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Dynamics of the one-dimensional transverse Ising model†

L L Gonçalves‡

Department of Theoretical Physics, University of Oxford, 1 Keble Road, Oxford OX1 3NP, UK

‡ Permanent Address: Departamento de Física da UFCe, Campus do Pici, Caixa Postal, 1262, 60000 Fortaleza, Ceará, Brazil

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Abstract. An approximate expression for the time-dependent longitudinal correlation function is given. It gives exact results in the limiting cases where the transverse field, or the exchange interaction, is zero. It is also shown that for arbitrary values of these parameters the approximation is only valid in the high-temperature limit. Some results are presented for the time-dependent and frequency transform of the spatial Fourier transform.

1. Introduction

The one-dimensional transverse Ising model ($s = \frac{1}{2}$, closed chain) is among the few many-body problems which can be solved exactly. Apart from that it has been used in the description of a large number of systems (Stinchcombe 1973). The one-dimensional model has received particularly great attention in recent years motivated by the discovery of the so-called quasi-one-dimensional systems (Zeller 1973). In the description of these systems the one-dimensional solution plays an important role due to the large anisotropy present (Sato 1961, Stout and Chisholm 1962).

The model is a particular case of the *XY* model (case of extreme anisotropy) introduced by Lieb *et al* (1961), and has been studied by many authors. The thermodynamic properties have been discussed in detail at $T = 0$ by Pfeuty (1970) and at finite temperature by Barouch and McCoy (1971).

Although the model is exactly soluble there are great difficulties in the calculation of some time-dependent correlation functions. These difficulties have been indicated by McCoy *et al* (1971) and discussed in detail by Capel *et al* (1974). Niemeijer (1967) and Tommet and Huber (1975) have calculated the transversal time-dependent correlation function at any temperature. The information about the time-dependent longitudinal correlation function is restricted to zero temperature and large separation between spins (McCoy *et al* 1971, Abraham 1972), short time expansion in the high-temperature limit (Capel *et al* 1974), and the exact result at infinite temperature (Brandt and Jacoby 1976, Capel and Perk 1977).

The purpose of this paper is to present in more detail an approximation to calculate these correlations at any temperature (Gonçalves and Elliott 1977). This approximation is an improvement over the so-called *c*-cyclic approximation (Mazur and Siskens

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1973, 1974). It gives the correct answer in special cases, namely when the exchange or the transverse field is zero.

In § 2 we present a review concerning the basic results and the difficulties of the calculation. In § 3 we calculate the correlations in the framework of the c -cyclic approximation and in § 4 we repeat the calculation in the framework of the new approach called the improved c -cyclic approximation. Finally in § 5 the results are presented and discussed.

2. Basic results

The Hamiltonian of the system can be written in the form

$$H = \sum_{j=1}^N 2JS_j^x S_{j+1}^x - \sum_{j=1}^N hS_j^z \quad (1)$$

where

$$S_1^v = S_{N+1}^v, \quad v = x, y, z \quad (2)$$

and S_i^v are half the Pauli spin matrices.

Introducing the lowering and raising operators (Lieb *et al* 1961)

$$a_j^+ = S_j^x + iS_j^y, \quad a_j = S_j^x - iS_j^y, \quad (3)$$

in terms of which the Pauli spin operators are

$$S_j^x = (a_j^+ + a_j)/2, \quad S_j^y = (a_j^+ - a_j)/2i, \quad S_j^z = a_j^+ a_j - \frac{1}{2}, \quad (4)$$

we obtain

$$H = \frac{1}{2} \sum_{j=1}^N J(a_j^+ a_{j+1} + a_{j+1}^+ a_j + a_j^+ a_{j+1} + a_{j+1} a_j) - \sum_{j=1}^N h \left(a_j^+ a_j - \frac{1}{2} \right). \quad (5)$$

Then if we introduce the Jordan–Wigner transformation (Jordan and Wigner 1928) defined by

$$a_j^+ = \exp \left[i\pi \sum_{l=1}^{j-1} c_l^+ c_l \right] c_j^+, \quad a_1^+ = c_1^+, \quad (6)$$

where c 's are fermion operators, the Hamiltonian (1) is written as (McCoy *et al* 1971)

$$H = H^+ P^+ + H^- P^-, \quad (7)$$

where P^+ and P^- are given by

$$P^\pm = \frac{1}{2} (1 \pm P) = \frac{1}{2} \left[1 \pm \exp \left(i\pi \sum_{l=1}^N c_l^+ c_l \right) \right], \quad (8)$$

and H^+ and H^- are:

$$H^\pm = \frac{1}{2} \sum_{j=1}^{N-1} J(c_j^+ c_{j+1} + c_j^+ c_{j+1}^+ + \text{HC}) - \sum_{j=1}^N h \left(c_j^+ c_j - \frac{1}{2} \right) \mp \frac{J}{2} (c_N^+ c_1^+ + \text{HC}). \quad (9)$$

The previous result is equal to that of McCoy *et al* (1971) when γ is considered equal to one.

The operator P defined in equation (8) satisfies the relations

$$[P, H] = [P, H^\pm] = 0, \quad P^2 = I, \tag{10}, (11)$$

and from these we conclude that P^+ and P^- are projector operators for states with positive and negative parity respectively, and 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^- differ by a boundary term (Capel *et al* 1974),

$$H^- - H^+ \equiv B = J(c_{Nc_1}^+ + c_{Nc_1}^+ + \text{HC}), \tag{12}$$

and they do not commute. Since they constitute bilinear forms on fermion operators, they can easily be diagonalised separately. The important step in this procedure is the imposition of boundary conditions on c operators, which should be anticyclic when diagonalising H^+ and cyclic when diagonalising H^- .

Defining the Fourier transform of c_j^+ as

$$c_j^+ = \frac{1}{N^{1/2}} \sum_k \exp(ikaj) c_k^+, \tag{13}$$

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

$$k = \pm 2\pi(n + \frac{1}{2})/Na \tag{14}$$

in the anticyclic case, and by

$$k = \pm 2\pi n/Na \tag{15}$$

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 equation (9) and the Bogoliubov-Valatin transformation (Bogoliubov 1959, Valatin 1961)

$$\beta_k = x_k c_k + y_k c_{-k}^+, \tag{16}$$

the inverse of which is

$$c_k = x_k^* \beta_k + y_k \beta_{-k}^+, \tag{17}$$

we obtain

$$H^\pm = \sum_k E_k \left(\beta_k^+ \beta_k - \frac{1}{2} \right), \tag{18}$$

where

$$E_k = [(J \cos ka - h)^2 + J^2 \sin^2 ka]^{1/2} \tag{19}$$

and the signs $+$ and $-$ in equation (18) hold for k 's given by equations (14) and (15) respectively. The x 's and y 's in equations (16) and (17) are given by

$$x_k = iJ \sin ka / [2E_k(E_k - \epsilon_k)]^{1/2}, \tag{20}$$

$$y_k = \left(\frac{E_k - \epsilon_k}{2E_k} \right)^{1/2}, \tag{21}$$

with

$$\epsilon_k = J \cos ka - h. \tag{22}$$

Using the results

$$[P^\pm, H^\pm] = 0, \quad (23)$$

$$(P^\pm)^2 = P^\pm, \quad P^+P^- = P^-P^+ = 0, \quad (24)$$

$$f(H) = f(H^+)P^+ + f(H^-)P^-, \quad (25)$$

where $f(z)$ is an analytic function of z , and

$$P^\pm S_j^x = S_j^x P^\mp, \quad (26)$$

the time-dependent longitudinal correlation function $\langle S_j^x(t)S_{j+n}^x(0) \rangle$ is given by

$$\langle S_j^x(t)S_{j+n}^x(0) \rangle = \frac{\text{Tr}[P^- \exp(-\beta H^-) \exp(iH^-t)S_j^x \exp(iH^+t)S_{j+n}^x] + \text{Tr}[P^+ \exp(-\beta H^+) \exp(iH^+t)S_j^x \exp(-iH^-t)S_{j+n}^x]}{\text{Tr}[P^+ \exp(-\beta H^+)] + \text{Tr}[P^- \exp(-\beta H^-)]} \quad (27)$$

where Tr stands for trace.

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

$$\langle S_j^x(t)S_{j+n}^x(0) \rangle = \frac{\text{Tr}[\exp(-\beta H^-) \exp(iH^-t)S_j^x \exp(-iH^+t)S_{j+n}^x]}{\text{Tr}[\exp(-\beta H^-)]}, \quad (28)$$

where the trace is calculated over the eigenstates of H^- .

Naturally the evaluation of equation (28) is very difficult since the time evolution is given by two different Hamiltonians. McCoy *et al* (1971) have avoided these difficulties by calculating the four-spin correlation function and using the cluster property:

$$\lim_{N \rightarrow \infty} \langle S_{1+N/2}^x(t)S_{1-n+N}^x(t)S_1^x(0)S_{1-n+N/2}^x(0) \rangle = \langle S_1^x(t)S_{1+n}^x(0) \rangle^2. \quad (29)$$

Within this approach they have been able to calculate the correlation $\langle S_j^x(t)S_{j+n}^x(0) \rangle$ for large n and $T = 0$. Unfortunately this method is very difficult to use at finite temperature.

Equation (28) can also be written in the form

$$\langle S_j^x(t)S_{j+n}^x(0) \rangle = \langle \exp(iH^-t)S_j^x \exp(-iH^-t)O(t)S_{j+n}^x \rangle, \quad (30)$$

where

$$O(t) = \exp(iH^-t) \exp(-iH^+t). \quad (31)$$

Capel *et al* (1974) have expanded this operator in powers of t and consequently equation (30) can be written as a power series. They have also 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.

3. The c -cyclic approximation

The so-called c -cyclic approximation (Mazur and Siskens 1973, 1974) consists of approximating the operator $O(t)$ by the identity. This means that in this approximation the correlation (30) is written as

$$\langle S_j^x(t)S_{j+n}^x(0) \rangle \cong \langle \exp(iH^-t)S_j^x \exp(-iH^-t)S_{j+n}^x \rangle. \quad (32)$$

Since we are considering the closed chain and assuming that the approximation does not break the translational symmetry, the correlation $\langle S_j^x(t)S_{j+n}^x(0) \rangle$ depends only on n and we can consider j equal to one. Proceeding in this way and after some rather lengthy algebraic manipulations we obtain

$$\langle S_1^x(t)S_{1+n}^x(0) \rangle = \frac{1}{4N} \sum_k \sum_{j=1}^{n+1} \cos(j-1)ka (-1)^{j-1} M_{n+1}^j \left[\cos E_k t - i \sin E_k t \tanh \frac{\beta E_k}{2} \right] \tag{33}$$

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

$$M = \begin{vmatrix} G(0) & G(-1) & \cdots & \cdots & \cdots & G(-n) \\ G(1) & & & & & \cdots \\ \cdots & & & & & \\ \cdots & & & & & \\ \cdots & & & & & \\ G(n) & \cdots & \cdots & \cdots & \cdots & G(0) \end{vmatrix}, \tag{34}$$

calculated with respect to the $(n+1)$ th row, j th column, and $G(n)$ is given by

$$G(n) = \frac{1}{N} \sum_k \tanh \frac{\beta E_k}{2} \frac{h \cos nka - J \cos(n+1)ka}{E_k}. \tag{35}$$

The details of this calculation can be found elsewhere (Gonçalves 1977).

If in equation (33) we consider the limit $h = 0$ we obtain

$$\langle S_1^x(t)S_{1+n}^x(0) \rangle = \frac{1}{4} (-1)^n (\tanh \frac{1}{2} \beta J)^n (\cos Jt - i \sin Jt \tanh \frac{1}{2} \beta J), \tag{36}$$

whereas the correct result is (McCoy and Wu 1973)

$$\langle S_1^x(t)S_{1+n}^x(0) \rangle = \frac{1}{4} (-1)^n (\tanh \frac{1}{2} \beta J)^n. \tag{37}$$

This has also been pointed out by Capel and Siskens (1975), and naturally makes clear in this simple limit 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.

4. The improved c -cyclic approximation

To obtain a better description of the dynamics of the system we have to treat the operator $O(t)$ by a better approximation. If instead of neglecting the difference between H^+ and H^- we neglect the commutator, we can write

$$O(t) \cong \exp[i(H^- - H^+)t], \tag{38}$$

and this constitutes the so-called improved c -cyclic approximation (Gonçalves and Elliot 1977). This new approximation is indeed an improvement over the previous one, although in a rather arbitrary way.

Equation (38) can be written as

$$O(t) \cong \cos Jt - i \sin Jt A_1 B_N \tag{39}$$

where

$$A_j = c_j^+ + c_j, \quad B_j = c_j^+ - c_j, \tag{40}, (41)$$

Substituting equation (39) in equation (30) we obtain

$$\langle S_j^x(t) S_{j+n}^x(0) \rangle = \langle \exp(iH^- t) S_j^x \exp(-iH^- t) S_{j+n}^x \rangle \cos Jt - i \sin Jt \langle \exp(iH^- t) S_j^x \exp(-iH^- t) A_1 B_N S_{j+n}^x \rangle. \tag{42}$$

As we see, the first term is the *c*-cyclic result multiplied by $\cos Jt$, and there is an additional term which can be calculated in the same way as the first one. The details of this calculation can be found elsewhere (Gonçalves 1977). Therefore the final result considering $j = 1$ is

$$\begin{aligned} \langle S_1^x(t) S_{1+n}^x(0) \rangle &= \frac{1}{4N} \sum_k^{n+1} \sum_{j=1}^{n+1} \left\{ \cos(j-1)ka \cos Jt (-1)^{j-1} M_{n+1}^j \right. \\ &\quad \times [\cos E_k t - i \sin E_k t \tanh(\beta E_k/2)] + i \sin Jt (-1)^j N_{n+1}^j \\ &\quad \left. \times \left(\tanh \frac{\beta E_k}{2} \cos E_k t - i \sin E_k t \right) \frac{[h \cos(j-2)ka - J \cos(j-1)ka]}{E_k} \right\} \end{aligned} \tag{43}$$

where N_{n+1}^j is the minor of the shifted Toeplitz determinant (Hartwig and Fischer 1969):

$$N = \begin{vmatrix} G(-1) & G(-2) & \cdots & \cdots & \cdots & G(-n-1) \\ G(0) & & & & & \cdots \\ \cdots & & & & & \cdots \\ \cdots & & & & & \cdots \\ \cdots & & & & & \cdots \\ G(n-1) & \cdots & \cdots & \cdots & \cdots & G(-1) \end{vmatrix}. \tag{44}$$

Considering equation (43) in the limit $h = 0$ we obtain

$$\langle S_1^x(t) S_{1+n}^x(0) \rangle = \frac{(-1)^n}{4} \left(\tan \frac{\beta J}{2} \right)^n, \tag{45}$$

which is the correct result. This certainly means an improvement over the *c*-cyclic approximation.

The introduction of the approximation shown in equation (39) implies the loss of the translational symmetry. As we shall see below, 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 as

$$c_n = \frac{1}{N} \sum_{j=1}^N \langle S_j^x(t) S_{j+n}^x(0) \rangle. \tag{46}$$

Unfortunately this expression cannot easily be 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.

5. Results and discussion

As mentioned in § 4, equation (43) gives the exact known result if we consider $h = 0$. It also gives the correct result in the limit $J = 0$, since in this case H^+ is equal to H^- and consequently $[H^+, H^-] = 0$.

Putting $n = 0$ in equation (43) we obtain the first two moments exactly, at any temperature. We also conclude from equation (43) that at $T = \infty$ only the autocorrelation differs from zero, which is exact (Brandt and Jacob 1976, Capel and Perk 1977).

The autocorrelation function, when the field is equal to the critical field (Pfeuty 1970), $h = J$, is written in a simple form, namely

$$\begin{aligned} \langle S_1^x(t) S_1^x(0) \rangle &= \frac{1}{4N} \sum_k \left(\cos E_k t - i \sin E_k t \tanh \frac{\beta E_k}{2} \right) \cos Jt \\ &+ \frac{i}{4N} \sum_k \sin \frac{ka}{2} \left(\tanh \frac{\beta E_k}{2} \cos E_k t - i \sin E_k t \right) \sin Jt \end{aligned} \quad (47)$$

where

$$E_k = 2J \sin(ka/2). \quad (48)$$

If $T = 0$, the integrals in the equation (47) can be performed exactly and the result takes the form (Gradshteyn and Ryzhik 1965)

$$\begin{aligned} \langle S_1^x(t) S_1^x(0) \rangle &= \frac{1}{4} [J_0(2Jt) \cos Jt + J_1(2Jt) \sin Jt - 2iE_0(2Jt) \cos Jt \\ &+ i(E_1(2Jt) - E_{-1}(2Jt)) \sin Jt] \end{aligned} \quad (49)$$

where the J 's are Bessel functions of the first kind and the E 's are Weber's functions. The asymptotic behaviour of this correlation is given by (Watson 1966)

$$\langle S_1^x(t) S_1^x(0) \rangle \sim \alpha / t^{1/2} \quad (50)$$

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

$$\langle S_1^x(t) S_1^x(0) \rangle \sim \alpha' / t^{1/4}. \quad (51)$$

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.

If $T = \infty$ the integral over k in equation (47) can again be performed exactly and the result is

$$\langle S_1^x(t) S_1^x(0) \rangle = \frac{1}{4} [J_0(2Jt) \cos Jt + J_1(2Jt) \sin Jt]. \quad (52)$$

This does not agree with the exact result (Capel and Perk 1977):

$$\langle S_1^x(t) S_1^x(0) \rangle = \frac{1}{4} \exp(-J^2 t^2 / 4). \quad (53)$$

More recently Capel and Perk (1977) and Brandt and Jacoby (1976) have been able to get exact results at $T = \infty$ for arbitrary values of J and h .

In figures 1, 2 and 3 we show the autocorrelation for different temperatures ($\beta = 2J/k_B T$) and $\lambda = J/h$. The real part is symmetric and the imaginary part antisymmetric. It should be noticed that as λ is increased the Ising case is approached, and consequently the real part of the correlation falls off less rapidly and the imaginary part decreases. For λ greater than 100 the system behaves essentially as the Ising case independently of temperature. As the temperature is increased the imaginary part decreases, and at $T = \infty$ the autocorrelation is real.

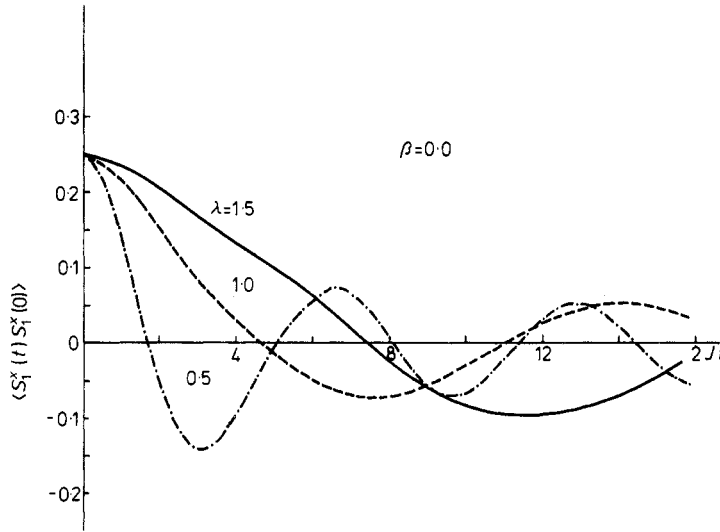


Figure 1. Self-correlation function at infinite temperature for various λ .

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

$$C_n(\omega) = \int_{-\infty}^{\infty} \exp(i\omega t) \langle S_1^x(t) S_{1+n}^x(0) \rangle dt \tag{54}$$

is immediately obtained from equation (43) and the result is

$$\begin{aligned}
 C_n(\omega) = \frac{\pi}{8N} \left\{ \sum_k \left(1 - \tanh \frac{\beta E_k}{2} \right) \delta(\omega + E_k + J) \left[\sum_j (F_n^j - G_n^j) \right] \right. \\
 + \sum_k \left(1 - \tanh \frac{\beta E_k}{2} \right) \delta(\omega + E_k - J) \left[\sum_j (F_n^j + G_n^j) \right] \\
 + \sum_k \left(1 + \tanh \frac{\beta E_k}{2} \right) \delta(\omega - E_k + J) \left[\sum_j (F_n^j + G_n^j) \right] \\
 \left. + \sum_k \left(1 + \tanh \frac{\beta E_k}{2} \right) \delta(\omega - E_k - J) \left[\sum_j (F_n^j - G_n^j) \right] \right\} \tag{55}
 \end{aligned}$$

where

$$F_n^j = \cos(j-1)ka (-1)^{j-1} M_{n+1}^j, \tag{56}$$

$$G_n^j = \frac{[h \cos(j-1)ka - J \cos jka] (-1)^j N_{n+1}^j}{E_k}. \tag{57}$$

The autocorrelation function and nearest-neighbour correlation function are shown in figures 4 and 5 for various λ and β . 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 frequencies is limited by h and $2J - h$. This is shown in figure 5 for $\lambda = 1.5$.

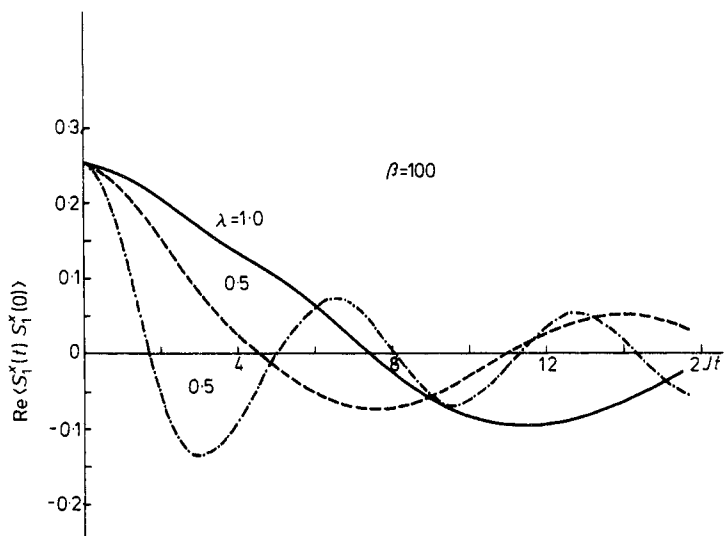


Figure 2. Real part of the self-correlation function at low temperature ($\beta = 100$) for various λ .

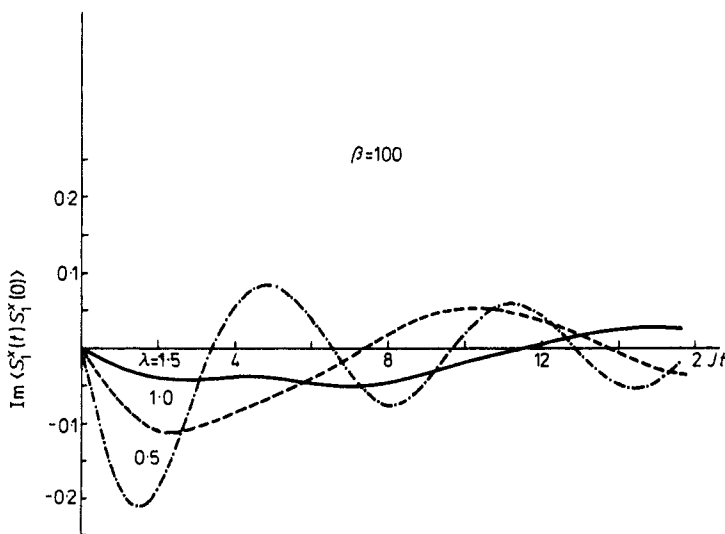


Figure 3. Imaginary part of the self-correlation function at low temperature ($\beta = 100$) for various λ .

The spatial Fourier transform of the time-dependent correlation function,

$$C_q(t) = \langle S_1^x(t) S_1^x(0) \rangle + 2 \sum_{n=1}^N \cos nqa \langle S_1^x(t) S_{1+n}^x(0) \rangle, \quad (58)$$

for various λ and wavevector $\pi/2a$ is shown in figures 6 and 7 for $\beta = 1.0$. Since we are considering the anti-ferromagnetic case, the correlation increases as we increase the wavevector. Unfortunately we have been unable to obtain the asymptotic behaviour of

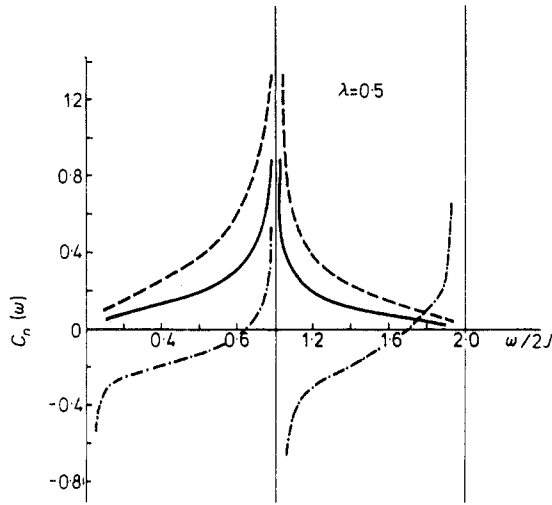


Figure 4. The frequency transforms of correlation functions at $\lambda = 0.5$. The full curve is the self-correlation function at high temperature $\beta = 0$. The broken curve is the self-correlation function at low temperature, $\beta = 100$. The chain curve is the near-neighbour correlation ($n = 1$) at $\beta = 100$.

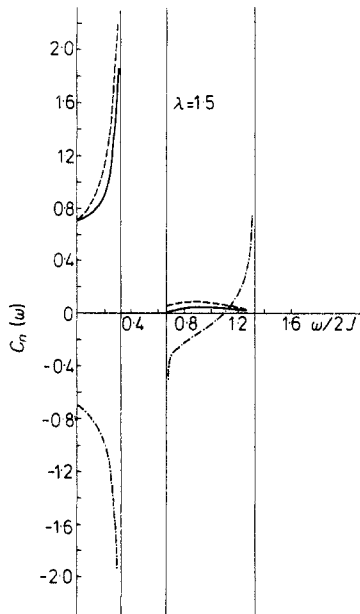


Figure 5. As figure 4, for $\lambda = 1.5$.

$\langle S_1^x(t)S_{1+n}^x(0) \rangle$ (large n), and consequently we cannot obtain the spatial Fourier transform at the very low-temperature limit. However it is possible numerically to obtain results as low as $\beta = 5$, which is lower than the critical temperature obtained using the mean-field approximation (for $\lambda = 1.5$, $\beta_c \sim 2$).

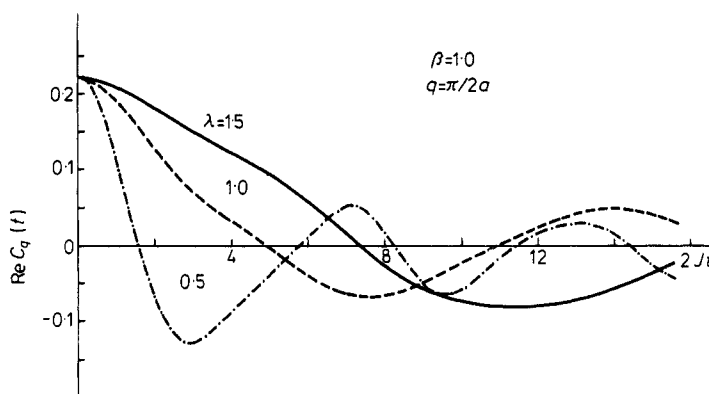


Figure 6. Real part of spatial transform for $\beta = 1.0$, wavevector $\pi/2a$ and various λ .

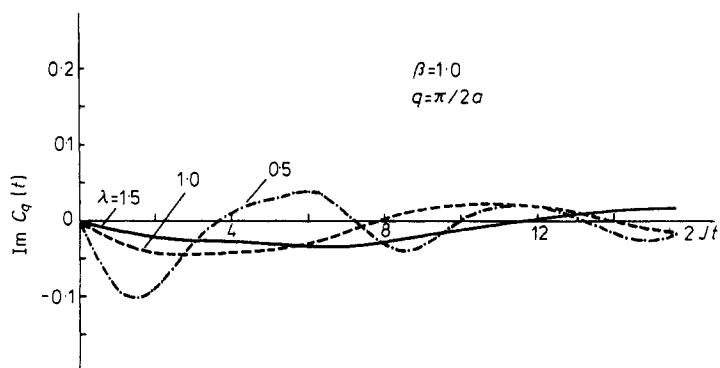


Figure 7. Imaginary part of spatial transform for $\beta = 1.0$, wavevector $\pi/2a$ and various λ .

Finally in figures 8 and 9 we present the transform of the spatial Fourier transform

$$C_q(\omega) = \int_{-\infty}^{\infty} \exp(i\omega t) C_q(t) dt \tag{59}$$

for various λ and β , and wavevectors $0, \pi/a$. As discussed previously there is a gap in the response for $\lambda > 1$ as shown in figure 9. These results, as expected, do not depend on the wavevector at high temperature ($\beta = 0.1$), and increase with the wavevector as we lower the temperature ($\beta = 1.0$).

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

$$\frac{1}{N} \langle\langle S_{-q}^x; S_q^x \rangle\rangle = \frac{1}{2\pi} \int_{-\infty}^{\infty} d\omega' \frac{\exp(-\beta\omega') [\exp(\beta\omega') - 1]}{\omega - \omega'} C_q(\omega'). \tag{60}$$

Due to translational symmetry we have

$$\langle\langle S_q^x; S_{-q}^x \rangle\rangle = \langle\langle S_{-q}^x; S_q^x \rangle\rangle, \tag{61}$$

and this implies that $\langle\langle S_q^x; S_{-q}^x \rangle\rangle$ must be a symmetric function of ω . To satisfy this

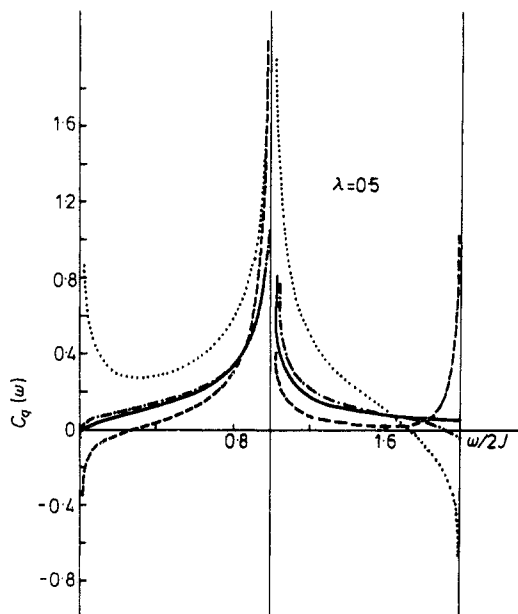


Figure 8. The frequency transforms of the spatial Fourier transforms at $\lambda = 0.5$. Full and broken curves are the transforms of wavevector 0 at $\beta = 0.1$ and 1.0 respectively. Transforms of wavevector π/a at $\beta = 0.1$ and 1.0 respectively.

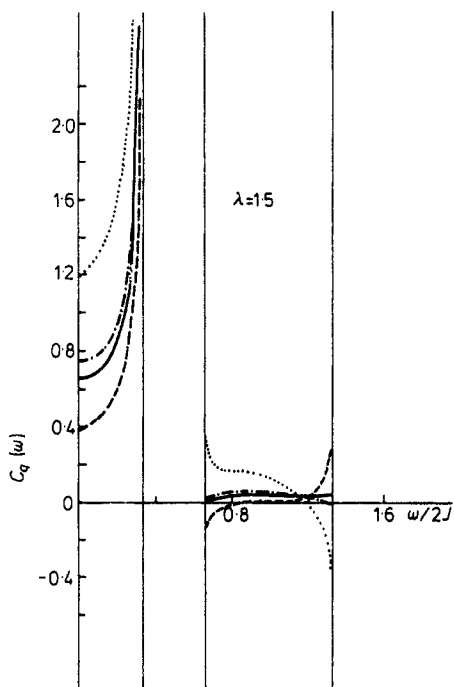


Figure 9. As figure 8, for $\lambda = 1.5$.

condition we conclude immediately from equation (60) that $C_q(\omega)$ should satisfy

$$C_q(\omega) = \exp(\beta\omega)C_q(-\omega). \quad (62)$$

This equation is only satisfied at $\beta = 0$, and consequently this clearly shows that the approximation breaks the translational symmetry at any finite temperature.

Defining \tilde{C}_q as

$$\tilde{C}_q(\omega) = \frac{1}{2}[C_q(\omega) + \exp(\beta\omega)C_q(-\omega)], \quad (63)$$

we see from equation (62) that \tilde{C}_q should be equal to C_q , had the translational symmetry not been broken. Therefore the parameter ϵ defined as

$$\epsilon = |(\tilde{C}_q - C_q)/C_q| \quad (64)$$

measures the quality of our approximation with respect to translational symmetry. To obtain a good approximation for $C_q(\omega)$, ϵ has to be small. At $\beta = 0.1$, ϵ is less than 10^{-3} ; however at $\beta = 1.0$ it becomes of order 1, which means that we have to restrict the use of the approximation for $\beta < 0.1$.

It should be noticed that we cannot at this stage of the calculation restore the translational symmetry by simply replacing C_q by \tilde{C}_q . The redefinition implies among other things that the static correlations which are known exactly are no longer correctly given by the approximation.

Finally we would like to point out that, as mentioned previously, in the c -cyclic approximation we considered $H^+ = H^-$, and in the improved one we neglected $[H^+, H^-]$. We can of course continue the calculation, and neglect higher-order terms, which are expected to give better approximations.

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