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Antiferromagnetic model with Néel states as ground states

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We discuss in one as well as three dimensions an antiferromagnetic model with Néel states as ground states. Long-range order exists for this Hamiltonian. Finite-temperature properties of this Hamiltonian can be computed through the usual Green-function method and the results obtained are identical with those of the isotropic Heisenberg Hamiltonian through a similar method. The reason for this identity and its implication in analysis of experimental data are discussed.

I. INTRODUCTION

Some time ago an antiferromagnetic model was discussed, for which the ground-state wave function could be written down explicitly.[1] That model and its extensions have been studied by several authors.[2,3] In particular, Shastry and Sutherland[4] show that it exhibits frustration and dimerization effects. The ground state has no long-range order in the two-spin correlation function but exhibits a type of long-range order in the four-spin correlation function.[4,5] Using group theoretic methods, Klein[6] has constructed a whole class of similar Hamiltonians with known ground-state properties. Van den Broek, Caspars, and Magnus[7] as well as Shastry and Sutherland[8] have formulated similar Hamiltonians and studied the excitation spectra in some cases. A cubic antiferromagnet with known ground state has been studied also.[9]

It is, however, well known that the elementary theory of the Heisenberg antiferromagnet is based on the Néel states and finite-temperature Green-function computations[10] derived from them continue to be used for analysis of experimental data.[11] In this paper we discuss a Hamiltonian with Néel states as ground states. The model has strong transverse anistropy. It can be discussed in one as well as three dimensions and its finite-temperature properties can be computed through the Green-function method. The results indicate that if the experimental material is known to be an isotropic Heisenberg antiferromagnet the results should be analyzed not by the elementary theory but by detailed computations through other methods like series expansions.[12]

II. THE ONE-DIMENSIONAL MODEL

The Hamiltonian with Néel states as ground states can be written in one dimension as

$$H_A(J,\Delta)=\sum_{i=1}^{N}\left[JS_i^zS_{i+1}^z+\tfrac{1}{2}\Delta(S_i^+S_{i+1}^+ +S_i^-S_{i+1}^-)\right] . \tag{1}$$

Here $J>0$, $\Delta>0$, $0\leq\Delta/J\leq1$, N is even, and $N+1=1$ (periodic boundary conditions). Let us write the Néel states as

$$\phi_1=\alpha_1\beta_2\alpha_3\beta_4\cdots\alpha_{N-1}\beta_N , \tag{2a}$$

$$\phi_2=\beta_1\alpha_2\beta_3\alpha_4\cdots\beta_{N-1}\alpha_N , \tag{2b}$$

with α and β the up and down spin functions, respectively. These states are the lowest eigenstates of the Ising part of the Hamiltonian (1) with energy $E_0=-JN/4$ and the remaining part of (1) being a sum of two raising or two lowering operators for nearest neighbors has no effect on these states and no contribution to the ground-state energy. Actually, a lot could be said about (1) because it is a special case of the XYZ model studied by Baxter,[13] but the results of interest to us can be obtained directly, because the structure of (2) is rather simple. Also, Fogedby[14] has studied the ferromagnetic version of (1) and given an approximate description of the excitation spectrum.

Consider the ferromagnetic linear chain with longitudinal anisotropy

$$H_F(-J,-\Delta)=\sum_{i=1}^{N}\left[-JS_i^zS_{i+1}^z-\tfrac{1}{2}\Delta(S_i^+S_{i+1}^- +S_i^-S_{i+1}^+)\right] . \tag{3}$$

The ground state Φ_F is the completely aligned state, and the ground-state energy is $-JN/4$. By a simple canonical transformation it can be shown to have the same energy spectrum as the Hamiltonian

$$H_F(-J,\Delta)=\sum_{i=1}^{N}\left[-JS_i^zS_{i+1}^z+\tfrac{1}{2}\Delta(S_i^+S_{i+1}^- +S_i^-S_{i+1}^+)\right] . \tag{4}$$

Now, consider the operator

$$A=\Pi'\sigma^x , \tag{5}$$

where σ^x is the Pauli matrix and the product is taken over alternate sites. The canonical transformation with A connects (4) to (1) by

$$AH_F(-J,\Delta)A^{-1}=H_A(J,\Delta)\ . \tag{6}$$

This means that the ground-state energy of (1) is $-JN/4$.

To discuss the spectrum, we must also consider the translation group of (1) and (5). If T denotes the translation operator of displacement from one site to the next, the ferromagnetic state Φ_F belongs to the wave vector $k=0$ as $T\Phi_F=\Phi_F$. Depending on whether we rotate the spins at the odd or the even sites, we have two operators A_o and A_e, respectively. Neither commutes with T but we have $A_e\Phi_F=\phi_1$ and $A_0\Phi_F=\phi_2$. We note that T^2 commutes with both A_e and A_o. Given the spectrum and eigenfunctions of (4) labeled by the wave vectors of the translation group, these eigenfunctions of (4) acted on by A will have to be suitably mixed to make the spectrum and eigenfunctions of (1).

Since T^2 has the eigenvalue $+1$ for Φ_F, the states ϕ_1 and ϕ_2 have the same eigenvalue. Two normalized ground states belonging to the eigenvalues ± 1 for T can be constructed:

$$\begin{aligned}\phi^+&=\frac{1}{\sqrt{2}}(\phi_1+\phi_2),\quad T\phi^+=\phi^+\ ,\\ \phi^-&=\frac{1}{\sqrt{2}}(\phi_1-\phi_2),\quad T\phi^-=-\phi^-\ .\end{aligned} \tag{7}$$

We note the following relations:

$$S_m^z\phi_1=\tfrac{1}{2}(-1)^{m+1}\phi_1,\quad S_m^z\phi_2=\tfrac{1}{2}(-1)^m\phi_2\ ,\qquad m=1,2,\ldots,N \tag{8}$$

and

$$\begin{aligned}&S_m^+\phi_1=0,\quad S_m^-\phi_2=0,\quad m \text{ odd}\\ &S_m^+\phi_2=0,\quad S_m^-\phi_1=0,\quad m \text{ even}\ .\end{aligned} \tag{9}$$

The excited states of (4) can be calculated by the Bethe ansatz. Following the same trick, we would construct the excited state of (1), but a double periodicity appears as there are two ground states ϕ^+ and ϕ^- belonging to wave vectors 0 and π, respectively. Thus the states

$$\psi_1^+=\sum_m e^{iqm}(S_m^++S_m^-)\phi^+ \tag{10}$$

can be easily shown to have the excitation energy

$$\epsilon=J(1+\sigma\cos q) \tag{11}$$

where $\sigma=\Delta/J$. The excited states built up from the ground state ϕ^-

$$\psi_1^-=\sum_m e^{iqm}(S_m^++S_m^-)\phi^- \tag{12}$$

have the energy

$$\epsilon=J(1-\sigma\cos q)\ . \tag{13}$$

From (11) and (13), the lower excitation branch has the spectrum

$$\epsilon=\begin{cases}J(1-\sigma\cos q), & 0\le q\le\pi/2\\ J(1+\sigma\cos q), & \pi/2\le q\le\pi.\end{cases} \tag{14}$$

For $\sigma=1$, the dispersion relation for small excitation energy and small wave vector is

$$\epsilon\sim Jq^2\ . \tag{15}$$

Other excited states can be computed by Bethe-type ansatz and rearrangement as in (14).

The ground states (7) have the alternating long-range order of the Néel states:

$$\langle\phi^\pm|S_i^zS_j^z|\phi^\pm\rangle=\tfrac{1}{4}\delta_{ij}+\tfrac{1}{4}(1-\delta_{ij})(-1)^{i-j}\ . \tag{16}$$

At finite nonzero temperature, the one-dimensional system will not exhibit long-range order.

III. THE THREE-DIMENSIONAL MODEL

A three-dimensional antiferromagnetic Hamiltonian with Néel states as ground states can now be easily constructed. Consider a bipartite lattice and the Hamiltonian with nearest neighbor interaction ($J>0$):

$$H=\tfrac{1}{2}\sum_{\langle ij\rangle}[-JS_i^zS_j^z+\tfrac{1}{2}\Delta(S_i^+S_j^-+S_i^-S_j^+)]\ , \tag{17}$$

where i runs through one sublattice and j through the other such that i and j are nearest neighbors. The factor $\frac{1}{2}$ avoids double counting of bonds. The ground-state energy is $E_0=-\frac{1}{8}JNq$, where q is the number of nearest neighbors. On (17) we apply the unitary transformation

$$C=\Pi'\sigma^x\ , \tag{18}$$

where the product runs over one sublattice, and generate the desired antiferromagnetic Hamiltonian

$$H_A=\tfrac{1}{2}\sum_{\langle ij\rangle}[JS_i^zS_j^z+\tfrac{1}{2}\Delta(S_i^+S_j^++S_i^-S_j^-)]\ . \tag{19}$$

We can have two C operators for the rotation of the two sublattices. They generate the two Néel states Φ_1 and Φ_2. In Φ_1, the up spins are on sublattice A, the down spins on sublattice B, while the reverse happens in Φ_2. We have now three primitive translations, each of which takes Φ_1 into Φ_2 and vice versa. The ground-state functions

$$\Phi^+=\frac{1}{\sqrt{2}}(\Phi_1+\Phi_2),\quad \Phi^-=\frac{1}{\sqrt{2}}(\Phi_1-\Phi_2) \tag{20}$$

are eigenfunctions of the translation operator. The excitation spectrum for $J=\Delta$ has the form $\epsilon\sim q^2$ as $q\to 0$.

The ground state (20) has the conventional long-range order. Dyson, Lieb, and Simon[15] have utilized the canonical transformation (18) to prove that the two-dimensional version of (19) will have long-range order at finite temperature. It is likely that the Hamiltonian (19) in three dimensions has long-range order at finite temperature also.

IV. GREEN-FUNCTION CALCULATION

We now apply the Green-function technique to (19) to calculate the finite temperature thermodynamics. The basic equation is ($\hbar=1$)

$$E\langle\langle A;B\rangle\rangle_E=\frac{1}{2\pi}\langle[A,B]_-\rangle+\langle\langle[A,H]_-;B\rangle\rangle\ . \tag{21}$$

Let $A=S_g^-$ and $B=S_h^+$ where g and h denote sites on the same sublattice. The last term of (21) requires decoupling. Following Lines[10] we do the simplest Tyablikov decoupling, we put the average value of S_i^z at a site as $\bar{S}$ (the "up sublattice") and $-\bar{S}$ (the "down sublattice"). This is expected from the structure of the Néel states. The equations for the Green function can be written as

$$EG_k^{-+}=\frac{1}{\pi}\bar{S}+\mu\bar{S}G_k^{-+}+\lambda\bar{S}G_k^{++}\ , \tag{22}$$

$$EG_k^{++}=\mu\bar{S}G_k^{++}+\lambda\bar{S}G_k^{-+}\ . \tag{23}$$

$G_k^{\alpha\alpha'}$ ($\alpha,\alpha'=+$ or $-$) is the Fourier transform of the Green function $\langle\langle S_g^\alpha;S_h^{\alpha'}\rangle\rangle_E$ with respect to the reciprocal sublattice. Also

$$\mu=Jq,\ \ \lambda=J\sum_{\vec{\delta}}\exp(i\vec{k}\cdot\vec{\delta})\ . \tag{24}$$

$\vec{\delta}$ joins a site to its nearest neighbor.

For the linear chain (1), $\Delta=J$, this leads at zero temperature to

$$G_k^{-+}=\frac{\bar{S}(E-2J\bar{S})}{\pi(E-2J\bar{S}+2J\bar{S}\cos k)(E-2J\bar{S}-2J\bar{S}\cos k)}\ . \tag{25}$$

For spin-$\frac{1}{2}$ particles, the poles give the exact elementary excitation energies (11), (13), and (14). In three dimensions

$$G_k^{-+}=\frac{\bar{S}}{2\pi}\left[\frac{1}{E-\alpha_1\bar{S}}+\frac{1}{E-\alpha_2\bar{S}}\right]\ , \tag{26}$$

where

$$\alpha_{1,2}=\mu\pm\lambda\ . \tag{27}$$

Now from the relation

$$\langle B(t')A(t)\rangle=\lim_{\epsilon\to 0} i\int_{-\infty}^{\infty}d\omega\, e^{-i\omega(t-t')}(e^{\omega/k_BT}-1)^{-1}\times(\langle\langle A;B\rangle\rangle_{\omega+i\epsilon}-\langle\langle A;B\rangle\rangle_{\omega-i\epsilon})\ , \tag{28}$$

we can obtain using (21)

$$\langle S_h^+S_h^-\rangle=\bar{S}\left[\left\langle\frac{\sinh(\mu\bar{S}/k_BT)}{\cosh(\mu\bar{S}/k_BT)-\cosh(\lambda\bar{S}/k_BT)}\right\rangle_k-1\right]\ , \tag{29}$$

where $\langle\ \rangle_k$ denotes an average for k over the $N/2$ values in the first Brillouin zone. The expression for sublattice magnetization is

$$\frac{1}{\bar{S}}=2\left\langle\frac{\sinh(\mu\bar{S}/k_BT)}{\cosh(\mu\bar{S}/k_BT)-\cosh(\lambda\bar{S}/k_BT)}\right\rangle_k\ . \tag{30}$$

At and above T_c, we have $\langle(S^x)^2\rangle=\langle(S^y)^2\rangle=\langle(S^z)^2\rangle=\frac{1}{3}S(S+1)$ and we obtain from (30) the expression

$$\tfrac{1}{3}S(S+1)=\bar{S}\left\langle\frac{\sinh(\mu\bar{S}/k_BT)}{\cosh(\mu\bar{S}/k_BT)-\cosh(\lambda\bar{S}/k_BT)}\right\rangle_k\ . \tag{31}$$

As $T\to T_c$ from below, $\bar{S}\to 0$ and we get

$$\frac{S(S+1)}{3k_BT_c}=\left\langle\frac{\mu}{\mu^2-\lambda^2}\right\rangle_k\ . \tag{32}$$

The expression is identical to that of Lines for the usual Heisenberg antiferromagnet.

To calculate the parallel susceptibility, we include the magnetic field term $-g\mu_BH\sum_i S_i^z$ in the Hamiltonian (19). The average spin per site $\bar{S}_u=\bar{S}+\delta S$ and $\bar{S}_d=-\bar{S}+\delta S$ on the up and down sublattices, respectively, are no longer equal and opposite. Starting with Green functions for the sublattice we get

$$\bar{S}\mp\delta S=\{2\langle[\sinh(a'/k_BT)\pm A'\sinh(b'/k_BT)]\times[\cosh(a'/k_BT)-\cosh(b'/k_BT)]^{-1}\rangle_k\}^{-1}\ , \tag{33}$$

where

$$\begin{aligned}a'&=\mu\bar{S}\ ,\\ b'&=[\mu^2(\delta S)^2-2\mu g\mu_BH\,\delta S+g^2\mu_B^2H^2-\lambda^2(\delta S)^2-\lambda^2\bar{S}^2]^{1/2}\ ,\\ A'&=(g\mu_BH-\mu\delta S)/b'\ .\end{aligned} \tag{34}$$

Combining the two equations (33), we get an expression for δS

$$\delta S=\tfrac{1}{2}A'\sinh(b'/k_BT)[\cosh(a'/k_BT)-\cosh(b'/k_BT)]\times[\sinh^2(a'/k_BT)-A'^2\sinh^2(b'/k_BT)]^{-1}\ . \tag{35}$$

To obtain the zero-field parallel susceptibility $\chi_{\|}$, we consider the limit $H\to 0$ in the expression

$$\chi_{\|}=Ng\mu_B\delta S/H\ . \tag{36}$$

Using the expression (30) for $\bar{S}$ we obtain for temperatures below the transition point

$$\chi_{\|}=\frac{Ng^2\mu_B^2\sinh(\lambda\bar{S}/k_BT)}{\lambda\sinh(\mu\bar{S}/k_BT)+\mu\sinh(\lambda\bar{S}/k_BT)}\ . \tag{37}$$

At $T=0$, $\chi_{\|}=0$. To evalute $\chi_{\|}$ at the transition temperature T_c we use the result (37) for the ordered state. Consider the limit $T\to T_c$ from below. Then $\bar{S}\to 0$ and we get

$$\chi_{\|}(T_c)=Ng^2\mu_B^2/2\mu\ . \tag{38}$$

For temperatures above T_c, $\bar{S}_u=\bar{S}_d=\delta S$ as $\bar{S}=0$. There is no long-range order and we put $\langle(S_u^z)^2\rangle=S(S+1)/3$; then

$$\frac{2S(S+1)}{3\delta S}=\left\langle\frac{A'\sinh(b'/k_BT)}{\cosh(b'/k_BT)-1}\right\rangle_k\ . \tag{39}$$

A' and b' have now simpler forms. The series expansion for susceptibility $\chi_{\|}$ in inverse temperature is

$$\chi_{\|}=\frac{Ng^2\mu_B^2}{\tau}\left[1+\frac{\alpha_1}{\tau}+\frac{\alpha_2}{\tau}+\cdots\right] \tag{40}$$

with $\tau=3k_BT/S(S+1)$ and α_1,α_2 are lattice-dependent constants.

V. DISCUSSION

The thermodynamic properties of Eqs. (32), (36), (38), and (40) are all identical with those of Lines for the isotropic Heisenberg antiferromagnet. This is so despite the fact that the Hamiltonian (19) is very different from the isotropic Heisenberg Hamiltonian. These formulas result from an approximate Green-function calculation, the crucial feature being the replacement of the mean value $\langle S_i^z \rangle$ by $\pm\bar{S}$ for the two sublattices. It is clear that this is justified in (19) much more than in the Heisenberg Hamiltonian. In the latter an additional hypothesis of broken symmetry has to be made but the broken symmetry has not been rigorously demonstrated.

If the experimental material is known to be described by the isotropic Heisenberg Hamiltonian, it would be better not to compare the results with Eqs. (32), (36), and (40), for they are more typical of a Hamiltonian like (19). Now more accurate calculations are available[12] and those should be used in analyzing data.

The Hamiltonian (19) should be studied further for excited states and perhaps it may be useful for some experimental materials. Since the ground-state structure is simple, it may serve as the start of perturbation theoretic investigations for the *XYZ*-type Hamiltonians for three-dimensional systems.

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