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Thermodynamics of $s = ½$ Magnetic Linear Chain

ANTONIO CALIRI and DANIEL MATTIS

Physics Department, University of Utah, Salt Lake City, Utah, USA

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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 c_n^* and c_n [1]. 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,

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

For $|J_z| << |J_X|$ 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

$$H_0 = -\sum_{n=1}^{N}\left[S_n^x S_{n+1}^x + S_n^y S_{n+1}^y\right] = (-1/2)\sum_{n=1}^{N}\left[S_n^+ S_{n+1}^- + \mathrm{H.C.}\right] \qquad (2)$$

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

2. HARTREE-I'OCK EQUATIONS

After the transformation to fermions, H_0 takes the form

$$H = (-1/2)\sum_{n=1}^{N}\left[c_n^* c_{n+1} + \mathrm{H.C.}\right] \qquad (3)$$

while H' assumes the form

$$H' = -J_z \sum_{n=1}^{N} (c_n^* c_n - 1/2)(c_{n+1}^* c_{n+1} - 1/2) \qquad (4)$$

Together, they represent a one-component fermi gas ("Majorana fermions") with weak nearest-neighbor interactions. Exact theories[2] have established that in the range $|J_z| \leqslant 1$ the picture of free fermions remains *essentially* **exact.** (It is only for $|J_z| > 1$ that fundamental changes occur: for $J_z > 1$ there develops an energy gap and the ground state is the particle vacuum. The ground state for $J_z < -1$ 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

$$H'_{\mathrm{HF}} = J_z \sum_{n=1}^{N}\left[c_n^* c_{n+1} \langle c_{n+1}^* c_n\rangle + \mathrm{H.C.}\right]$$

$$- J_z \sum_{n=1}^{N} |\langle c_n^* c_{n+1}\rangle|^2 \qquad (5)$$

In selecting the terms to be retained one determines the outcome of the calculation. Thus, we have *not* considered contractions such as

$$<c_n \, c_{n+1}> \tag{6a}$$

and have assumed

$$<c_n^* \, c_n - 1/2> = 0 \tag{6b}$$

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

The novanishing brackets are thermal averages. Let us define $\mu(T)$ as,

$$<c_n^* \, c_{n+1}> = <c_{n+1}^* \, c_n> = \mu \tag{7}$$

making the further assurnption that μ is real, again verified at the conclusion. The internal energy is

$$<H_0 + H'_{\mathrm{HF}}> = -N(\mu - J_z\mu^2) \tag{8}$$

with

$$\begin{aligned} \mu &= \frac{1}{N} \sum_k <a_k^* a_k> \cos k \\ &= \frac{1}{2\pi} \int^{2\pi} dk \cos k \left[1/(e^{-\beta J_{\mathrm{eff}} \cos k} + 1) \right] \end{aligned} \tag{9}$$

and

$$J_{\mathrm{eff}} = 1 - 2J_z\mu \tag{10}$$

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

$$\beta^* \equiv \beta J_{\mathrm{eff}} \tag{11}$$

in terms of which we obtain

$$\mu(\beta^*) = \frac{1}{2\pi} \int_0^{2\pi} dk \cos k \left[e^{-\beta^* \cos k} + 1 \right]^{-1} \tag{12}$$

$$\beta = \beta^* \left[1 - 2J_z \, \mu\,(\beta^*) \right]^{-1} \tag{13}$$

and

$$\partial\mu/\partial\beta = \dot{\mu} \left[(1-2J_z\mu)^2/(1 - 2J_z(\mu - \dot{\mu}\beta^*)) \right] \tag{14}$$

with $\dot{\mu} \equiv \partial\mu(\beta^*)\partial\beta^*$.

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

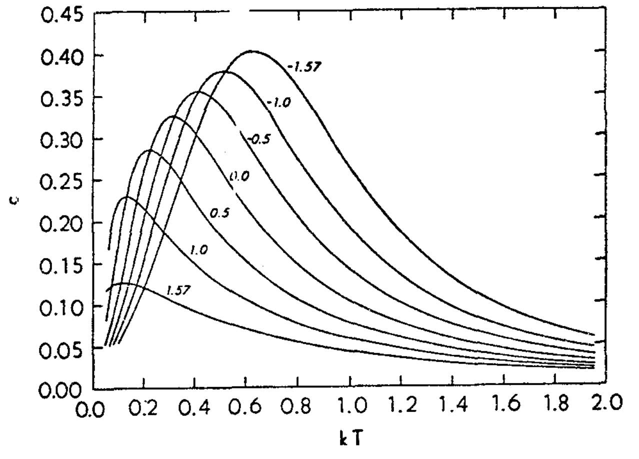

Fig.1 - Specific heat in units of k, eq. (15), for various J_z, as a function of kI' (in units of $J_x = J_y = 1$).

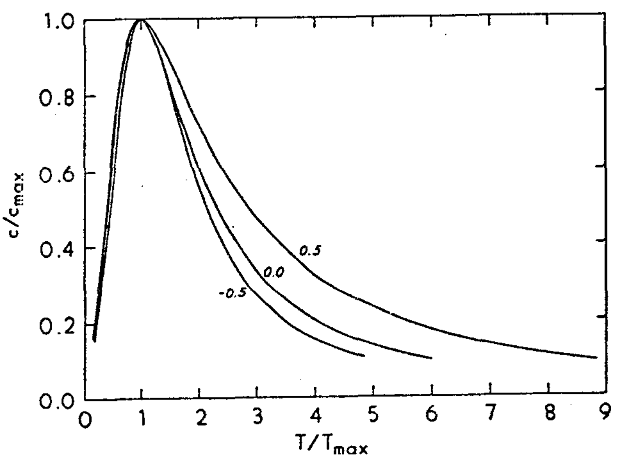

Fig.2 - Approximate scaling: c/c_{max} vs T/T_{max} yields a universal curve only for $T < T_{max}$.

as a function of β^* alone

$$c_{H=0} = k\,\beta^{*2}\,(1 - 2J_z\mu)\,\dot{\mu}/[1 - 2J_z(\mu - \dot{\mu}\beta^*)] \tag{15}$$

The procedure we adopted was to specify β^*, then calculate β, μ and $\dot{\mu}$ 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 = I 1 or 11.57, the results are well--behaved.

Figure 2 shows an approximate scaling. Plotting c/c_{max} vs. T/T_{max} (where the maximum specific heat c_{max} occurs at a temperature T_{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 $T > T_{max}$. How-wever, this scaling seems accurate only for the low-temperature range.

3. DISCUSSION

At $\beta^{*-1}=0$, $\mu=1/\pi$. Thus, for $|J_z| > \pi/2$, we have trouble at T=O 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[6]. 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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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.