Thermodynamics of $s = \frac{1}{2}$ Magnetic Linear Chain

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Abstract We solve the thermal Hartree-Fock equations for the anisotropic Heisenberg model in 1D in the neighborhood of the exactly soluble XY model. This paper displays the specific heat.

1. INTRODUCTION

The anisotropic Heisenberg Hamiltonian is characterized by three coupling constants $J_x$, $J_y$, and $J_z$. The thermodynamics of the $s=1/2$ XY model (Heisenberg model with $J_z=0$) is exactly calculable in one dimension (1D) by a "trick": transformation of spin operators $S_n^\pm$ into fermion creation and destruction operators $\alpha_n^*$ and $\alpha_n$. The anisotropic Heisenberg model ($J_z \neq 0$) cannot be so easily reduced to quadrature; the ground state for the cases $J_x=J_y$ is obtainable by Bethe's ansatz$^2$ but the thermodynamics is given by formidable coupled nonlinear equations$^3$, the validity of which has not been fully established. Our basic knowledge of the thermodynamics of $s=1/2$ magnetic systems in 1D comes, therefore, from numerical extrapolations on finite chains$^4$, and not from fundamental theory.

In this paper, we seize upon a remark by several researchers$^5$ that the elementary excitations of magnetic systems in 1D are fermionic i.e. "spin waves" carry spin one-half. This is precisely the situation for the XY model, and suggests that the general anisotropic Heisenberg model may be modeled on the XY model. For the ground state, this modeling yields excellent results$^6$ if "exchange" and "correlation" terms are retained in the treatment of the perturbation,

$$H' = -J_z \sum_{n=1}^{N} S_n^z S_{n+1}^z$$

(1)

For $|J_z| \ll |J_x|$ or $|J_y|$ the exchange terms are sufficient, because the correlation energy contributes only $O(J_z^2)$$^6$. The "exchange" contributions are given exactly by Hartree-Fock theory, and so we have the
motivation for the present work: We derive, and solve, the rather simple Hartree-Fock equations for the Hamiltonian $H = H_0 + H'$, where $H_0$ is

$$H_0 = -\sum_{n=1}^{N} \left[ \frac{S^x_n S^x_{n+1}}{2} + \frac{S^y_n S^y_{n+1}}{2} \right] = (-1/2) \sum_{n=1}^{N} \left[ S^+_n S^-_{n+1} + H.C. \right]$$

choosing $\langle J_z \rangle = J_y = 1$ as the unit. We display the specific-heat curves obtained by this method in the accompanying figures. In an concluding paragraph, we indicate possible extensions of these calculations to include the aforementioned correlation terms, as well as externally applied fields and XY anisotropy ($J_z \neq J_y$).

2. HARTREE-FOCK EQUATIONS

After the transformation to fermions, $H_0$ takes the form

$$H = (-1/2) \sum_{n=1}^{N} \left[ \bar{\sigma}^*_n \bar{\sigma}^f_{n+1} + H.C. \right]$$

while $H'$ assumes the form

$$H' = -J_B \sum_{n=1}^{N} (\sigma^*_n \sigma^f_n - 1/2) (\sigma^*_n \sigma^f_{n+1} - 1/2)$$

Together, they represent a one-component fermi gas ('Majorana fermions') with weak nearest-neighbor interactions. Exact theories have established that in the range $|J_B| \leq 1$ the picture of free fermions remains essentially exact. (It is only for $|J_B| > 1$ that fundamental changes occur: for $J_B > 1$ there develops an energy gap and the ground state is the particle vacuum. The ground state for $J_B < -1$ is also characterized by a gap, but vacuum fluctuations introduce additional complications into this Ising-antiferromagnetic limit.)

The Hartree-Fock treatment of $H'$ thus models it on $H_0$, approximating it by a simpler operator

$$H'_{HF} = J_B \sum_{n=1}^{N} \left[ \bar{\sigma}^*_n \bar{\sigma}^f_{n+1} <\sigma^*_n \sigma^f_{n+1}> + H.C. \right]$$

$$-J_B \sum_{n=1}^{N} |<\sigma^*_n \sigma^f_{n+1}>|^2$$

In selecting the terms to be retained one determines the outcome of the calculation. Thus, we have not considered contractions such as
and have assumed
\[ \langle c_n c_{n+1} \rangle \]
\[ \langle c_n^* c_{n} \rangle - 1/2 = 0 \]  \tag{6b}

At the outcome of the calculation, one verifies that eqs. (6a) and (6b) vanish.

The vanishing brackets are thermal averages. Let us define \( \mu(T) \) as,
\[ \langle c_n^* c_{n+1} \rangle = \langle c_{n+1}^* c_n \rangle = \mu \]  \tag{7}
making the further assumption that \( \mu \) is real, again verified at the conclusion. The internal energy is
\[ \langle H_0 + H_{\text{HF}} \rangle = -N(\mu - J_{\text{eff}} \mu^2) \]  \tag{8}

with
\[ \mu = \frac{1}{N} \sum_k \langle a_k^* a_k \rangle \cos k \]
\[ = \frac{1}{2\pi} \int_{0}^{2\pi} d\cos k \left[ \frac{1}{\cos k} + 1 \right] \]  \tag{9}

and
\[ J_{\text{eff}} = 1 - 2J_z \mu \]  \tag{10}
The operators \( a_k^* \) create fermions in plane wave states, \( a_k \) destroy them. At this point, one may verify that eqs. (6a) and (6b) vanish.

To solve these equation, it is efficient to define an auxiliary variable
\[ \beta^* \equiv \beta J_{\text{eff}} \]  \tag{11}
in terms of which we obtain
\[ \mu(\beta^*) = \frac{1}{2\pi} \int_{0}^{2\pi} d\cos k \left[ e^{-\beta^* \cos k} + 1 \right]^{-1} \]  \tag{12}
\[ \beta = \beta^* \left[ 1 - 2J_z \mu(\beta^*) \right]^{-1} \]  \tag{13}
and
\[ \partial \mu/\partial \beta = \dot{\mu} \left[ (1-2J_z \mu)^2/(1 - 2J_z (\mu - \dot{\mu} \beta^*)) \right] \]  \tag{14}
with \( \dot{\mu} \equiv \partial \mu/\partial \beta \). The r.h.s. of eqs.(12)-(14) involve only the auxiliary variable. Similarly, the specific heat (the thermal derivative of eq. (8)) is obtained
Fig. 1 - Specific heat in units of $k$, eq. (15), for various $J_z$, as a function of $kT'$ (in units of $J_z = J_y = 1$).

Fig. 2 - Approximate scaling: $c/c_{max} \ vs \ T/T_{max}$ yields a universal curve only for $T < T_{max}$.
as a function of $\beta^*$ alone

$$
\sigma_{H=0} = k \beta^* (1 - 2J_z \mu) \sqrt{1 - 2J_z (\mu - \mu \beta^*)} \tag{15}
$$

The procedure we adopted was to specify $\beta^*$, then calculate $\beta, \mu$ and $\cdot$ so as to obtain the zero-field specific heat eq. (15). Fig. 1 gives the results of such calculations, showing that even outside the range of validity of the theory, at $J_z = 11$ or 11.57, the results are well-behaved.

Figure 2 shows an approximate scaling. Plotting $c/c_{\text{max}}$ vs. $T/T_{\text{max}}$ (where the maximum specific heat $c_{\text{max}}$ occurs at a temperature $T_{\text{max}}$) one would obtain a universal curve at all $J_z$ if $c(T)$ were linear at low $T$ and satisfied an Inverse power law, say $T^{-2}$ at $T > T_{\text{max}}$. However, this scaling seems accurate only for the low-temperature range.

3. DISCUSSION

At $\beta^* = 0$, $\mu = 1/\pi$. Thus, for $|J_z| > \pi/2$, we have trouble at $T=0$ with eq. (10). (The correct critical $|J_z|$ is eq. 1). If we retained the correlation terms, the approximate critical $|J_z|$ becomes $\pi/4$, a decided improvement over the present results. However, to retain the correlation terms at finite temperature, one requires a temperature-dependent bosonization scheme (an interesting project for the future).

To study small $J_z$ corrections to the anisotropic XY model ($J_x \neq J_y$), one requires averages of type eq. (6a). In the presence of an external field, or at values of $|J_z|$ exceeding the critical value, one similarly requires nonzero averages for eq. (6b). But, for the stated conditions of small $|J_z|$ and $J_x = J_y = 1$ in zero external field, the present solution of the exact Hartree-Fock equations appears to be satisfactory.

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6. Using "bosonization" of the fermion Hamiltonian, with all that implies (linearization procedures), M. Fowler succeeded in finding an excellent approximation to the ground state; see M. Fowler, J. Phys. **C13**, 1459 (1980).

**Resumo**

Resolvemos as equações de Hartree-Fock para o modelo de Heisenberg anisotrópico em 1D na vizinhança do modelo XY exatamente solúvel. Neste trabalho apresentamos o calor específico.