may be described by the spin $\frac{1}{2}$ Hamiltonian

$$H = \sum_i J_0 S_i^z S_{i+1}^z + \sum_i J (S_i^x S_{i+1}^x + S_i^y S_{i+1}^y). \quad (4.26)$$

The ration J_0/J is

$$\frac{J_0}{J} \sim 10^{-2} \quad (4.27)$$

which means that the Hamiltonian (4.26) is very close to the ideal XY Hamiltonian. Another interesting aspect of praseodymium ethyl sulphate is the non-appearance of three dimensional order, which is exhibited by the isomorphic compound PrCl_3 (Harrison et al., 1976).

The specific heat exhibits a broad one-dimensional peak as a function of temperature. The location of the peak agrees with the result obtained by Katsura (1962; 1963), nevertheless its value is substantially less than the value of the XY-model. Folinsbee et al. (1976) have argued that this is mainly due to the presences of Pr hyperfine interaction, namely $AS_i^Z I_i^Z$. They have considered the effect of this term in the Hamiltonian (4.26) as an effective field in the z-direction and in this approximation they have been able to fit the experimental results. Naturally this is a very poor approximation and a more accurate treatment is necessary.

The Hamiltonian (4.26), when neglecting the first term and adding the hyperfine interaction is written as

$$H = \sum_j J(S_j^x S_{j+1}^x + S_j^y S_{j+1}^y) + A \sum_j S_j^z I_j^z \quad (4.28)$$

The operator I_j^z commutes with H , and consequently the hyperfine interaction can be treated as a random field. Since the nuclear spin is $5/2$ (Abragam and Bleaney, 1970) the random field has six components.

In the approximate calculation which we present we will neglect the thermal fluctuations in the occupancy of the nuclear levels, and consider the situation where they are equally populated. This means that we have to consider equal probabilities for the different components of the random field which will be expressed in the CPA equation as concentrations. This approximation is justified by the assumption that at temperatures of interest the thermal average of the interaction term is small compared with $k_B T$. Since the average random field is zero, and the system develops short range order only in the XY-plane, we have $\langle S^Z \rangle$ equal to zero, and consequently the mentioned approximation is acceptable.

From eq. (2.53) taking h and ΔJ equal to zero we get

$$T_{kk'} = - \frac{h'}{1 + h'A} \quad , \quad (4.29)$$

which in site representation becomes

$$T(\ell, \ell') = - \frac{h' \delta_{\ell,2} \delta_{\ell',2}}{1 - h'A} \quad . \quad (4.30)$$

Making the suitable changes in the previous expression, the CPA equation, namely eq. (4.25) yields

$$\sum_{j=1}^6 \frac{x_j (h_j - \Sigma)}{1 - (h_j - \Sigma)G} = 0 \quad , \quad (4.31)$$

where

$$G = \frac{1}{N} \sum_k \frac{1}{\omega - \epsilon_k - \Sigma} \quad , \quad (4.32)$$

and

$$x_j = \frac{1}{6} ; \quad h_j = \pm \frac{5}{2}, \pm \frac{3}{2}, \pm \frac{1}{2} ; \quad j = 1, 2, \dots, 6 .$$

(4.33)

Eqs. (4.31) and (4.32) are solved numerically by using the Newton-Raphson method (see for instance McCracker and Dorn, 1966), and of course using the exact expression for G given in eqs. (4.22) and (4.23). The density of states is obtained by using eq. (4.7) and from this the specific heat given by eq. (4.10). The result obtained by using the praseodymium ethyl sulphate parameters (Folinsbee et al., 1976) is shown in fig. (4.4) and compared with the experimental result. As we see, the maximum of the C/R is 0.315, in which case it has changed very little when compared to Katsura's result, which is 0.325. We tried to find a value of A which could fit the experimental results, considering a two-component ($S = \frac{1}{2}$) random field. Unfortunately the minimum value obtained for the peak was 0.303 for $A/J = 1$, which is much larger than experimental result, 0.25. These results rule out the possibility of the hyperfine interaction being responsible for the anomalous behaviour of the specific heat. In view of all these facts we believe that the splitting of the ground doublet due to random strains is responsible for the anomalous behaviour of the specific heat. Since this term is represented in the Hamiltonian as a field in the X direction, any calculation, even approximate, is very complicated and we leave the problem at this point.

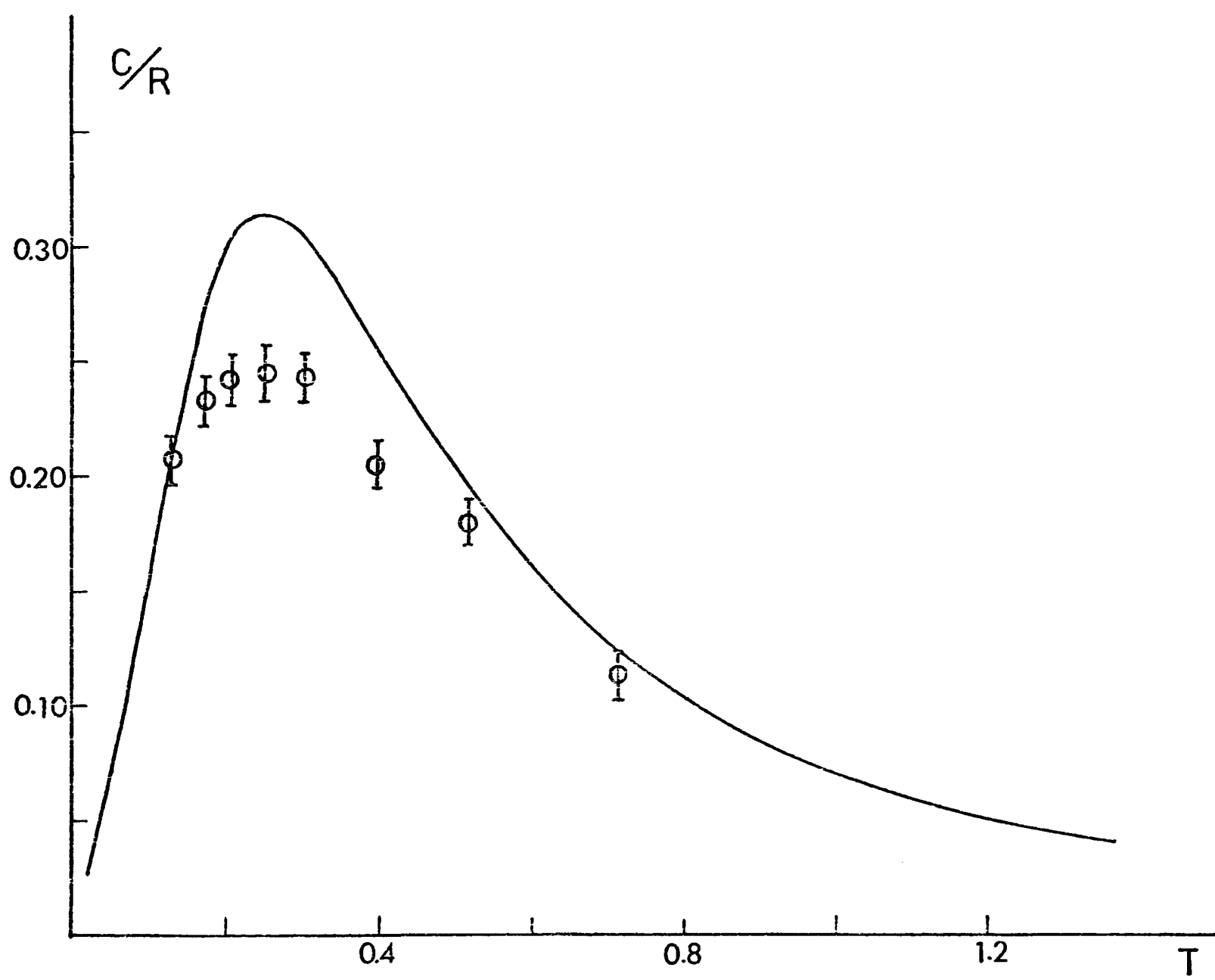


Fig. 4.4

4.3 The Thermal Conductivity of the Isotropic XY-chain in a Transverse Random Field

Before we consider specific applications we will express the thermal conductivity in terms of configurational average Green functions, when there are many impurities in the system. Let us start by considering the heat-flux operator, eq. (2.68), which can be written as:

$$Q = \sum_{\ell, \ell'} J(\ell, \ell') c_{\ell}^{\dagger} c_{\ell'} \quad . \quad (4.34)$$

Following Flicker and Leath (1973) we can write eq. (2.68) as:

$$K = \frac{1}{LT} \frac{d}{d\omega} \text{Im} \langle\langle Q, Q \rangle\rangle \Big|_{\omega=0} \quad , \quad (4.35)$$

where the Green function on the left hand side is defined in terms of the commutator. Putting this result together with eq. (4.25) it is clear that we need the commutator Green function $\langle\langle c_{\ell}^{\dagger} c_{\ell'} ; c_m^{\dagger} c_m \rangle\rangle^{(-)}$. Since the Hamiltonian, even in the presence of impurities, is a bilinear form in fermion operators, we have the decomposition

$$\begin{aligned} \langle\langle c_{\ell}^{\dagger} c_{\ell'} ; c_m^{\dagger} c_m \rangle\rangle^{(-)} &= \langle c_{\ell}^{\dagger}(t) c_m(0) \rangle \langle\langle c_{\ell}^{\dagger} ; c_m \rangle\rangle - \\ &\quad - \langle c_m^{\dagger}(0) c_{\ell'}(t) \rangle \langle\langle c_{\ell'} ; c_m^{\dagger} \rangle\rangle \quad , \end{aligned} \quad (4.36)$$

where the Green functions on the right hand side are defined in terms of anti-commutator. This result is easily obtained by considering the transformation that diagonalizes the Hamiltonian in the isotropic case, namely (Tyablikov, 1967)

$$c_\ell = \sum_j \varphi_{\ell j} \beta_j \quad , \quad (4.37)$$

and Wick's theorem.

Performing the Fourier transform of eq. (4.28) we get:

$$\begin{aligned} \langle\langle c_\ell^+ c_{\ell'}; c_m^+ c_{m'} \rangle\rangle^{(-)} = \frac{1}{2\pi} \int_{-\infty}^{\infty} dz \left[\langle c_\ell^+ c_{m'} \rangle_z \langle\langle c_{\ell'}; c_m^+ \rangle\rangle_{\omega-z} - \right. \\ \left. - \langle c_m^+ c_{\ell'} \rangle_z \langle\langle c_\ell^+; c_{m'} \rangle\rangle_{\omega-z} \right] \end{aligned} \quad (4.38)$$

where $\langle c^+ \rangle_\omega$ and $\langle\langle c^+; c \rangle\rangle_\omega$ are the Fourier transforms of $\langle c^+(t) c(0) \rangle$ and $\langle\langle c^+(t); c \rangle\rangle$ respectively.

Introducing in the previous equation the results (Parry, 1973):

$$\langle c_\ell^+ c_{m'} \rangle_z = \frac{e^{\beta z}}{e^{\beta z} + 1} 2 \operatorname{Im} \langle\langle c_\ell^+; c_{m'} \rangle\rangle = 2 n(-z) \operatorname{Im} \langle\langle c_\ell^+; c_{m'} \rangle\rangle \quad , \quad (4.39)$$

$$\langle c_m^+ c_{\ell'} \rangle = \frac{2}{e^{\beta z} + 1} \operatorname{Im} \langle\langle c_m; c_{\ell'}^+ \rangle\rangle = 2 n(z) \operatorname{Im} \langle\langle c_m; c_{\ell'}^+ \rangle\rangle \quad , \quad (4.40)$$

where $n(z)$ is the fermion occupation number, and considering the transformation $z \rightarrow -z$ in the first term, we obtain

$$\begin{aligned} \operatorname{Im} \langle\langle c_\ell^+ c_{\ell'}, c_m^+ c_{m'} \rangle\rangle^{(-)} = \frac{1}{\pi} \int_{-\infty}^{\infty} n(z) dz \left[\operatorname{Im} \langle\langle c_\ell^+; c_{m'} \rangle\rangle_{-z} \operatorname{Im} \langle\langle c_{\ell'}; c_m^+ \rangle\rangle_{\omega+z} \right. \\ \left. - \operatorname{Im} \langle\langle c_{\ell'}; c_m^+ \rangle\rangle_z \operatorname{Im} \langle\langle c_\ell^+; c_{m'} \rangle\rangle_{\omega-z} \right] \quad . \quad (4.41) \end{aligned}$$

From this we get immediately that

$$\begin{aligned} & \frac{d}{d\omega} \operatorname{Im} \langle\langle c_{\ell}^+ c_{\ell'}; c_m^+ c_{m'} \rangle\rangle^{(-)} = \\ & = \frac{1}{\tilde{\Pi}} \int_{-\infty}^{\infty} n(z) dz \left[\operatorname{Im} \langle\langle c_{\ell'}^+; c_{m'} \rangle\rangle_{-z} \frac{d}{dz} \operatorname{Im} \langle\langle c_{\ell'}; c_m^+ \rangle\rangle_z \right. \\ & \quad \left. + \operatorname{Im} \langle\langle c_{\ell'}; c_m^+ \rangle\rangle_z \frac{d}{dz} \operatorname{Im} \langle\langle c_{\ell}^+; c_{m'} \rangle\rangle_{-z} \right], \end{aligned} \quad (4.42)$$

and using the property shown in eq. (1.10) we obtain

$$\begin{aligned} & \frac{d}{d\omega} \operatorname{Im} \langle\langle c_{\ell}^+ c_{\ell'}; c_m^+ c_{m'} \rangle\rangle \Big|_{\omega=0} = \\ & = - \frac{1}{\tilde{\Pi}} \int_{-\infty}^{\infty} n(z) \frac{d}{dz} \left[\operatorname{Im} \langle\langle c_{m'}; c_{\ell}^+ \rangle\rangle_z \operatorname{Im} \langle\langle c_{\ell'}; c_m^+ \rangle\rangle_z \right] dz. \end{aligned} \quad (4.43)$$

Integrating by parts the last equation and using eq. (4.26), the thermal conductivity is written as

$$K = - \frac{1}{LT} \sum_{\ell \ell'} \sum_{m m'} J(\ell, \ell') J(m, m') \frac{1}{\tilde{\Pi}} \int_{-\infty}^{\infty} \frac{dn(z)}{dz} \operatorname{Im} \langle\langle c_{m'}; c_{\ell}^+ \rangle\rangle_z \operatorname{Im} \langle\langle c_{\ell'}; c_m^+ \rangle\rangle_z dz \quad (4.44)$$

or in a more compact form

$$K = - \frac{1}{\tilde{\Pi} LT} \int_{-\infty}^{\infty} \frac{dn(z)}{dz} \operatorname{Tr} [\operatorname{Im} \tilde{G} \tilde{J} \operatorname{Im} \tilde{G} \tilde{J}] dz, \quad (4.45)$$

where $\tilde{J}$ is a matrix with elements $J(l, l')$.

Of course, when many impurities are present, the trace in eq. (4.45) can be evaluated only approximately, and it should be understood that in this case we are considering the configurational average Green function. The $\operatorname{Tr} \langle \tilde{I}_m \tilde{G} \tilde{I}_m \tilde{G} \rangle_{av}$ can be written as

$$\text{Tr} \langle \text{Im} \tilde{G} \tilde{J} \text{Im} \tilde{G} \tilde{J} \rangle_{av} = \frac{1}{4i} \text{Tr} \langle (\tilde{G} - \tilde{G}^*) \tilde{J} (\tilde{G} - \tilde{G}^*) \tilde{J} \rangle_{av} , \quad (4.46)$$

and from this it is clear that we need to calculate terms like $\text{Tr} \langle \tilde{G} \tilde{J} \tilde{G} \tilde{J} \rangle_{av}$ and $\text{Tr} \langle \tilde{G} \tilde{J} \tilde{G}^* \tilde{J} \rangle_{av}$. In order to calculate these terms we follow the procedure adopted by Flicker and Leath (1973), since we are considering only site diagonal impurities. Then let us consider $\text{Tr} \langle \tilde{G} \tilde{J} \tilde{G} \tilde{J} \rangle_{av}$. Expanding $\tilde{G}$ in terms of the effective medium propagator G and the single-site t -matrices as

$$\tilde{G} = G + G t G + G t G t G + \dots , \quad (4.47)$$

we get

$$\begin{aligned} \text{Tr} \langle \tilde{G} \tilde{J} \tilde{G} \tilde{J} \rangle_{av} = \sum_{\ell} \langle J(\ell, n) [G(n, m) + \sum_1 G(n, 1) t_1 G(1, m) + \\ + \dots] J(m, p) [G(p, \ell) + \sum_1 G(p, 1') t_{1'} G(1', \ell) + \dots] \rangle_{av} . \end{aligned} \quad (4.48)$$

Since in the CPA the average value of the single-site t -matrix is zero, in order to be consistent with the appropriate Ward identity, only terms with an even number of t 's will contribute in the average of eq. (4.48). If we decouple average of product of t 's in a nested fashion:

$$\begin{aligned} \langle t_1 t_2 \dots t_n \rangle_{av} &\cong \langle t_1 \langle t_2 \langle t_3 \langle \dots \rangle t_{n-2} \rangle t_{n-1} \rangle t_n \rangle_{av} = \\ &= \langle t_n^2 \rangle_{av}^{n/2} \delta_{1,n} \delta_{2,n-1} \dots , \end{aligned} \quad (4.49)$$

and use the result in eq. (4.48), there is left in each term a quantity of the form

$$\sum_m G(n, m) J(m, p) G(p, n) , \quad (4.50)$$

which is zero, since G is even under inversion and J is odd.

Therefore the average is factorized as

$$\langle \tilde{G} \tilde{J} \tilde{G} \tilde{J} \rangle_{av} = \langle \tilde{G} \tilde{J} \rangle_{av} \langle \tilde{G} \tilde{J} \rangle_{av} . \quad (4.51)$$

Applying the same procedure we could factorize $\langle \tilde{G} \tilde{J} \tilde{G}^* \tilde{J} \rangle_{av}$, and then write

$$\langle I_m \tilde{G} \tilde{J} I_m \tilde{G} \tilde{J} \rangle_{av} = \langle I_m \tilde{G} \tilde{J} \rangle_{av} \langle I_m \tilde{G} \tilde{J} \rangle_{av} . \quad (4.52)$$

This equation can also be written as

$$\langle I_m \tilde{G} \tilde{J} I_m \tilde{G} \tilde{J} \rangle_{av} \cong \tilde{J} I_m G \tilde{J} I_m G , \quad (4.53)$$

where in this expression the elements of $\tilde{J}$ are obtained from eq. (2.68) considering all J 's equal. In this approximation the effect of impurities appear only through the configurational average Green function. Using the translational symmetry of G and eq. (4.53) the thermal conductivity is then expressed as

$$\mathcal{K} = - \frac{1}{\tilde{V} L T} \int_{-\infty}^{\infty} \frac{dn(z)}{dz} \sum_k v_k^2 \mathcal{E}_k^2 [I_m \langle G(k) \rangle]^2 \quad (4.54)$$

where v_k is the group velocity and $\langle G(k) \rangle_{av}$, defined as in eq. (4.6), is the averaged single particle Green function. The sum over k 's in eq. (4.54), namely

$$\mathcal{I} = \sum_k v_k^2 \mathcal{E}_k [I_m \langle G(k) \rangle]^2 , \quad (4.55)$$

is expressed in terms of G defined in eq. (4.8) as follows:

$$\begin{aligned} \mathbb{I} = & -N(\Sigma - \Sigma^*)^2 a^2 + N(\omega - \Sigma)^3 a^2 G + N(\omega - \Sigma^*)^3 a^2 G^* \\ & + \frac{2(\omega - \Sigma)(\omega - \Sigma^*)N}{\Sigma^* - \Sigma} [J^2 - (\omega - \Sigma)^2] a^2 G \\ & + \frac{2(\omega - \Sigma)(\omega - \Sigma^*)a^2 N}{\Sigma^* - \Sigma} [(\omega - \Sigma^*)^2 - J^2] G^* . \end{aligned} \quad (4.56)$$

For the case of the praseodymium ethyl sulphate the thermal conductivity can be evaluated immediately using G obtained from eqs. (4.31) and (4.32). The results are obtained numerically and shown in fig. (4.5). Apart from a small region in the lowest temperature limit, the calculated thermal conductivity due to spins is at least one order of magnitude smaller than the experimental results (dashed line). Also it decreases as the temperature increases, showing an opposite behaviour. The results clearly suggest that the phonons are really responsible for the thermal conductivity, agreeing with Folinsbee et al. They have reached this conclusion on grounds of very strong temperature dependence of the thermal conductivity ($K \propto T^5$) between 0.2° and 2°K . However, they overlooked the thermal conductivity due to spins which in principle could give a non-negligible contribution as suggested by the crude estimate of the thermal conductivity at low temperature considering only boundary scattering and using the kinetic theory result (see for instance Ziman, 1965):

$$K = \frac{1}{3} \sum c_q v_q \ell_q , \quad (4.57)$$

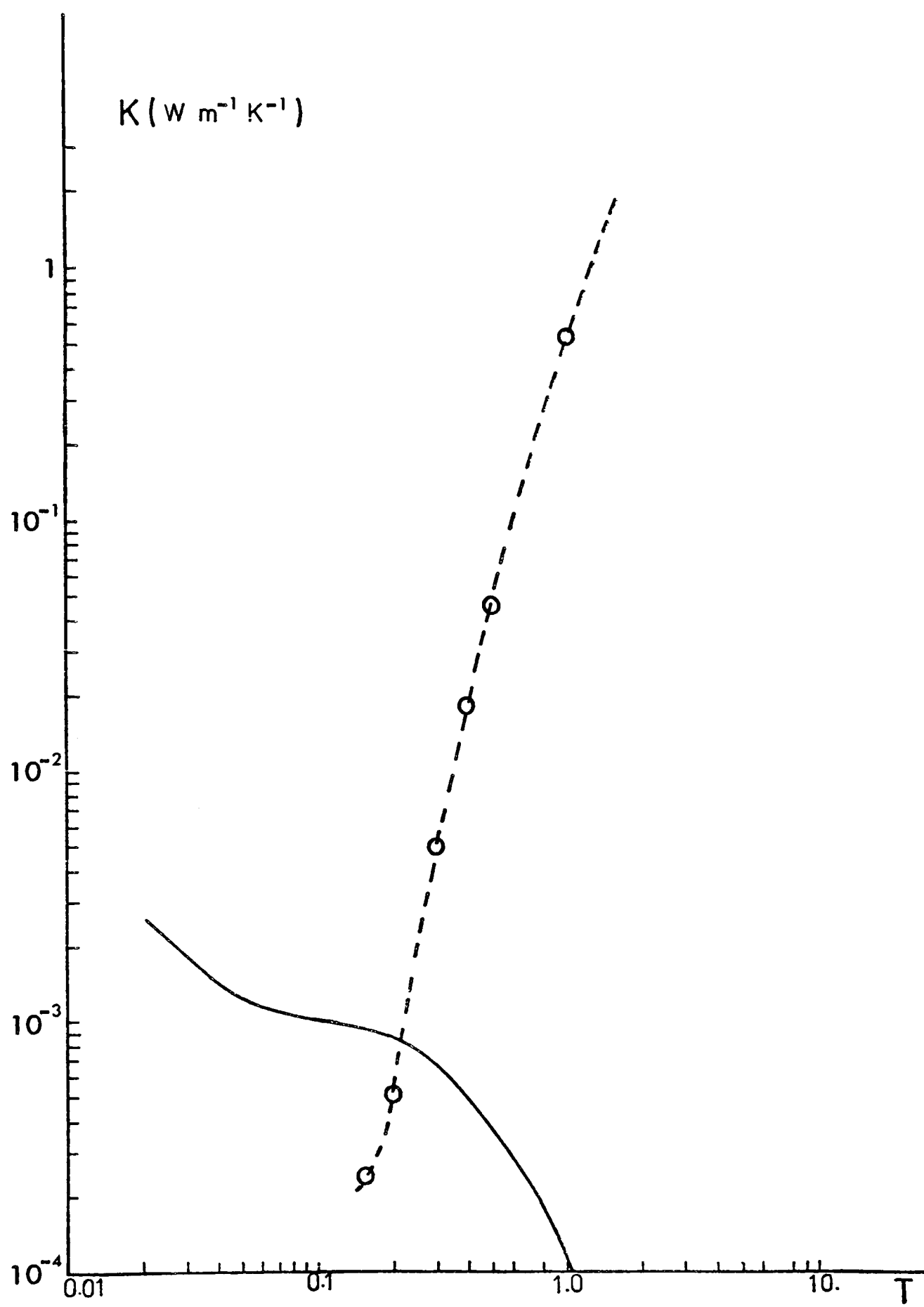


Fig. 4.5

where ℓ_q the mean-free path, v_q the group velocity and e_q the specific heat, which gives $k_p/k_s \sim 10^{-4}$. The hyperfine interaction, although not explaining the anomalous behaviour of the specific heat, is very effective in damping the otherwise non-interacting spin excitation, because they are one-dimensional.

Chapter 5

Peierls Instability in One-dimensional Systems

In this chapter we discuss the phonon dispersion and instability in two one-dimensional systems. The first one is an interacting electron-phonon system, where the instability is a giant Kohn anomaly (Kohn, 1959) which drives a Peierls instability (Peierls, 1955), and the second an interacting spin-phonon system. As we will see later these results constitute the basis for getting the behaviour of quasi-one-dimensional systems. However, we will restrict our discussion to one-dimensional cases. We also present a brief discussion of the Peierls transition as it was proposed originally.

5.1 The One-dimensional Peierls Instability

Although this effect has been discussed on many occasions since its original publication, we present here a simple discussion of it, for the sake of completeness and to make clear the ideas presented in this chapter.

Let us start by considering a one-dimensional lattice, of lattice parameter a , Fig. (5.1), and for simplicity let us assume that there is one electron per unit cell. It is well known (see for instance Peierls, 1955) that the energy levels of an electron in presence of a periodic potential present a band structure, and that these bands are limited by the limits of the Brillouin zones. The first band is limited by the wave-vectors $\frac{\pi}{a}$ and $-\frac{\pi}{a}$, and since we have one electron per unit

cell this band is half-filled. This situation is shown in fig. (5.2), where it is also clear that the Fermi surface reduces to two points. Naturally this system is a conductor.

Suppose now that we distort the chain in such a way that the new lattice parameter becomes $2a$, fig. (5.3). Thus, in this new situation where we have reduced the translational symmetry, the first Brillouin zone is limited by the wave-vectors $-\frac{\pi}{2a}$ and $\frac{\pi}{2a}$, and consequently a gap appears in the spectrum exactly at the Fermi surface as shown in fig. (5.4). This implies that the total energy of the electrons is lowered. Assuming this variation of energy proportional to the deformation, the total energy of the system is lowered and it undergoes a metal-insulation or metal-semiconductor transition, since the upper bands are empty. This is the so-called Peierls instability, and was proposed by Peierls in 1955.

Naturally the mechanism that causes the distortion is the electron-phonon interaction, and it is driven by the softening of a particular phonon mode which is a giant Kohn anomaly. The distorted phase just discussed is obtained by the condensation of the phonon mode of wave-vector $\frac{\pi}{a}$. There is also associated with this instability the formation of a charge density wave (CDW), which is the electron response to the instability.

5.2 The Coupled Electron-phonon System

The discover of quasi-one-dimensional materials (Zeller, 1973; Steiner et al., 1976; Berlinsky, 1976) which exhibit critical behaviour has renewed interest in the physics of low

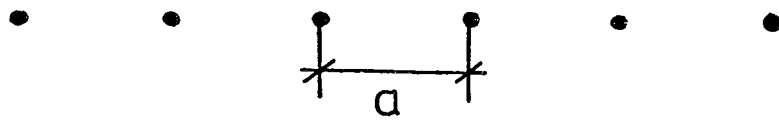


Fig. 5.1

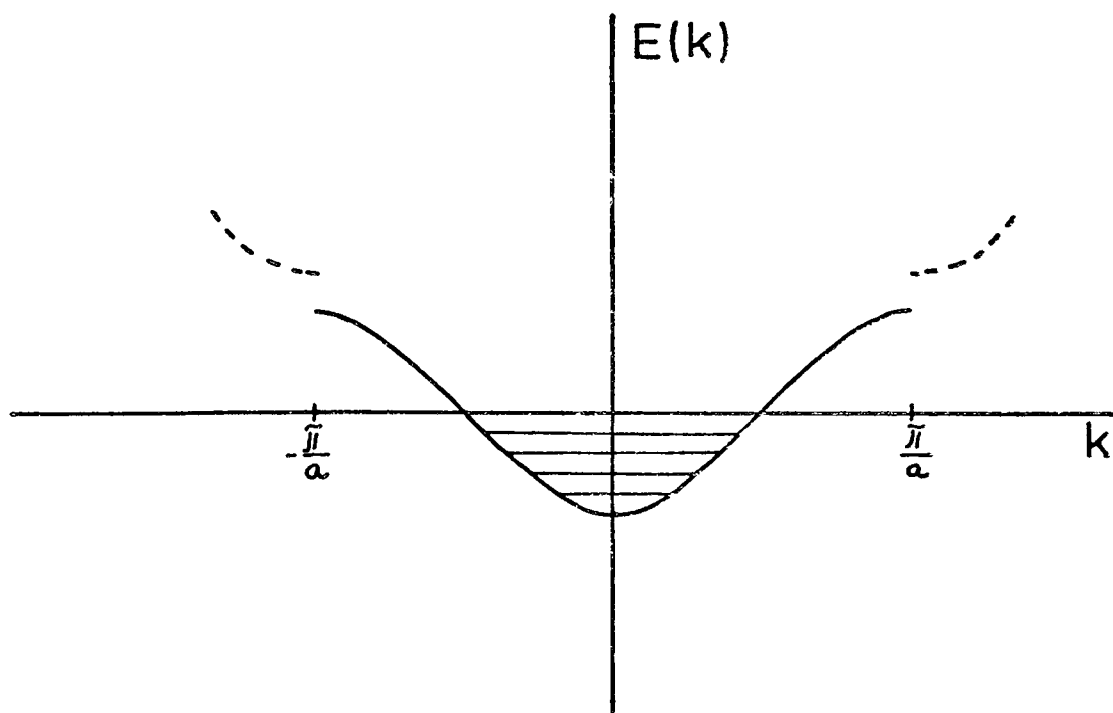


Fig. 5.2

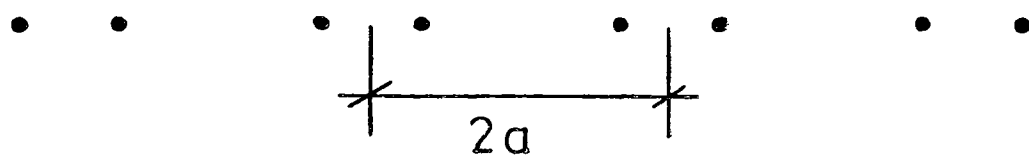


Fig.5.3

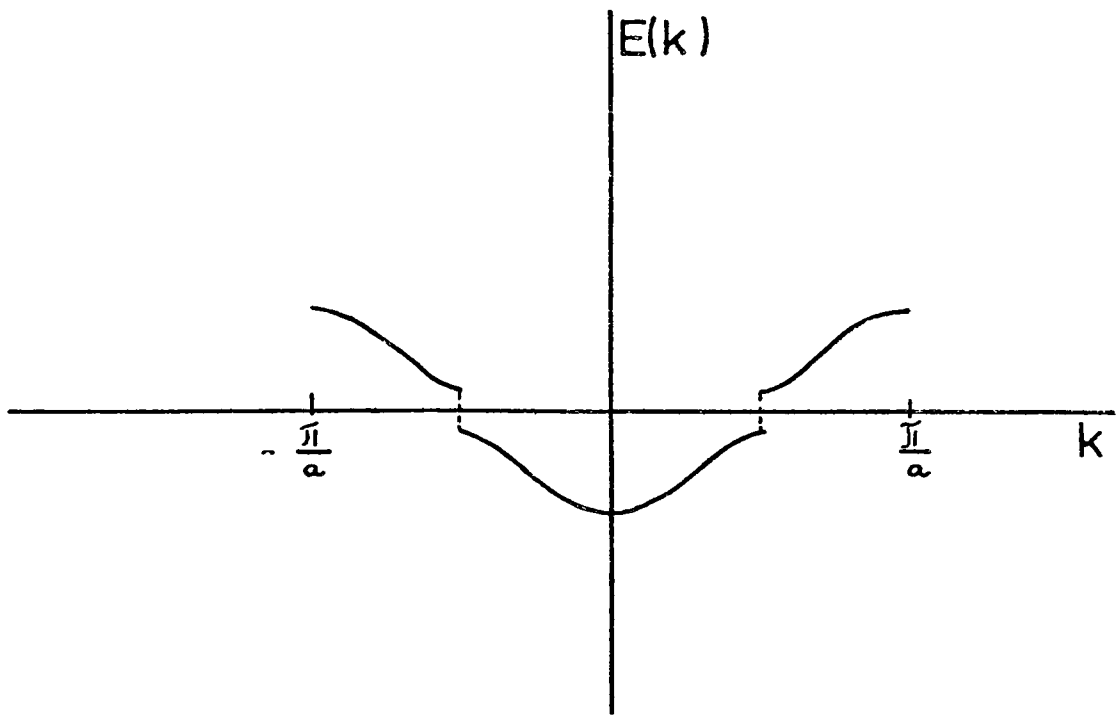


Fig. 5.4

dimensional systems. The high anisotropy presented in these materials allows us to obtain the three-dimensional behaviour in good approximation from the exact solution of the problem in one-dimension. The idea put in more precise terms consists in treating exactly the intrachain interactions, and approximating the interchain interactions by a mean-field. This idea has been used in the study of the quasi-one-dimensional Ising systems by Sato (1961), and by Stout and Chisholm (1962), and in the study of the quasi-one-dimensional classical Heisenberg system by Stanley and Kaplan (1967) and recently by Scalapino et al. (1975).

A Peierls transition has been suggested for some quasi-one-dimensional materials like the organic conductor (TTF-TCNQ) tetrathiofulvalene tetracyanoquinodimethane charge transfer salt (Berlinsky, 1976) and in the Krogman compounds, such as $K_2Pt(CN)_4 \cdot Br_{0.3} \cdot 3H_2O$ (KCP), (Zeller, 1973), with transition temperatures given respectively by $T_p \approx 60^\circ K$ and $T_p \approx 77^\circ K$. The quasi-one-dimensional behaviour of these materials is reflected in the ratio of the electrical conductivity along ($\sigma_{\parallel}$) and across ($\sigma_{\perp}$) the chains, which is given by $\sigma_{\perp}/\sigma_{\parallel} \sim 10^{-3}$ for TTF-TCNQ and by $\sigma_{\perp}/\sigma_{\parallel} \sim 10^{-5}$ for KCP at room temperature. Naturally these finite transition temperatures characterize the three-dimensional ordering induced by the weak intrachain interaction. As pointed out at the beginning, provided the one-dimensional solution is known, we can get the three-dimensional behaviour of these systems. Therefore the first step towards the solution of this problem is to solve the one-dimensional problem. In order to get this solution we will use the results obtained in the first chapter, which give the exact transition temperature and of course represent

a great improvement over the results obtained using the mean field theory. As stressed at the beginning we will restrict ourselves to the one-dimensional case.

We consider then the half-filled band metal in which the electron-phonon interaction is described by the simplest Hamiltonian, eq. (1.11):

$$H = \sum_k \epsilon_k c_k^\dagger c_k + \sum_q \omega_q a_q^\dagger a_q + \sum_{kq} V_q (a_q + a_{-q}^\dagger) c_k^\dagger c_{k-q} \quad (5.1)$$

where c_k , a_q are annihilation operators for electrons in a Bloch state and for longitudinal phonons, and

$$\omega_q = \omega^0 \sqrt{2(1 - \cos qa)} \quad , \quad (5.2)$$

$$\epsilon_k = -\epsilon_F \cos ka \quad , \quad (5.3)$$

$$V_q = \frac{g_q}{\sqrt{2MN\omega_q}} \quad (5.4)$$

where ϵ_k is obtained in the tight binding approximation and measured from the Fermi level, M the mass of the ions in the chain, N the total number of particles, and g_q is the coupling constant that in principle can have any q -dependence.

Naturally we can also consider ω_q having any q -dependence.

The simple form was assumed for the sake of simplicity. From this point we can use the results obtained in the first chapter, in order to obtain all the relevant properties of the system.

Then the commutator Green function $\tilde{G}_q$, eq. (1.52), is given by eq. (1.64):

$$\tilde{G}_q = \frac{G_q^0 \left(1 - 2 \frac{V_q V_{-q}}{\omega_q} \langle\langle \rho_q; \rho_{-q} \rangle\rangle_{\text{eff}} \right)}{1 - G_q^0 \frac{\omega^2}{\omega_q} V_q V_{-q} \langle\langle \rho_q; \rho_{-q} \rangle\rangle_{\text{eff}}} \quad , \quad (5.5)$$

where $\frac{V_q V_{-q}}{\omega_q}$ is given by

$$\frac{V_q V_{-q}}{\omega_q} = \frac{g_q g_{-q}}{2 N M \omega_q^2} \quad , \quad (5.6)$$

and $\langle\langle \rho_q; \rho_{-q} \rangle\rangle_{\text{eff}}$ is calculated using H_{eff} given by eq. (1.66).

Let us consider first the mean-field solution of the problem.

This approximation has been considered by several authors (Rice and Strässler, 1973; Allender et al., 1974; Horovitz et al., 1974) and we mentioned here the basic results, considering the interaction V_q , as defined in eq. (5.4). Therefore we get

$$\tilde{G}_q = \frac{2 \omega_q}{\omega^2 - \omega_q^2 - 2 \omega_q V_q V_{-q} f_q} \quad , \quad (5.7)$$

where

$$f_q = \sum_k \frac{n_k - n_{k-q}}{\omega + \epsilon_k - \epsilon_{k-q}} \quad , \quad (5.8)$$

and

$$n_k = \frac{1}{e^{\beta \epsilon_k} + 1} \quad (5.9)$$

is the Fermi occupation number.

Observe that the result (5.7) is obtained from eq. (1.64) when we consider the R.P.A. result for $\langle\langle \rho_q; \rho_{-q} \rangle\rangle_{\text{eff}}$ calculated using H_{eff} without the correction shown in eq. (1.68). The transition temperature is therefore obtained from eq. (5.7) by considering the softening of the phonon mode of wave-vector

$2k_F = \frac{\pi}{a}$ which gives:

$$\frac{2f_q V_q V_{-q}}{\omega_q} = -1 \quad . \quad (5.10)$$

In order to solve the previous equation we have to calculate the integral

$$\frac{1}{N} f_{2K_F} = - \frac{1}{N} \sum_k \frac{\tanh \frac{\beta_c \epsilon_k}{2}}{2 \epsilon_k} \quad . \quad (5.11)$$

It can be evaluated approximately (Allender et al., 1974) by considering the cut-off X such that

$$2 K_B T \ll X \leq \epsilon_F \quad . \quad (5.12)$$

Then we can write eq. (5.11) as

$$\frac{1}{N} f_{2K_F} = - \frac{2}{\pi} \left[\int_0^X \frac{\tanh \frac{\beta_c \epsilon}{2}}{\epsilon \sqrt{\epsilon_F^2 - \epsilon^2}} d\epsilon + \int_X^{\epsilon_F} \frac{\tanh \frac{\beta_c \epsilon}{2}}{\epsilon \sqrt{\epsilon_F^2 - \epsilon^2}} d\epsilon \right] , \quad (5.13)$$

where we have used eq. (5.3). Therefore using the condition (5.2) we obtain

$$\frac{1}{N} f_{2K_F} \cong - \frac{2}{\pi} \left[\int_0^X \frac{\tanh \frac{\beta_c \epsilon}{2}}{\epsilon_F \epsilon} d\epsilon + \int_X^{\epsilon_F} \frac{d\epsilon}{\epsilon \sqrt{\epsilon_F^2 - \epsilon^2}} \right] , \quad (5.14)$$

and finally the result

$$\frac{1}{N} f_{2K_F} \cong - \frac{2}{\pi \epsilon_F} \left(\ln \frac{\epsilon_F}{K T_c} - \gamma \right) , \quad (5.15)$$

where γ is given by (see for instance Gradshteyn and Ryzhik, 1965):

$$\gamma = \int_0^\infty \ln z \operatorname{sech}^2 z dz = 0.81878 \quad . \quad (5.16)$$

In order to get the transition temperature we have to assume an explicit form for V_q , and we will choose it in such a way that $\frac{V_q V_{-q}}{\omega_q}$ does not depend on q and is given by:

$$\frac{V_q V_{-q}}{\omega_q} = \frac{\bar{t}^2}{2NM\omega^2} \quad (5.17)$$

Although this choice appears to be rather arbitrary, as we will see later it will make possible the solution of the model exactly in the framework of the approximation discussed in the first chapter. The model is simple but not trivial, and certainly not completely unrealistic since we can consider complicated phonon dispersion relation.

Substituting the results obtained in eqs. (5.15) and (5.16) in eq. (5.9) we get:

$$k_B T_c = 2.28 \mathcal{E}_F \exp \left(- \frac{\bar{\Pi} \mathcal{E}_F M \omega^2}{2 \bar{t}^2} \right) \quad (5.18)$$

which can be written as

$$k_B T_c = 2.28 \mathcal{E}_F \exp \left(- \frac{\bar{\Pi}}{2 \alpha \delta} \right) \quad (5.19)$$

where

$$\alpha = \left(\frac{\bar{t}}{\omega^0} \right)^2 \quad (5.20)$$

$$\delta = \frac{\omega^0}{\mathcal{E}_F} \quad (5.21)$$

with $\bar{t}$ given by

$$\bar{t} = \frac{t}{\sqrt{M \omega^0}} \quad (5.22)$$

Of course the finite transition temperature obtained was expected, since we have neglected fluctuations.

The renormalized phonon excitations at any temperature are obtained by solving the equation

$$\omega^2 - \omega_q^2 - 2 \omega_q V_q V_{-q} f_q = 0 \quad (5.23)$$

which gives two branches, one of which is undamped. The damping is calculated by considering the imaginary part of f_q obtained through the analytical continuation of ω into complex plane, which is given by:

$$f_q(\omega) = \lim_{\epsilon \rightarrow 0} f_q(\omega - i\epsilon) \quad (5.24)$$

Similarly we can get the real and imaginary parts of $\tilde{G}_q$ obtained from the equation

$$\tilde{G}_q(\omega) = \lim_{\epsilon \rightarrow 0} \tilde{G}_q(\omega - i\epsilon) \quad (5.25)$$

The undamped excitations will be characterized by the appearance of a delta function in the $\text{Im} \tilde{G}_q$ which is of course in the region where $\text{Im} f_q$ is different from zero.

Let us consider the solution of the problem in the framework of the approximation discussed in the first chapter. From eq. (1.64) we have

$$\tilde{G}_q = \frac{G_q^0 \left(1 - \frac{2V_q V_{-q}}{\omega_q} \langle \rho_q, \rho_{-q} \rangle_{\text{eff}} \right)}{1 - G_q^0 \frac{V_q V_{-q}}{\omega_q^2} \omega^2 \langle \rho_q, \rho_{-q} \rangle_{\text{eff}}} \quad (5.26)$$

Since $\frac{V_q V_{-q}}{\omega_q}$ is a constant, eq. (5.17), the effective Hamiltonian, eq. (1.66), is given by:

$$H_{\text{eff}} = \sum_k \varepsilon_k c_k^\dagger c_k - \sum_q \frac{\chi^2}{2NM\omega^2} \rho_q \rho_{-q} \quad , \quad (5.27)$$

which after subtracting the self-energy term, eq. (1.68) gives

$$H_{\text{eff}} = \sum_k \varepsilon_k c_k^\dagger c_k \quad . \quad (5.28)$$

Therefore in this model, the Green function, $\langle\langle \rho_q; \rho_{-q} \rangle\rangle_{\text{eff}}$, can be calculated exactly, and is given by:

$$\langle\langle \rho_q; \rho_{-q} \rangle\rangle_{\text{eff}} = \sum_q \frac{n_k - n_{k-q}}{\omega + \varepsilon_k - \varepsilon_{k-q}} \quad , \quad (5.29)$$

which is equal to f_q . In this particular model the electron-electron interaction generated by electron-phonon interaction contains only the spurious term which has to be eliminated from calculations. If we try now to reproduce the mean-field result as discussed in first chapter, eq. (1.55), (1.56) and (1.57), we see that we have to consider the interacting term as it appears in eq. (1.66). This therefore means that the mean-field approximation not only neglects fluctuations but also includes the contribution of spurious terms. This has been pointed out by Pytte (1974), although in his problem there were no dynamical effects. Even when we do not know how to calculate $\langle\langle \rho_q; \rho_{-q} \rangle\rangle_{\text{eff}}$ exactly, the use of the random-phase-approximation after we have discarded the self-energy term represents a great improvement when compared with the usual mean-field result.

In order to calculate the real and imaginary parts of $\tilde{G}_q$, as given by eq. (5.26), we have to calculate first of all the real and imaginary parts of $\langle\langle \rho_q; \rho_{-q} \rangle\rangle_{\text{eff}}$. Using then eq. (5.29) we get immediately

$$\operatorname{Re} \langle \langle \rho_q; \rho_{-q} \rangle \rangle_{\text{eff}} = \frac{\rho}{2N} \sum_k \frac{1}{\omega_k + \varepsilon_k - \varepsilon_{k-q}} \left(\tanh \frac{\beta \varepsilon_k}{2} - \tanh \frac{\beta \varepsilon_{k-q}}{2} \right), \quad (5.30)$$

$$\operatorname{Im} \langle \langle \rho_q; \rho_{-q} \rangle \rangle_{\text{eff}} = -\frac{\pi}{2N} \sum_k \delta(\omega + \varepsilon_k - \varepsilon_{k-q}) \left(\tanh \frac{\beta \varepsilon_k}{2} - \tanh \frac{\beta \varepsilon_{k-q}}{2} \right). \quad (5.31)$$

Due to translational symmetry we have that

$$\langle \langle \rho_{-q}; \rho_q \rangle \rangle_{\text{eff}} = \langle \langle \rho_q; \rho_{-q} \rangle \rangle_{\text{eff}}, \quad (5.32)$$

and from this and eq. (1.10) we conclude that $\langle \langle \rho_q; \rho_{-q} \rangle \rangle_{\text{eff}}$ is a symmetric function of ω . This symmetry property implies then that the real and imaginary parts of $\langle \langle \rho_q; \rho_{-q} \rangle \rangle$ are symmetric and antisymmetric, respectively. These results are easily verified using the expressions (5.30) and (5.31). Of course the Green function $\tilde{G}_q$ satisfies the same properties.

The imaginary part of $\langle \langle \rho_q; \rho_{-q} \rangle \rangle$ can be calculated analytically at any temperature, and at $T \neq 0$ is given by:

$$\operatorname{Im} \langle \langle \rho_q; \rho_{-q} \rangle \rangle_{\text{eff}} = 0, \quad \text{if } |\omega| > 2\varepsilon_F \sin \frac{qa}{2}, \quad (5.33)$$

$$\begin{aligned} \operatorname{Im} \langle \langle \rho_{-q}; \rho_q \rangle \rangle_{\text{eff}} = & \frac{1}{(4\varepsilon_F^2 \sin^2 \frac{qa}{2} - \omega^2)^{1/2}} \left\{ \tanh \left\{ \frac{\beta}{4} \left[\cos \frac{qa}{2} \sqrt{4\varepsilon_F^2 - \left(\frac{\omega}{\sin \frac{qa}{2}} \right)^2} \right] + \right. \right. \\ & \left. \left. + \omega \right\} - \tanh \left\{ \frac{\beta}{4} \left[\cos \frac{qa}{2} \sqrt{4\varepsilon_F^2 - \left(\frac{\omega}{\sin \frac{qa}{2}} \right)^2} - \omega \right] \right\} \right\}, \quad \text{if } |\omega| < 2\varepsilon_F \sin \frac{qa}{2}. \end{aligned} \quad (5.34)$$

At $T = 0$, the real and imaginary parts can be calculated analytically and are given by

$$\begin{aligned} \operatorname{Re} \langle \langle \rho_q; \rho_{-q} \rangle \rangle_{\text{eff}} = & \frac{2}{\pi \sqrt{4\varepsilon_F^2 \sin^2 \frac{qa}{2} - \omega^2}} \tanh^{-1} \left[\frac{4\varepsilon_F \sin^2 \frac{qa}{2} \sqrt{4\varepsilon_F^2 \sin^2 \frac{qa}{2} - \omega^2}}{4\varepsilon_F^2 \sin^2 \frac{qa}{2} (1 + \sin^2 \frac{qa}{2}) - \omega^2} \right] \\ & \text{for } |\omega| < 2\varepsilon_F \sin \frac{qa}{2}, \end{aligned} \quad (5.35)$$

$$\text{Re} \langle \langle \rho_q; \rho_{-q} \rangle \rangle_{\text{eff}} = \frac{2}{\pi \sqrt{\omega^2 - 4\varepsilon_F^2 \sin^2 \frac{qa}{2}}} \tan^{-1}(E_q + \pi) , \quad (5.36)$$

$$\text{for } |\omega| > 2\varepsilon_F \sin \frac{qa}{2} , \quad E_q < 0$$

and

$$\text{Re} \langle \langle \rho_q; \rho_{-q} \rangle \rangle_{\text{eff}} = \frac{2}{\pi \sqrt{\omega^2 - 4\varepsilon_F^2 \sin^2 \frac{qa}{2}}} \tan^{-1}(E_q) , \quad (5.37)$$

$$\text{for } |\omega| > 2\varepsilon_F \sin \frac{qa}{2} , \quad E_q > 0 ,$$

where

$$E_q = \frac{4\varepsilon_F \sin^2 \frac{qa}{2} \sqrt{4\varepsilon_F^2 \sin^2 \frac{qa}{2} - \omega^2}}{\omega^2 - 4\varepsilon_F^2 \sin^2 \frac{qa}{2} (1 + \sin^2 \frac{qa}{2})} , \quad (5.38)$$

and

$$\text{Im} \langle \langle \rho_q; \rho_{-q} \rangle \rangle_{\text{eff}} = 0 , \quad \text{for } |\omega| < \varepsilon_F \sin qa , \quad |\omega| > 2\varepsilon_F \sin \frac{qa}{2} \quad (5.39)$$

$$\text{Im} \langle \langle \rho_q; \rho_{-q} \rangle \rangle_{\text{eff}} = \frac{2 \text{sign}(\omega)}{\sqrt{4\varepsilon_F^2 \sin^2 \frac{qa}{2} - \omega^2}} , \quad \text{for } |\omega| < 2\varepsilon_F \sin \frac{qa}{2} . \quad (5.40)$$

These are identical to the results obtained by Katsura et al.

(1970) in the study of the isotropic one-dimensional XY-model.

Our results differ from those just by a factor 2 that comes from the density of states in the case of electrons.

At $\omega = 0$, $\langle \langle \rho_q; \rho_{-q} \rangle \rangle_{\text{eff}}$ diverges only for $q = \frac{\pi}{a}$ and $T = 0$, and from eq. (5.15) we see that it is given by

$$\left. \langle \langle \rho_q; \rho_{-q} \rangle \rangle_{\text{eff}} \right|_{q=\frac{\pi}{a}} = -\frac{2}{\pi} \left(\ln \frac{\varepsilon_F}{kT} - \gamma \right) . \quad (5.41)$$

From eq. (5.26) we have that the renormalized phonon excitations are given by the equation

$$\omega^2 = \frac{\omega_q^2}{1 - 2 \frac{V_q V_{-q}}{\omega_q} \langle \langle \rho_q; \rho_{-q} \rangle \rangle_{\text{eff}}} , \quad (5.42)$$

and as already discussed in the first chapter ω will go to zero, only if $\langle\langle\rho_q; \rho_{-q}\rangle\rangle_{\text{eff}}$ goes to infinity as $\omega \rightarrow 0$. Since this happens only at $T = 0$ and $q = \frac{\pi}{a}$, there is the appearance of a soft mode of wave-vector $\frac{\pi}{a}$ at $T = 0$. As a function of temperature the soft mode varies as

$$\omega^2 = \frac{2\omega^2}{1 + \frac{\hbar^2}{M\omega^2} \left(\ln \frac{\epsilon_F}{KT} - \gamma \right)}, \quad (5.43)$$

and therefore in this model we get that $T_c = 0$, which is the correct transition temperature.

The Green function $\tilde{G}_q$ for $q = \frac{\pi}{a}$ and $\omega = 0$, diverges as

$$G_q \sim - \ln KT. \quad (5.44)$$

The real and imaginary parts of $G_q(\omega)$ for $q = \frac{\pi}{a}$ and various temperatures ($\beta = \frac{\epsilon_F}{K_B T}$) are shown in figs. (5.5) to (5.10). The coupling constant is defined in terms of the parameters δ and α defined in eqs. (5.20) and (5.21). For a given set of parameters, figs. (5.5), (5.6) and (5.7), as we lower the temperature the real part exhibits a peak at $\omega = 0$ which becomes a divergence at $T = 0$. It also exhibits a singularity in the region where $\text{Im} \langle\langle\rho_q; \rho_{-q}\rangle\rangle$ is equal to zero, which of course means the presence of undamped excitations. The imaginary part increases as we decrease the temperature, and the arrows in figs. (5.8), (5.9) and (5.10) represent the delta functions which are relaxations of the undamped excitations. They are expressed as

$$\text{Im } G_q(\omega) = \frac{\hbar\omega_q}{\bar{\omega}_q} \left[\delta(\omega - \bar{\omega}_q) - \delta(\omega + \bar{\omega}_q) \right], \quad (5.45)$$

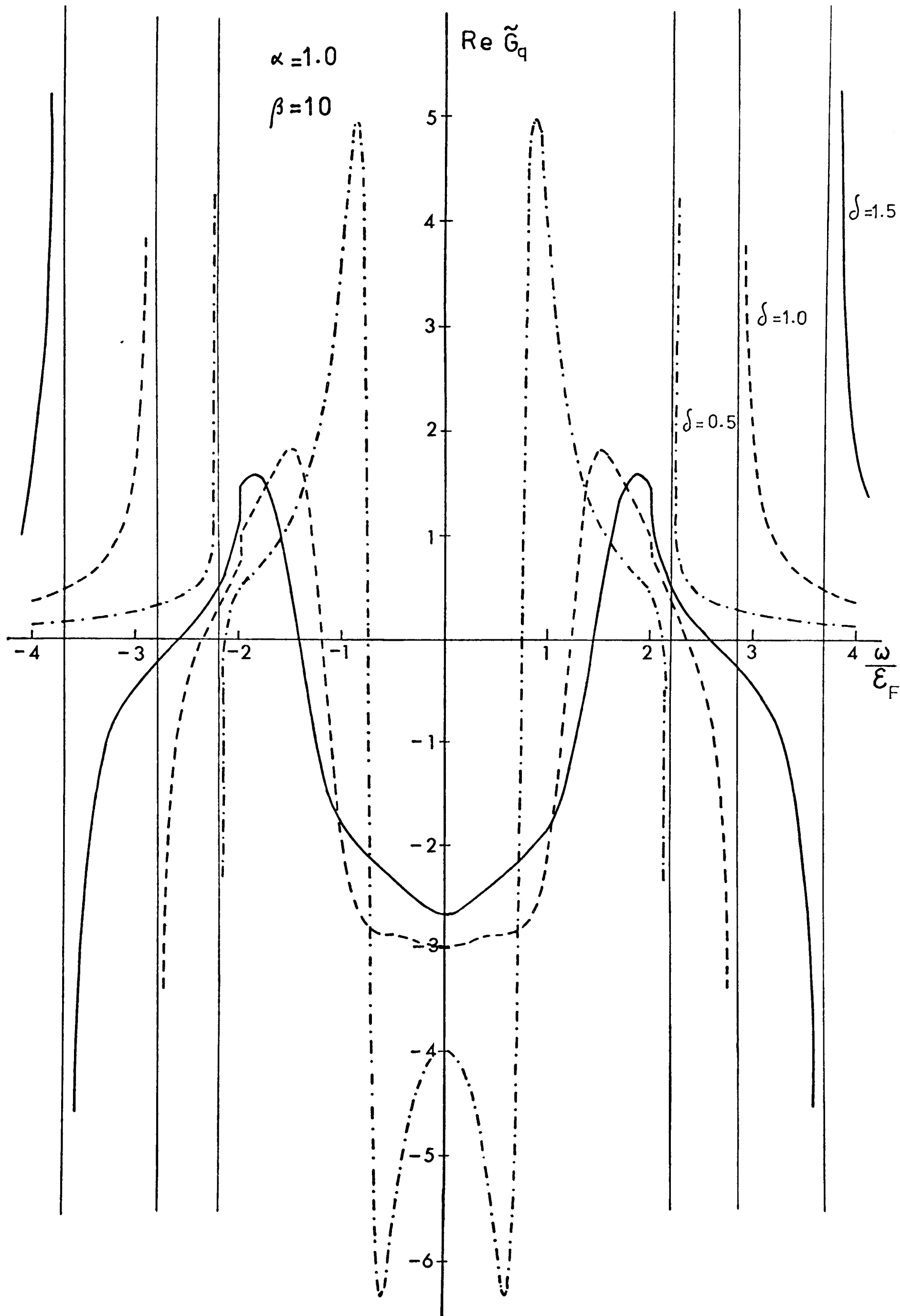


Fig. 5.5

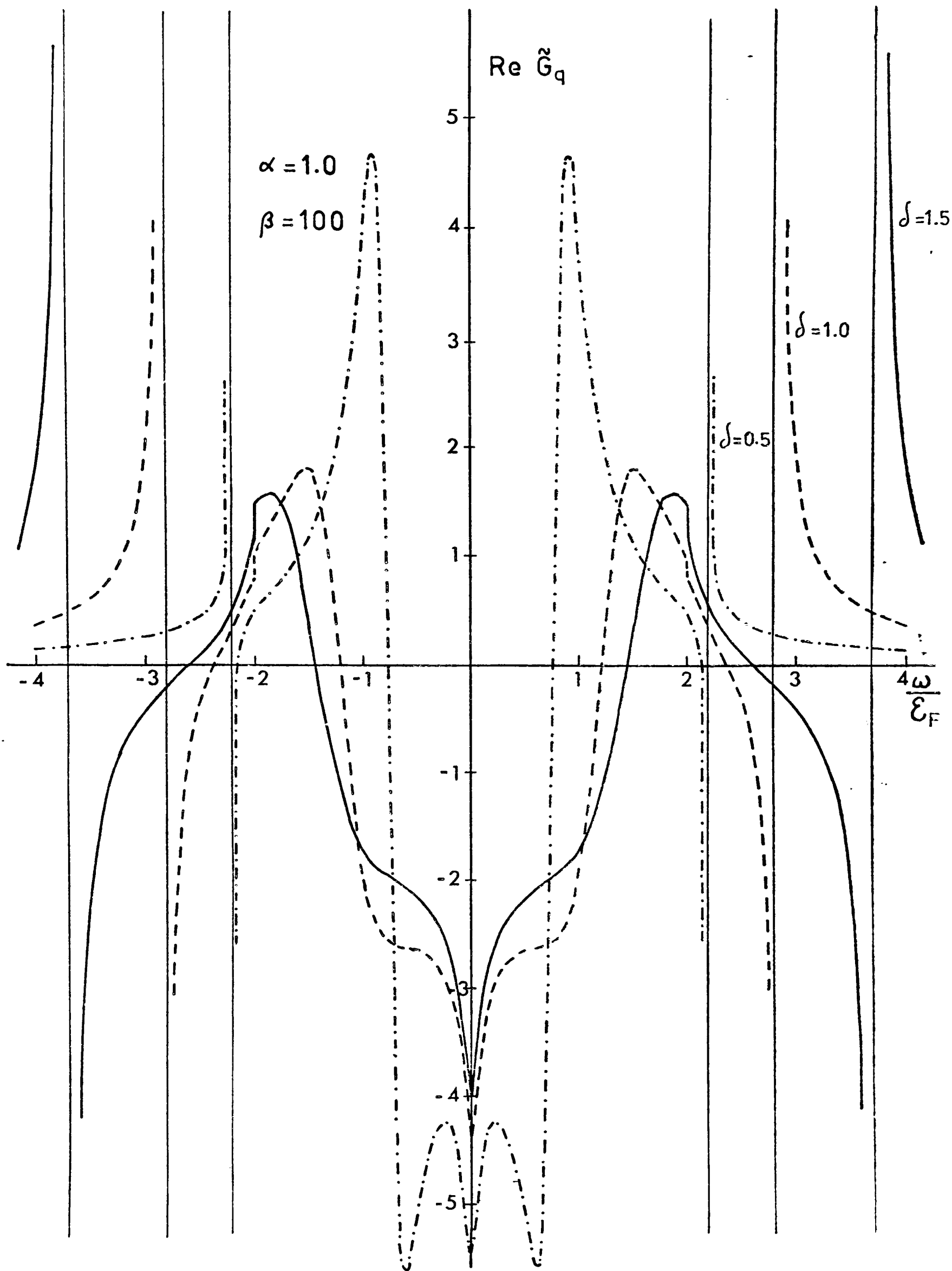


Fig 5.6

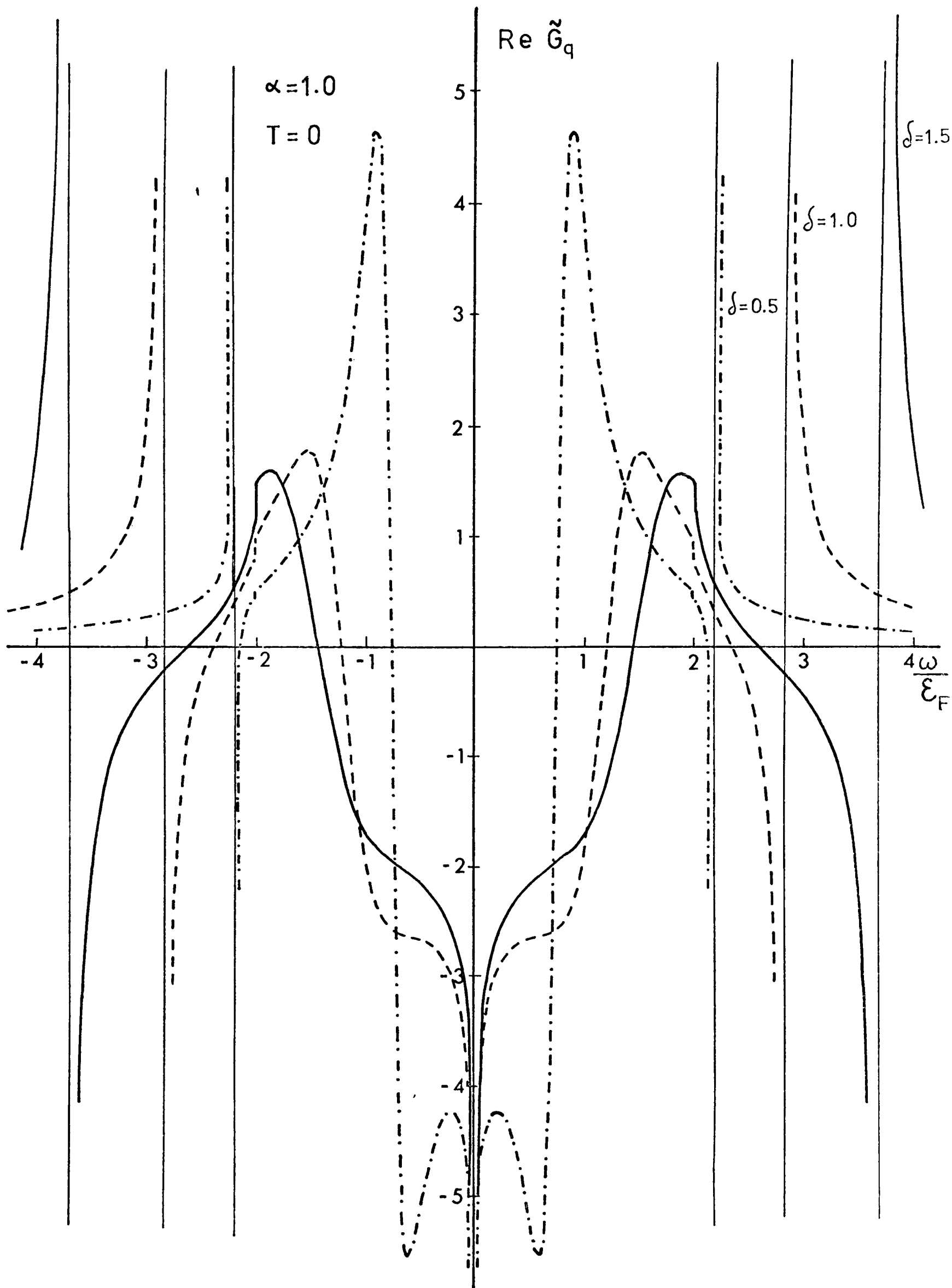


Fig. 5.7

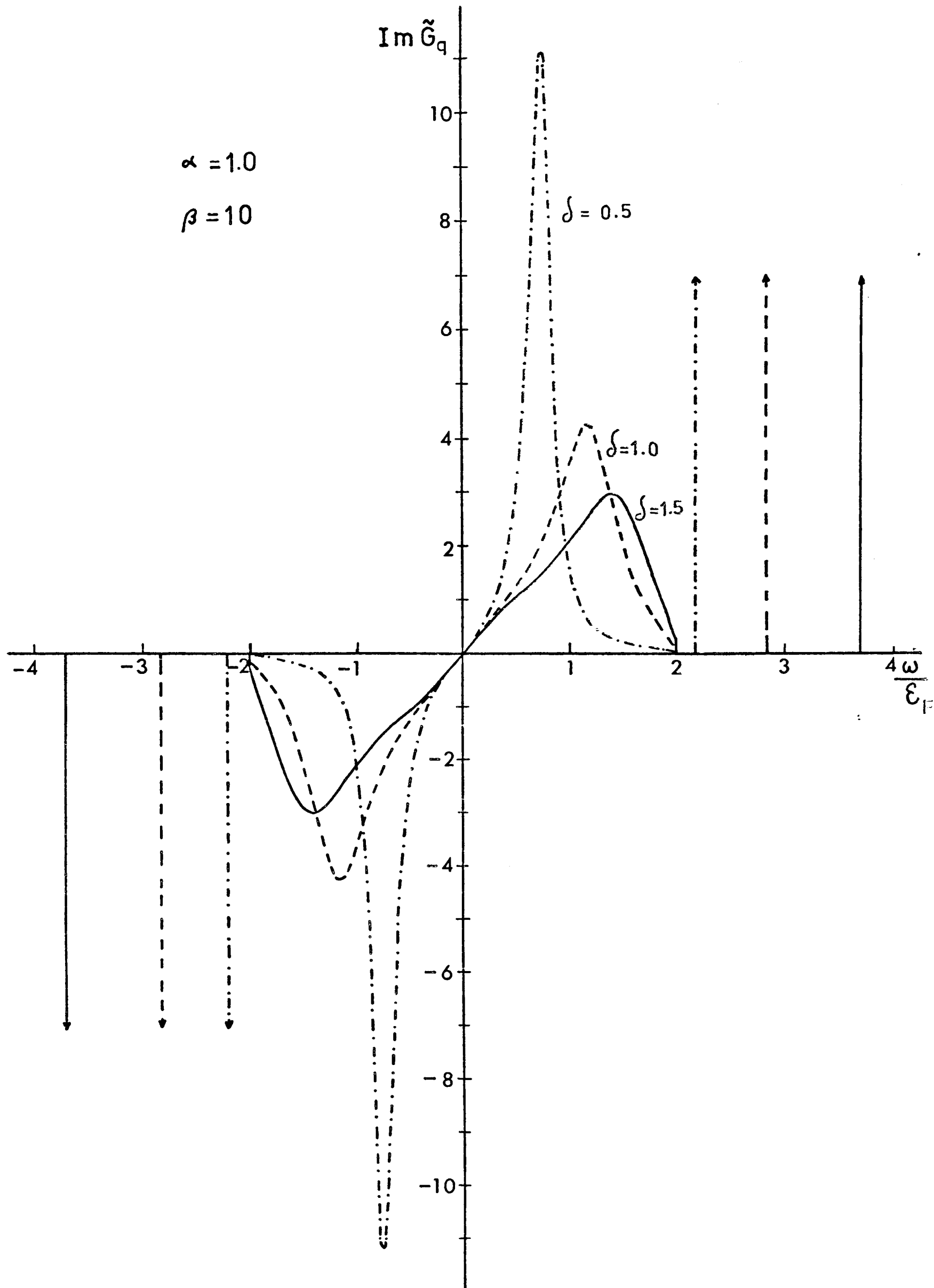


Fig. 5.8

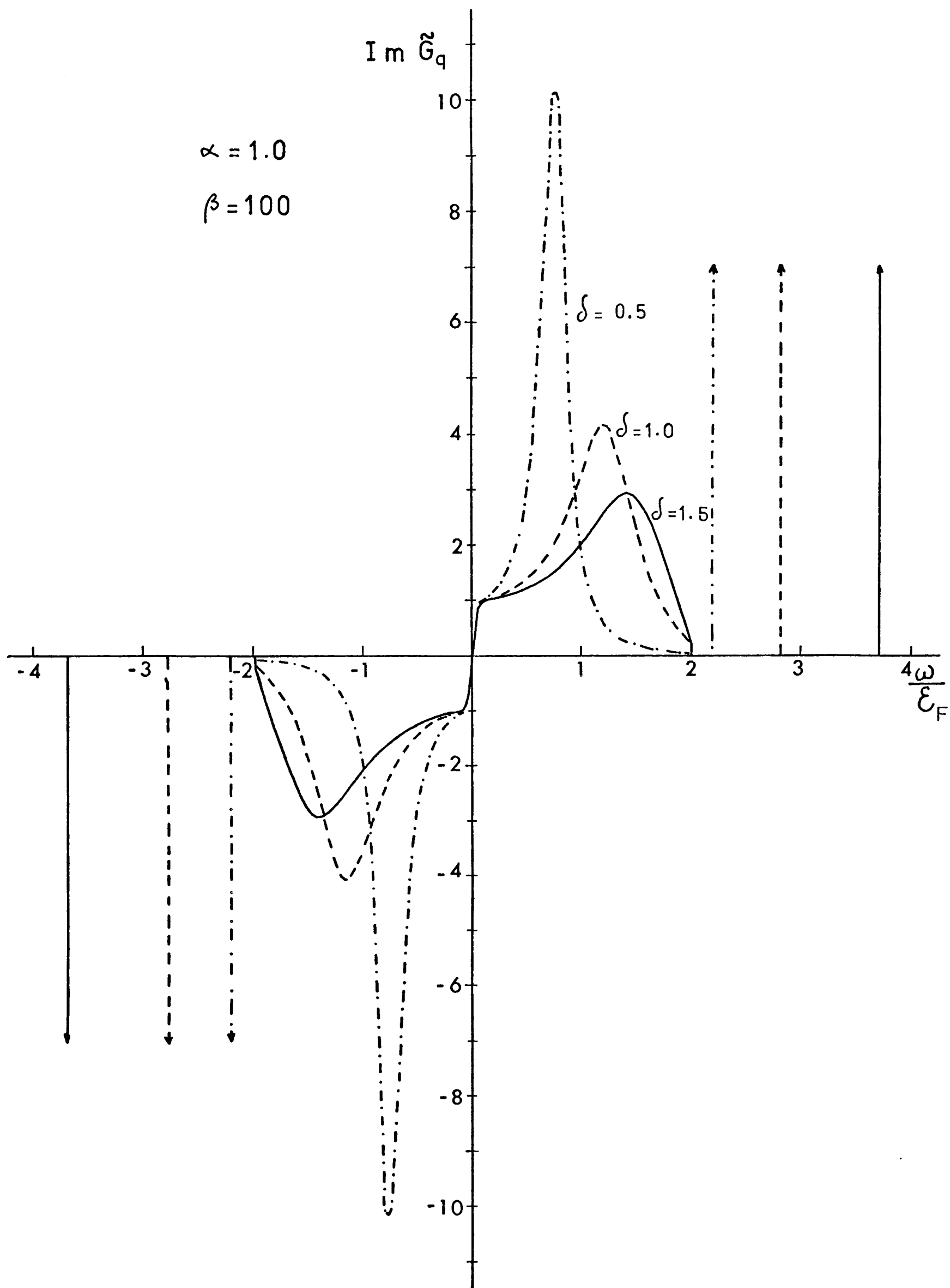


Fig. 5.9

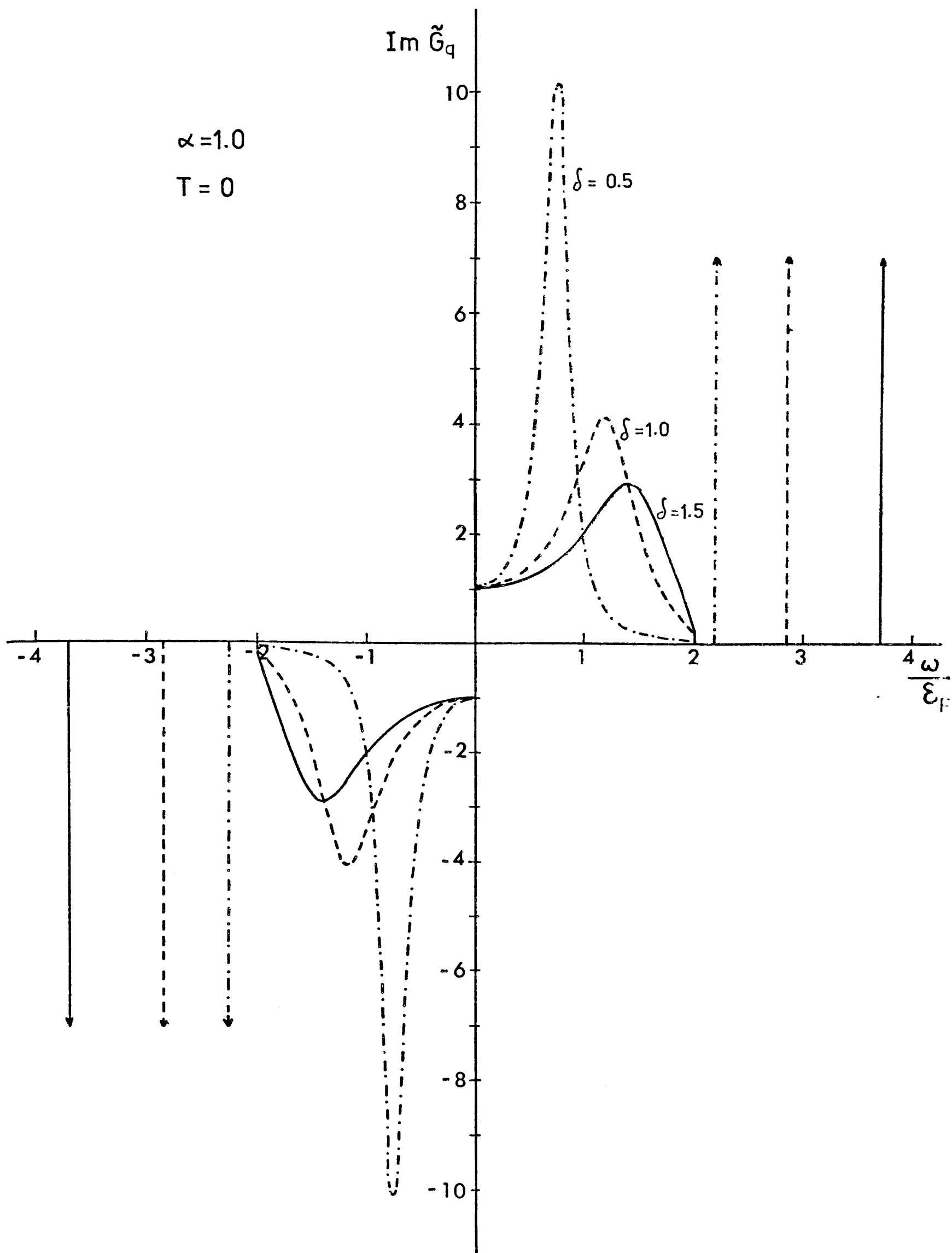


Fig. 5.10

where $\bar{\omega}_q$ is the renormalized phonon excitations which is given by eq. (5.43). Observe that as the coupling becomes weaker or the temperature increases these modes move toward the band. At $T = 0$ $\text{Im}G_q$ is discontinuous at $\omega = 0$, and this immediately implies a divergence of the neutron cross section calculated in Born approximation.

The important aspect of this whole calculation is the fact that we have been able to describe correctly the behaviour of the one-dimensional system. Certainly the next step should include the interaction between chains in order to get the three-dimensional behaviour. The simplest interaction should be a hopping term between chains in which case ϵ_K should be written as

$$\epsilon_{\vec{K}} = -\epsilon_F \cos k_z a - \eta (\cos k_x b + \cos k_y b) , \quad (5.46)$$

which could be treated exactly in the framework of our approximation. The mean-field calculation of this model has been done by Horowitz et al. (1975). There certainly are some difficulties when treating the three-dimensional case, for instance the non-existence of the Peierls transitions due to the Fermi surface shape. Certainly we are still able to see a giant Kohn anomaly (Alfanas'ev and Kagan, 1963), although there is no Peierls transition.

5.3 The Coupled Spin-phonon System

Let us consider finally a one-dimensional coupled spin-phonon system whose Hamiltonian is given by

$$H = \sum_q \omega_q a_q^\dagger a_q + H_S + \sum_q V_q (a_q + a_{-q}^\dagger) S_q^x , \quad (5.47)$$

where the a 's are annihilation operators for longitudinal phonons. ω_q and V_q are identical to those defined in eqs. (5.2) and (5.17) respectively, and H_s is the spin part of the Hamiltonian. We will not assume any special form for H_s for the moment.

The Hamiltonian (5.47) has been studied in the first chapter, and then from eq. (1.65) we get:

$$\tilde{G}_q = \frac{G_q^0 \left(1 - \frac{2V_q V_{-q}}{\omega_q} \langle\langle S_{-q}^x, S_q^x \rangle\rangle_{\text{eff}} \right)}{1 - G_q^0 V_q V_{-q} \frac{\omega^2}{\omega_q} \langle\langle S_{-q}^x, S_q^x \rangle\rangle_{\text{eff}}}, \quad (5.48)$$

where $\langle\langle S_{-q}^x, S_q^x \rangle\rangle_{\text{eff}}$ is evaluated using the effective Hamiltonian, eq. (1.67),

$$H_{\text{eff}} = H_s - \sum_q v(q) S_q^x S_{-q}^x, \quad (5.49)$$

where $v(q)$ is given by eq. (1.68). Since $\frac{V_q V_{-q}}{\omega_q}$ does not depend on q , eq. (5.17), $v(q)$ is identical to zero, and consequently H_{eff} is equal to H_s . The critical behaviour of the system will depend on H_s and we will write it as:

$$H_{\text{eff}} = \sum_j 2J S_j^x S_{j+1}^x - \sum_j h S_j^z, \quad (5.50)$$

which is the transverse Ising model. We have chosen the antiferromagnetic case because we are interested in the condensation of the phonon mode of wave-vector $\frac{\pi}{a}$. The softening of this phonon-mode will correspond to a transition to an ordered antiferromagnetic state of the spin system. Naturally the electron-phonon system, neglecting

the electronic spin, can be solved in terms of spin $\frac{1}{2}$ due to the Jordan-Wigner transformation, eqs. (2.3), (2.6) and (2.7), and H_{eff} is equivalent to the anisotropic Heisenberg model. There is, however, the difficulty associated with the boundary term as discussed in the second chapter, which clearly shows that the two systems are not completely equivalent. This equivalence was used by Falk and Ruijbroek (1965) in the study of the anti-ferromagnetic Heisenberg chain, although they overlooked the problem of the boundary term. In this case it is obvious that the softening of the phonon mode will induce a Peierls transition, although it is represented as an ordered magnetic state.

Even when we consider electron with spins it is possible to find equivalent spin systems. In this case we have to extend the Jordan-Wigner transformation and write it as:

$$S_j^+ = S_j^x + i S_j^y = e^{i\pi \sum_{l=1}^{j-1} (c_{l\uparrow}^+ c_{l\uparrow} + c_{l\downarrow}^+ c_{l\downarrow})} c_{j\uparrow}^+ \quad (5.51)$$

$$T_j^+ = T_j^x + i T_j^y = e^{i\pi \left(\sum_{l=1}^j c_{l\uparrow}^+ c_{l\uparrow} + \sum_{l=1}^{j-1} c_{l\downarrow}^+ c_{l\downarrow} \right)} c_{j\downarrow}^+ \quad (5.52)$$

where the S's and T's constitute two independent sets of spin $\frac{1}{2}$ operators. A similar result has been pointed out by Shiba (1972) and Camp (1974), however, they have written the transformation in different forms.

Since H_{eff} is the transverse Ising model, $\langle\langle S_{-q}^x; S_q^x \rangle\rangle_{\text{eff}}$ is given by eq. (3.70), and we can immediately evaluate G_q . Unfortunately as discussed in chapter three, we can calculate $\langle\langle S_{-q}^x; S_q^x \rangle\rangle_{\text{eff}}$ only in the high temperature limit, which obviously rules out the possibility of any anomalous behaviour. Even so for

completeness we calculate $\tilde{G}_q$ for $q = \frac{\pi}{a}$, $\beta = 0.1$, $\lambda = 1.5$ and various δ , where δ and λ are defined as

$$\lambda = \frac{J}{\hbar} \quad (5.53)$$

$$\delta = \frac{\omega^0}{2J} \quad (5.54)$$

and for simplicity we assume that J is given by:

$$J \equiv \frac{t^2}{4MN} \quad (5.55)$$

The results are shown in figs. (5.11), (5.12) and (5.13) where we present the real and imaginary parts of the phonon Green function. The divergences present in the real part correspond to undamped excitations which are essentially the unperturbed phonon frequencies. This is all we can get from these results.

The problem now consists simply in improving the results for the dynamics of the transverse Ising model in order to describe the critical behaviour of this interacting spin-phonon system. Improvement has also to be made in the interaction fermion system which will make it possible to consider more realistic interaction for the electron-phonon system. Naturally not only these two systems, but any other one-dimensional system, where the results shown in the first chapter are applied, should be considered. We believe that this general result better describes these interacting one-dimensional systems, and consequently will provide better understanding of the related quasi-one-dimensional systems.

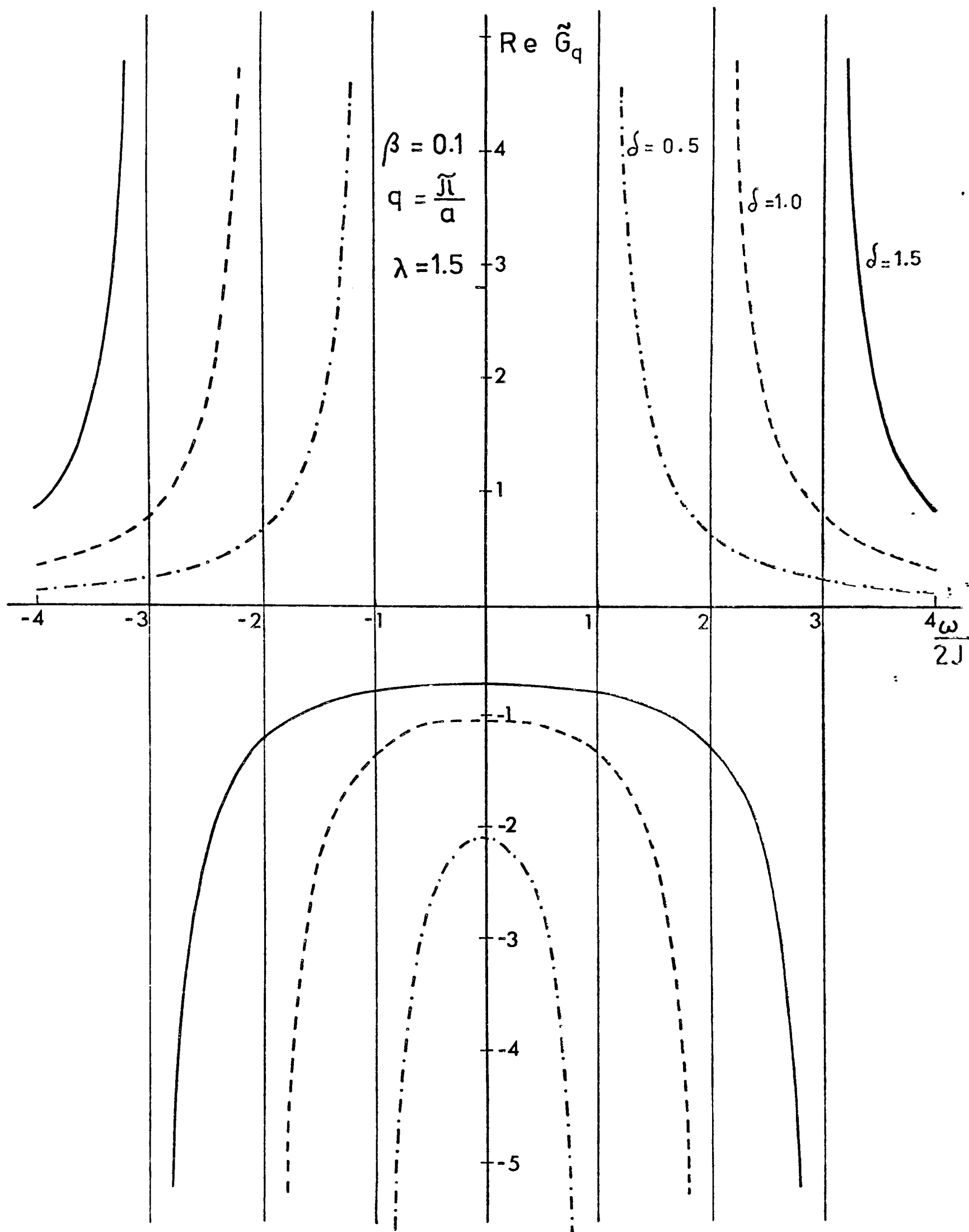


Fig. 5.11

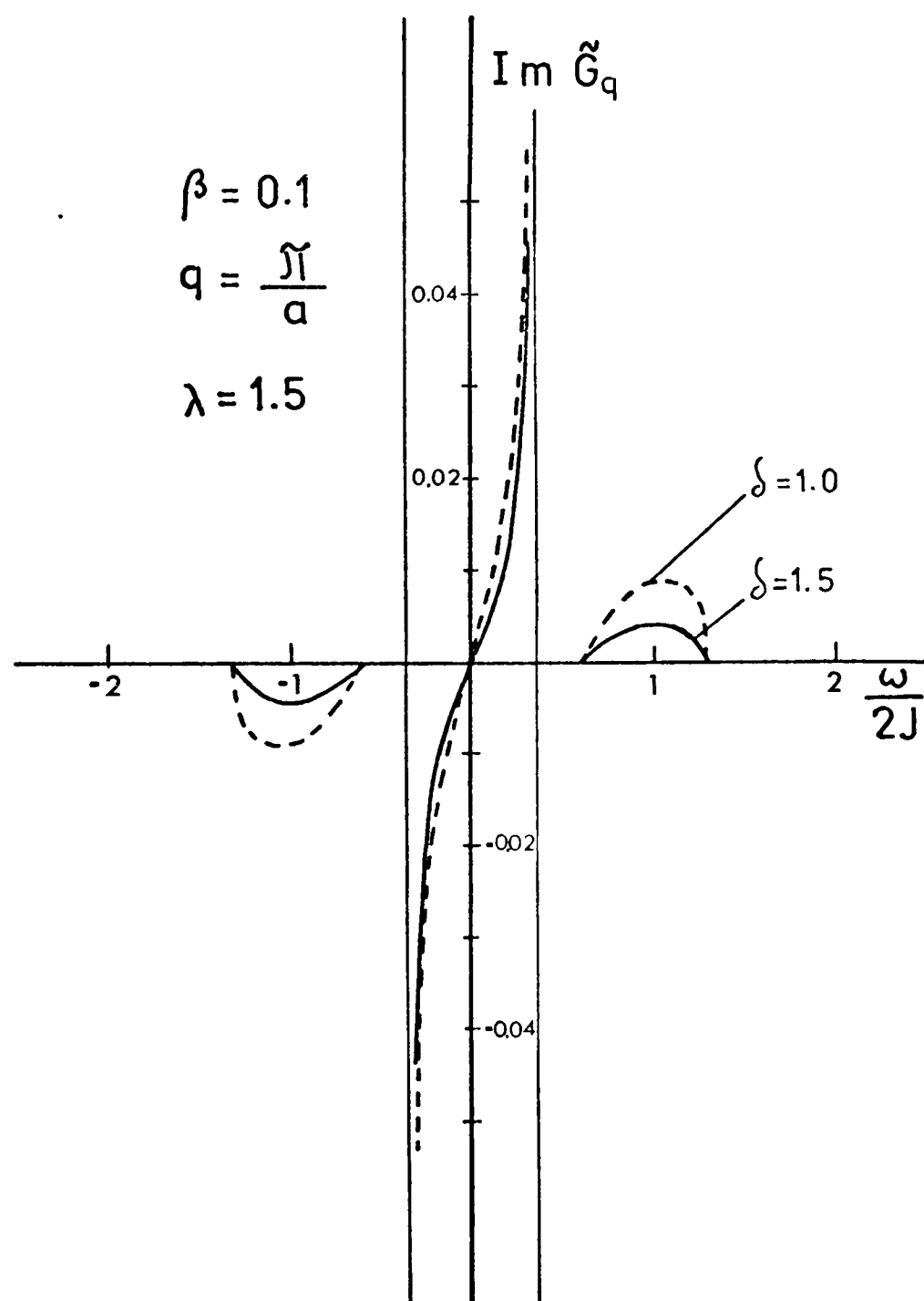


Fig. 5.12

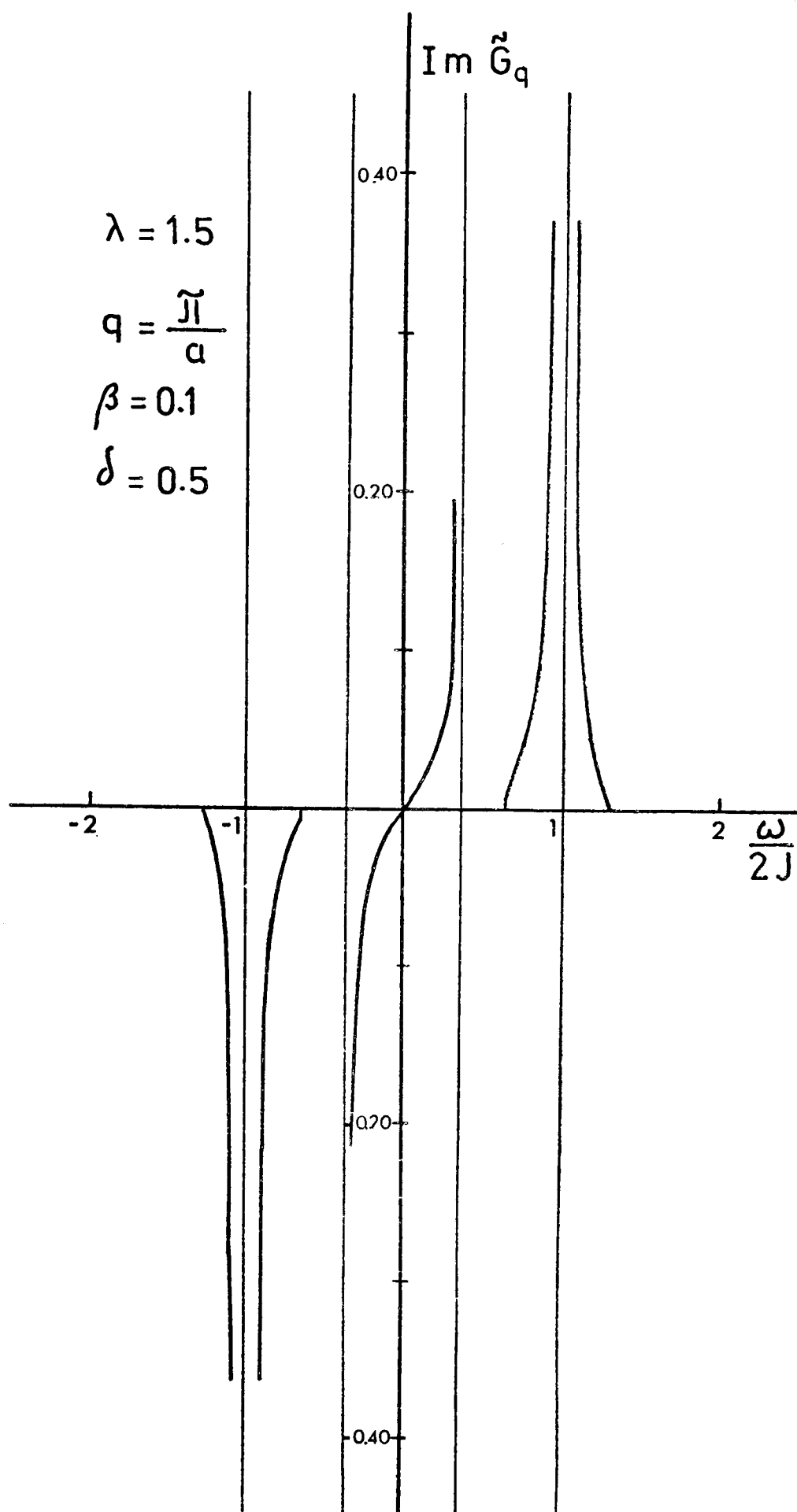


Fig. 5.13

CONCLUSIONS

We have been able to express the properties of the interacting electron-phonon and spin-phonon systems in terms of an effective electron-electron and spin-spin Green function, respectively, when the interaction is linear in displacement. The approximation gives the correct transition temperature in the one-dimensional case, namely $T = 0$, provided the effective Green function is calculated exactly. This represents a great improvement on the result obtained using mean-field approximation, and has no restrictions in its use as far as dimensionality is concerned. Although the approximation does not give the entire solution of the problem, it is put in a more tractable form, in which exact results can be obtained.

The solution of the impure one-dimensional XY-chain in a transverse field was shown to be equivalent to a diagonalization of bilinear forms of fermion operators, as in the pure case. The boundary term plays as expected a special role in the dynamics of the system and only in some cases can be neglected, as again in the pure case. The calculation of the heat-flux operator by solving the continuity equation shows that time-evolution of this operator can be evaluated neglecting the boundary term.

In the study of the pure transverse Ising model, the importance of the boundary term was brought to light in some simple calculations. In the analysis of the model under better approximation, taking into account this term, we have been able to reproduce some known exact results. However, the approximation

was satisfactory only in the high temperature limit, since the breaking of the translational symmetry became apparent as we lowered the temperature. The natural way to recover the translational symmetry led to complicated expressions which are very difficult to evaluate. Therefore, no critical behaviour was observed within the approximation in which the model was studied. Certainly further studies have to be made on this model in order to obtain reasonable results at low temperatures.

The specific heat of the dilute XY-chain was obtained using the average t-matrix approximation and the agreement with exact numerical results for finite chains was quite good even in the high concentration limit. This was rather surprising bearing in mind the simplicity of the approximation.

From the study of the specific heat and thermal conductivity of the isotropic XY-chain in a random field it became clear that the hyperfine interaction could not explain all the low temperature thermal properties of praseodymium ethyl sulphate. This interaction is very effective in damping the spin excitations; however, it does not explain the anomalous behaviour of the specific heat. We believe that this behaviour is due to random splitting of the ground doublet.

In the framework of the decoupling scheme introduced for the study of coupled electron-phonon and spin-phonon systems, we solved exactly one electron-phonon model which exhibited critical behaviour at zero temperature. This giant Kohn anomaly drives the Peierls instability in this one-dimensional system. There is in addition to a damped renormalized phonon branch one undamped branch outside the electron band.

The spin-phonon case studied led to the solution of the problem in terms of the transverse Ising model in which case only the high temperature result was attainable. Therefore we got information just about the excitations in this temperature limit, which showed to be equal to the unperturbed phonon excitations and consequently undamped.

We believe that the decoupling scheme introduced offers hope of progress in the study of the critical behaviour of these systems, particularly better description of the quasi-one-dimensional systems. Naturally the main problem is to look for solutions of one-dimensional systems which can be used in the description of interacting models, implying that one-dimensional problems are still alive as objects of theoretical study.

Appendix

The Decoupling Scheme Approximation: Special Cases

We will consider firstly the case where the transverse field is zero. Eq. (3.11) is then written as:

$$f_{jl}^{xx} \ddot{f}_{jl}^{xx} - \left(\dot{f}_{jl}^{xx} \right)^2 = 0 \quad , \quad (\text{A.1})$$

and so we get immediately

$$f_{jl}^{xx}(t) = f_{jl}^{xx}(0) \exp \left[\left(\dot{f}_{jl}^{xx}(0) / f_{jl}^{xx}(0) \right) t \right] \quad . \quad (\text{A.2})$$

Imposing then the exact boundary conditions (McCoy and Wu, 1973):

$$f_{jl}^{xx}(0) = \frac{(-1)^n}{4} \left(\tanh \frac{\beta J}{2} \right)^n , \quad n = |j-l| \quad (\text{A.3})$$

and

$$\dot{f}_{jl}^{xx}(0) = 0 \quad , \quad (\text{A.4})$$

we get

$$f_{jl}^{xx}(t) = \frac{(-1)^n}{4} \left(\tanh \frac{\beta J}{2} \right)^n \quad , \quad (\text{A.5})$$

which is the exact result.

On the other hand, when the exchange interaction is zero, we have to consider two cases. The first one is when $j = 1$, and in this case we have immediately

$$f_{jj}^{zz}(t) = \frac{1}{4} \quad , \quad (\text{A.6})$$

$$\langle S_j^z \rangle = \frac{1}{2} \tanh \frac{\beta h}{2} \quad , \quad (\text{A.7})$$

and from eq. (3.11) we get:

$$f_{jj}^{xx} \ddot{f}_{jj}^{xx} - \left(\dot{f}_{jj}^{xx} \right)^2 = - \frac{h^2}{16} \left(- \tanh^2 \frac{\beta h}{2} + 1 \right) , \quad (\text{A.8})$$

with the boundary conditions:

$$f_{jj}^{xx}(0) = \frac{1}{4} \quad (\text{A.9})$$

and

$$\dot{f}_{jj}^{xx}(0) = \frac{-ih}{4} \tanh \frac{\beta h}{2} . \quad (\text{A.10})$$

Introducing in eq. (A.8) the transformation

$$f_{jj}^{xx} = e^{\phi} , \quad (\text{A.11})$$

we get

$$\ddot{\phi} = - C e^{-2\phi} , \quad (\text{A.12})$$

where

$$C = \frac{h^2}{16} \left(- \tanh^2 \frac{\beta h}{2} + 1 \right) . \quad (\text{A.13})$$

From eq. (A.12) we obtain:

$$\frac{1}{2} \dot{\phi}^2 = \frac{C}{2} e^{-2\phi} + C' , \quad (\text{A.14})$$

and from this equation, and using transformation (A.11) we get:

$$\left(\dot{f}_{jj}^{xx} \right)^2 = C + 2 C' f_{jj}^{xx} . \quad (\text{A.15})$$

Using the boundary conditions (A.9) and (A.10) the previous equation can be written as:

$$h^2 \left(f_{jj}^{xx} \right)^2 + \left(\dot{f}_{jj}^{xx} \right)^2 = C \quad , \quad (\text{A.16})$$

and finally we get:

$$f_{jj}^{xx}(t) = \frac{1}{4} \cos(ht) - \frac{i}{4} \tanh \frac{\beta h}{2} \sin(ht) \quad . \quad (\text{A.17})$$

The exact result is of course given by:

$$f_{jj}^{xx}(t) = \langle e^{iHt} S_j^x e^{-iHt} S_j^x \rangle \quad , \quad (\text{A.18})$$

where

$$H = -h \sum_{j=1}^N S_j^z \quad . \quad (\text{A.19})$$

Using the identity (see for instance Merzbacher, 1970)

$$e^{i\Theta S_j^z} = \cos \frac{\Theta}{2} + 2i \sin \frac{\Theta}{2} S_j^z \quad , \quad (\text{A.20})$$

we get

$$f_{jj}^{xx}(t) = \frac{1}{4} \cos(ht) - \frac{i}{2} \sin(ht) \langle S_j^z \rangle \quad , \quad (\text{A.21})$$

which can be expressed as

$$f_{jj}^{xx}(t) = \frac{1}{4} \cos(ht) - \frac{i}{4} \sin(ht) \tanh \frac{\beta h}{2} \quad . \quad (\text{A.22})$$

This expression is identical to the result obtained in eq. (A.17).

If $j \neq 1$ we have:

$$f_{j\ell}^{zz}(t) = \frac{1}{4} \tanh^2 \frac{\beta h}{2} \quad , \quad (\text{A.23})$$

and from eq. (3.11) we obtain

$$f_{jl}^{xx} \ddot{f}_{jl}^{xx} - \left(\dot{f}_{jl}^{xx} \right)^2 = 0 \quad , \quad (\text{A.24})$$

the solution of which is given by eq. (A.2). The boundary conditions in this case are:

$$f_{jl}^{xx}(0) = 0 \quad (\text{A.25})$$

and

$$\dot{f}_{jl}^{xx}(0) = 0 \quad , \quad (\text{A.26})$$

and obviously they imply

$$f_{jl}^{xx}(t) = 0 \quad . \quad (\text{A.27})$$

The exact result is obtained by proceeding as in the previous case, and we get immediately

$$f_{jl}^{xx}(t) = \cos(ht) \langle S_j^x S_l^x \rangle + \sin(ht) \langle S_j^y S_l^x \rangle \quad , \quad (\text{A.28})$$

and then

$$\dot{f}_{jl}^{xx}(t) = 0 \quad , \quad (\text{A.29})$$

which is identical to eq. (A.27).

REFERENCES

- Abraham A. and Bleaney B., Electron Paramagnetic Resonance of Transition Ions (Oxford University Press, London, 1970)
- Abraham D.B., Studies in Applied Math. 51, 179 (1972)
- Alfanas'ev A.M. and Kagan Yu, Sov. Phys. JETP 13, 1030 (1963)
- Algra H.A., Jongh L.J. de, Blöte H.W.J., Huiskamp W.J. and Carlin R.L., Physica 82B, 239 (1975)
- Allender D., Bray J.W. and Bardeen J., Phys. Rev. B9, 119 (1974)
- Barouch E. and McCoy B.M., Phys. Rev. A3, 786 (1971)
- Bartolomé J.G., Algra H.A., Jongh L.J. de and Huiskamp W.J., Proceedings of the International Conference on Magnetism, Amsterdam (1976), to be published in Physica B+C
- Berlinsky A.J., Contemp. Phys. 17, 331 (1976)
- Blöte H.W.J., Physica 79B, 427 (1975)
- Bogoliubov N.N., Uspekhi Fiz. Nauk. 67, 549 (1959)
- Brandt U. and Jacoby K., Z. Physik B25, 181 (1976)
- Camp W.J., Phys. Rev. B10, 2903 (1974)
- Capel H.W., Van Dongen E.J. and Siskens Th. J., Physica 76, 445 (1974)
- Capel H.W. and Siskens Th. J., Physica 81A, 214 (1975)
- Capel H.W. and Perk J.H.H., to be published (1977)
- Elliott R.J. and Dawber P.G., Proc. R. Soc. Lond. 273, 222 (1963)
- Elliott R.J., Harley R.T. and Smith S.P., Proc. R. Soc. Lond. A328, 217 (1972)
- Elliott R.J., Krumhansl J.A. and Leath P.L., Rev. Mod. Phys. 46, 465 (1974)

- Falk H. and Ruigrok Th. W., Phys. Rev. 139, 1203 (1965)
- Fisher M.E. and Hartwig R.E., Adv. Chem. Phys. 15, 333 (1969)
- Flicker J.K. and Leath P.L., Phys. Rev. B7, 2296 (1973)
- Folinsbee J.T., Harrison J.P., McColl D.B. and Taylor D.R.
to be published (1976)
- Gehring G.A. and Gehring K.A., Rep. Prog. Phys. 38, 1 (1975)
- Gonçaves L.L. and Elliott R.J., Proceedings of the International
Conference on Magnetism, Amsterdam (1976), to be published
in Physica B+C
- Gradshteyn I.S. and Ryzhik I.M., Table of Integrals, Series and
Products (Academic Press, New York, 1965)
- Hardy R.J., Phys. Rev. 132, 168 (1963)
- Harrison J.P., Hessler J.P. and Taylor D.R. Phys. Rev. B14,
2979 (1976)
- Hartwig R.E. and Fisher M.E., Arch. Ratl. Mech. Anal. 32, 190
(1969)
- Hone D.W. and Richards P.M., Annu. Rev. Mater. Sci. 4, 337 (1974)
- Horovitz B., Weger M. and Gutfraund H., Phys. Rev. B9, 1246 (1974)
- Horovitz B., Gutfraund H. and Weger M., Phys. Rev. B12, 3174 (1975)
- Imry Y., Montano P.A. and Hone D., Phys. Rev. B12, 253 (1975)
- Jha D.K. and Valatin J.G., J. Phys. A6, 1679 (1973)
- Johnson D.J. and McCoy B.M. Phys. Rev. A4, 2314 (1971)
- Jordan P. and Wigner E., Z. Physik 47, 631 (1928)
- Katsura S., Phys. Rev. 127, 1508 (1962)
Phys. Rev. 129, 2835 (1963)
- Katsura S., Horiguchi T. and Suzuki M., Physica 46, 67 (1970)

- Kawasaki K., Prog. Theo. Phys. 29, 801 (1963)
- Kohn W., Phys. Rev. Letts. 2, 393 (1959)
- Kubo R., J. Phys. Soc. Jap. 12, 570 (1957)
- Lajzerowicz J. and Pfeuty P., Phys. Rev. B11, 4560 (1975)
- Landau L. and Lifshitz E., Physique Statistique (Éditions MIR, Moscow, 1967)
- Lieb E.H., Schultz T. and Mattis D.C., Ann. Phys. 16, 407 (1961)
- Lieb E.H. and Mattis D.C., Mathematical Physics in One Dimension (Academic Press, New York, 1966)
- Madhukar A., Solid State Commun. 15, 921 (1975)
- Mazur P. and Siskens Th. J. Physica 69, 259 (1973)
- Physica 71, 560 (1974)
- McCoy B.M., Phys. Rev. 173, 531 (1968)
- McCoy B.M., Barouch E. and Abraham D.B., Phys. Rev. A4, 2331 (1971)
- McCoy B.M. and Wu T.T., The Two-dimensional Ising Model (Harvard University Press, Cambridge, 1973)
- McCracken D.D. and Dorn S.W., Numerical Methods and Fortran Programming (John Wile and Sons, New York, 1966)
- Merzbacher E., Quantum Mechanics, 2nd edition (John Wile and Sons, New York, 1970)
- Niemeijer Th., Physica 36, 377 (1967)
- Parry W.E., The Many-body Problem (Oxford University Press, London, 1973)
- Peierls R.E., Quantum Theory of Solids (Oxford University Press, London, 1955)
- Pfeuty P., Ann. Phys. 57, 79 (1970)

- Pytte E., Phys. Rev. B10, 2039 (1974)
- Rice M.J. and Strässler S., Solid State Commun. 13, 125 (1973)
- Sato H.J., J. Phys. Chem. Solids 19, 54 (1961)
- Scalapino D.J., Imry Y. and Pincus P., Phys. Rev. B11, 2042 (1975)
- Shiba H., Prog. Theo. Phys. 48, 2171 (1972)
- Soven P., Phys. Rev. 156, 809 (1967)
- Stanley H.E. and Kaplan T.A., J. Appl. Phys. 38, 975 (1967)
- Stanley H.E., Introduction to Phase Transitions and Critical Phenomena (Oxford University Press, London, 1971)
- Steiner M., Villain J. and Windsor C.G., Adv. Phys. 25, 87 (1976)
- Stout J.W. and Chisholm R.C., J. Chem. Phys. 36, 979 (1962)
- Suzuki M., Phys. Letts. 34A, 94 (1971)
- Taylor D.W., Phys. Rev. 156, 1017 (1967)
- Tjon J.A., Phys. Rev. B7, 2411 (1970)
- Tommet T.N. and Huber D.L., Phys. Rev. B11, 450 (1975)
- Tyablikov S.V., Methods in Quantum Theory of Magnetism (Plenum Press, New York, 1967)
- Valatin J.G., Phys. Rev. 122, 1012 (1961)
- Vinikovetsky I.A., Frishman A.M. and Khokhlov V.I., Ukrainian Phys. Journal 18, 810 (1973)
- Watson G.N., A Treatise on the Theory of Bessel Functions, 2nd edition (Cambridge University Press, London, 1966)
- Whittaker E.T. and Watson G.N., A Course of Modern Analysis, 4th edition (Cambridge University Press, London, 1973)
- Yonezawa F. and Morigaki K., Prog. Theo. Phys. 53, 1 (1973)

Young A.P., J. Phys. C8, 3158 (1975)

Zeller H.R., Adv. Solid State Phys. 13, 31 (1973)

Ziman J.M., Principles of the Theory of Solids (Cambridge
University Press, London, 1965)

Zubarev D.N., Sov. Phys. Usp. 3, 320 (1960)