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Thermal Properties of the Anisotropic Heisenberg Linear Chain

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Abstract We study the specific heat of the anisotropic Heisenberg closed linear chain by using two different formalisms. These two approaches give the same result and reproduce the well known exact results for the Ising and XY models. These methods seem to be more suitable and powerful for better approximation when compared with other similar works. We present explicit expressions for the internal energy and the specific heat, which are valid for any temperature, and we compare the results with the exact ones obtained for the anisotropic chain in the low temperature limit.

1. INTRODUCTION

The most commonly studied system in statistical mechanics, on which exact calculations have been performed is the one - dimensional Ising model[1]. The reason is because it is one of richest and most profound model investigated so far and it can describe fairly well inumerous physical systems of interest. Indeed much of the theoretical study in magnetism has been based on this model together with the Heisenberg spin Hamiltonian[2,3].

The solution of the one-dimensional spin 1/2 Ising model with nearest-neighbour interaction has been given by several authors[4]. For the one-dimensional anisotropic XY-model nearest-neighbour interaction only Lieb *et al*[5] and Katsura[6] calculated the exact partition function and investigated the magnetic properties. The exact results for the isotropic Heisenberg chain have been obtained by Fisher[7] and are restricted to the classical model.

Exact results have been also obtained for the classical aniso-

tropic chain by Rae[8] and for the quantum model there has been a renewed surge of interest in the model with and without externa1 magnetic field, although so far they are restrict to the low-temperature limit[9-12].

It is the aim of this work to present two treatments to study the specific heat of the one-dimensional ferromagnetic spin 1/2 system. In the first one the results are derived from a Green function formalism via Dyson's equation; the infinite set of equations for these functions are solved exactly with the use of a transfer function. On the other hand, the same results can be found by mapping the spin system in an interacting fermion system by introducing the Jordan-Wigner transformation[13]. Although these two formalisms are different, they bear a reasonably close resemblance as far as the nature of the problem is concerned.

Sections 2 and 3 are devoted to the presentation of the Hamiltonian and the two methods of calculation, with the scope to find the density of states of the system, In section 4 we calculate the specific heat for both isotropic and anisotropic chain and cqmpare these results with the known exact ones. The conclusions of this paper are in section 5.

2. THE HAMILTONIAN: TRANSFER MATRIX TREATMENT

We consider the Hamiltonian for the one-dimensional system in which spin j interacts only with spin $j \pm 1$, namely

$$H = - \sum_j \left[J^z S_j^z S_{j+1}^z + J^{xy} (S_j^x S_{j+1}^x + S_j^y S_{j+1}^y) \right] \qquad (1)$$

where the sum on j runs from 1 to N; J is the effective nearest neighbour exchenge and S^x, S^y, and S^z are half the Pauli spin matrices a.

The ground state of our ferromagnet, corresponding to the state of complete spin alignment, is denoted by $|0\rangle$. We may define a complete set of orthonormal single spin deviation states $\{|m\rangle, m = 1 \ldots a\}$ where

$$|m\rangle = S_m^- |0\rangle \qquad (2)$$

Using this basis, the matricial representation of the Hamiltonian (1) is

$$\langle n|H|m\rangle = \frac{J^z}{2}\,\delta_{nm} - \frac{J^{xy}}{2}\,(\delta_{n,m+1} + \delta_{n,m-1}) \tag{3}$$

where we have considered in (3) as zero of energy the ground state energy $-NJ^2/4$ minus $J^z/2$, and δ_{nm} is the Kronecker delta. This rather artifical zero of energy has been chosen in order to get the correct results in the lirnit $J^{xy} \to 0$.

The Green function matrix elements satisfy Dyson's equations ($\hbar = 1$)

$$\omega\, G_{jk}(\omega) = \delta_{jk} + \sum_{\ell} H_{j\ell}\, G_{\ell k} \tag{4}$$

which, together with (3) yields

$$\begin{aligned}
(\omega - J^z/2)\, G_{nm} &= 1 - \frac{J^{xy}}{2}\,(G_{n,n-1} + G_{n,n+1}) \\
(\omega - J^z/2)\, G_{n,n+1} &= -\frac{J^{xy}}{2}\,(G_{nn} + G_{n,n+2}) \\
&\vdots \\
(\omega - J^z/2)\, G_{n,n+m} &= -\frac{J^{xy}}{2}\,(G_{n,n+m-1} + G_{n,n+m+1})
\end{aligned} \tag{5}$$

This infinite set of coupled equation can be solved using the transfer function** defined by

$$T(\omega) = \frac{G_{n,n+m+1}}{G_{n,n+m}} \quad \text{for } m > 0 \tag{6}$$

and

$$T'(\omega) = \frac{G_{n,n+m-1}}{G_{n,n+m}} \quad \text{for } m < 0 \tag{7}$$

As we can assume that the coupling with the nearest neighbours spins are indentical we have $T(\omega) = T'(\omega)$. Equation (6) together with (5) therefore yields

$$T(\omega) = \frac{(\omega - J^z/2) \pm \left[(\omega - J^z/2)^2 - J^{xy\,2}\right]^{1/2}}{J^{xy}} \tag{8}$$

The Pfunction above is complex in the interval

$$-J^{xy} < \omega - J^z/2 < J^{xy} \tag{9}$$

which correspond to the energy band of the systern. The diagonal elements of the Green functions are given by

$$G_{nn} = \left[\omega - J^z/2 + J^{xy}\, T(\omega)\right]^{-1} \tag{10}$$

The density of states is

$$D(\omega) = -\frac{1}{\pi} \operatorname{Im} \sum_{n=1}^{N} G_{nn} \tag{11}$$

or

$$D(\omega) = \frac{N}{\pi} \left| J^{xy\,2} - (\omega - J^z/2)^2 \right|^{-1/2} \tag{12}$$

where the signal in (8) was choosen in such a way that we have a physical density of states.

In the special cases of the Ising model ($J^{xy} = 0$), XY model ($J^z = 0$) and isotropic Heisenberg model ($J^{xy} = J^z = J$) we have respectively, from (12)

$$D_I(\omega) = N\, \delta\, (\omega - J^z/2) \tag{13}$$

$$D_{xy}(\omega) = \frac{N}{\pi} \left(J^{xy\,2} - \omega^2\right)^{-1/2} \tag{14}$$

$$D_H(\omega) = \frac{N}{\pi} \left(3J^2/4 + J\omega - \omega^2\right)^{-1/2} \tag{15}$$

3. THE FERMION REPRESENTATION APPROACH

The Hamiltonian (1) can also be studied by introducing the Wigner-Jordan transformation[13] which maps the set of spins in a system of interacting fermions[15]. In order to make clear the method we will present the basic and formal results concerning the treatment of the Hamiltonian.

Introducing in the Hamiltonian (1) the lowering and raising operators[5]

$$a_j^+ = S_j^x + iS_j^y \ , \quad a_j = S_j^x - iS_j^y \tag{16}$$

in terms of which the spin operators are

$$S_j^x = \frac{a_j^+ + a_j}{2} \ ; \quad S_j^y = \frac{a_j^+ - a_j}{2i} \ ; \quad S_j^z = a_j^+ a_j - 1/2$$

we obtain

$$H = -\frac{J^{xy}}{2}\sum_j (a_j^+ a_{j+1} + a_{j+1}^+ a_j) - J^z \sum_j (a_j^+ a_j a_{j+1}^+ a_{j+1} - a_j^+ a_j + \frac{1}{4}) \tag{17}$$

If we introduce the Wigner-Jordan transformation[13] defined by

$$a_j^+ = \exp\ (i\pi \sum_{\ell=1}^{j-1} c_\ell^+ c_\ell)\ c_j^+ \qquad a_1^+ = c_1 \ , \tag{18}$$

where c's are fermion operators, (17) can be written as:

$$H = H^+ P^+ + H^- P^- \tag{19}$$

with

$$P^\pm = \frac{1}{2}\ (1 \pm P) = \frac{1}{2}\left[1 \pm \exp\ (i\pi \sum_{j=1}^{N} c_j^+ c_j)\right] \tag{20}$$

and $H^\pm$ is

$$H^\pm = -\frac{J^{xy}}{2} \sum_{j=1}^{N-1} (c_j^+ c_{j+1} + c_{j+1}^+ c_j) \pm \frac{J^{xy}}{2} (c_N^+ c_1 + c_1^+ c_N) -$$

$$- J^z \sum_{j=1}^{N} (c_j^+ c_j c_{j+1}^+ c_{j+1} - c_j^+ c_j + \frac{1}{4}) \qquad (21)$$

The operator P satisfies the relations

$$[P,H] = [P,H^{\pm}] = 0, \quad P^2 = I , \qquad (22)$$

and we conclude that the eigenstates of $H^{\pm}$ have definite parity. It is important to note that P^+ and P^- are projector operators for states with positive and negative parity respectively. Therefore the eigenstates of H are the eigenstates of H^+ with positive parity and the eigenstates of H^- with negative parity.

In order to deal with H^+ and H^- we have to impose anticyclic and cyclic boundary conditions on c operators[16,17]. In the thermodynanic limit the static properties can be evaluated by considering only H^-. On the other hand, in the calculation of some dynamic properties we cannot neglect H^+ and this fact makes these calculations very difficult to be performed[16]. However, since we are interested only in static properties we will indentify H with H^-. The interacting term of H^- will be considered in the so called virtual crystal approximation[18] by assuming that $J^z c_{j+1}^+ c_{j+1}$ behaves as random field which takes the values 0 and J^z[19]. The average field is obtained by considering equal probabilities forthe random values (1/2) and doing so we obtain

$$\bar{J} = \frac{J^z}{2} \qquad (23)$$

Therefore in this approximation we can write H^- in the form

$$H = - \frac{J^{xy}}{2} \sum_{x=1}^{N} (c_j^+ c_{j+1} + c_{j+1}^+ c_j) - \frac{J^z}{2} \sum_{j=1}^{N} (\frac{1}{2} - c_j^+ c_j) , \qquad (24)$$

where we have assumed cyclic boundary conditions on C operators. H^- is diagonalised by introducing the Fourier transform

$$c_j^+ = \frac{1}{\sqrt{N}} \sum_k \exp(ikj)\, c_k \quad \text{with} \quad k = \pm \frac{2\pi n}{N} \qquad (25)$$

where n runs from 0 to $N/2$ (N is assumed to be even for convenience) . Then we get

$$H = \sum_k \omega_k \left(c_k^+ c_k - \frac{1}{2} \right) , \tag{26}$$

where

$$\omega_k = - J^{xy} \cos k + \frac{J^z}{2} \tag{27}$$

It should be noticed that $2J^z$ appearsas a transverse field in the XY-model. Naturally in this approach we get correctly the limit $J_z \to 0$ [5].

The Ising limit is obtained by $J^{xy} = 0$ and in this case we get the correct energy for the ground state namely $E_0 = - NJ^z/4$.

The density of states is immediately obtained and is given by:

$$D(\omega) = \frac{N}{\pi} \frac{1}{\left[J^{xy^2} - (\omega - \frac{J^z}{2})^2 \right]^{1/2}} \tag{28}$$

which is identical to the one obtained using the transfer matrix technique. Therefore the different approaches will give the same result for the therrnodynamic properties.

4. THE SPECIFIC HEAT

Using (15) or (28) we can easily calculate the internal energy of the system defined by

$$U(T) = \int \omega \, D(\omega) \, f(\omega) \, d\omega \tag{29}$$

where $f(\omega)$ is the Fermi-Dirac occupation factor given by

$$f(\omega) = \left[\exp(\beta\omega) + 1 \right]^{-1} \tag{30}$$

and $\beta = 1/K_B T$.

Explicitly the internal energy is given by

$$U(T) = \frac{N}{\pi} \int_{-J^{xy} + J^z/2}^{J^{xy} + J^z/2} \frac{\omega}{\left[J_{xy}^2 - (\omega - \frac{J^z}{2})^2\right]^{1/2}} \frac{d\omega}{e^{\beta\omega}+1} \qquad (31)$$

4.1 - Ising, XY and Heisenberg models

In the limit $J_{xy} \to 0$ rhe internal energy is obtained from eq. (31) by calculating Cauchy's principal value and we find apart from a constant term.

$$U(T) = - \frac{NJ^z}{4} \tanh (\beta J^z/4) \qquad (32)$$

The specific heat is

$$C(T) = \frac{\partial U(T)}{\partial T} = \frac{NJ^{z^2}}{16 K_B T^2} \operatorname{sech}^2 (\beta J^z / 4) \qquad (33)$$

which has a rmooth maximum in the neighbourhood of $K_B T = J^z/4$ but exhibits no phase transition at finite T. The specific heat goes to zero at T = 0 in agreement with the third law of thermodynamics. Also, (32, 33) agree with the well known exact results found by severa1 authors.

The partition function is defined from the internal energy by

$$U(T) = - \frac{\partial \ln Z}{\partial \beta} \qquad (34)$$

and gives

$$Z = \left[2 \cosh (\beta J^z/4)\right]^N \qquad (35)$$

From the partition function we can find now all the other thermodynamic potentials such as the entropy, Helmholtz free energy etc., as we are looking for.

Using (31) the internal energy in the XY model is given by

$$\frac{U(T)}{NJ^{xy}} = - \frac{1}{\pi} \int_0^{\pi/2} \tanh (k \cos \theta) \cos\theta \, d\theta \qquad (36)$$

where $k = \beta J^{xy}/2$.

The specific heat is

$$\frac{C(T)}{NK_B} = \frac{k^2}{\pi} \int_0^{\pi} \frac{\cos^2 \theta \, d\theta}{\cosh^2 (k \cos\theta)} \tag{37}$$

and both the results are in agreement with Katsura[6].

In a similar way, we can find the integral expressions for the internal energy and specific heat for the Heisenberg model, namely

$$\frac{U(T)}{NJ} = \frac{1}{8K^{3/2}\pi} \int_0^{4k} \frac{(y-k)\,[1 - \tanh(y-k)]\,dy}{y^{1/2}\,(1-y/4k)^{1/2}} \tag{38}$$

and

$$\frac{C(T)}{NK_B} = \frac{K^{1/2}}{\pi\beta} \int_0^{4K} \frac{(y-k)^2 dy}{y^{1/2}\,(1-y/4k)^{1/2}\,[\cosh(y-k)+1]} \tag{39}$$

4.2 - Anisotropic Chain

The specific heat for this case can be obtained from (31) as

$$C(T) = \frac{N}{2\pi K_B T^2} \int_0^{2\pi} \frac{\omega_k^2 \, e^{\beta\omega_k} \, dk}{(e^{\beta\omega_k} + 1)^2} \tag{40}$$

where ω_k is given by *(27)*

In order to compare with the exact results surveyed by Johnson[20] we restrict our calculation for the low-temperature regime although (40) is valid for any temperature.

For large β the asymptotic behaviour of (40) can be obtained by using Laplace's method[21] and we get the results

$$C(T) \sim \frac{N(J^{xy})^{3/2}}{(\pi K_B)^{1/2}} \left(1 - \frac{J^z}{2J^{xy}}\right)^2 T^{-3/2} \exp\left[\frac{J^{xy}}{K_B T}\left(1 - \frac{J^z}{2J^{xy}}\right)\right] \tag{41}$$

for $|J^z/J^{xy}| > 2$, and

$$C(T) \sim \frac{2K_B^2 T}{\pi\left[(4J^{xy})^2 - (J^z)^2\right]^{1/2}} \tag{42}$$

for $|J^z/J^{xy}| < 2$.

A comparison between our results (41) and (42) with the exact ones shows a difference in the interval $1 < |J^z/J^{xy}| < 2$ where the behaviour is like (41). This disagreement can be justified due to our crude approximation in considering no correlation effects in our treatment.

5. CONCLUSIOIUS

The main purpose of this paper was to show new derivations of the thermal properties of the spin 1/2 anisotropic Heisenberg chain. Analytic expression were obtained for the interna1 energy and specific heat for the special cases of Ising, XY and Heisenberg models while a low-temperature expansion for the anisotropic chain was also shown.

The elegant way to treat the Green functions via Dyson's equation with ths transfer function technique was one of the main feature of the calculat'ion presented here.

The other important features was concerned with the fermion operator formalism, first introduced by Jordan and Wigner. This formalism, since then, has been used extensively and always it seems to be very powerful. The results obtained by using both formalisms are in agreement and they reproduce the known exact results for the Ising and XY models.

Thr: little discrepancy found in the anisotropic chain, we believe can be overcome by including correlation effects into our methods.

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RESUMO

Estudamos o calor específico de uma cadeia linear fechada usando o modelo de Heisenberg anisotrópico, por meio de dois diferentes formalismos. Estes formalismos fornecem o mesmo resultado e reproduzem, como casos-limite, os já bem conhecidos resultados exatos dos modelos de Ising e XY. Os métodos de cálculo utilizados nos parecem ser mais convenientes e poderosos quando comparados com outros trabalhos similares. Apresentamos expressões explícitas para a energia interna e calor específico, válidas para qualquer temperatura, e comparamos nossos resultados com os resultados exatos obtidos para uma cadeia anisotrópica no limite de baixa temperatura.