PHYSICAL REVIEW B VOLUME 40, NUMBER 4 1 AUGUST 1989

# Spin-wave results for the triangular Heisenberg antiferromagnet

Th. Jolicoeur
*Service de Physique Théorique, Commissariat à l'Énergie Atomique, Centre d'Études Nucleaires de Saclay, F-91191 Gif-sur-Yvette CEDEX, France*

J. C. Le Guillou
*Laboratoire de Physique Théorique et Haute Energies, Université Pierre et Marie Curie (Paris VI), Tour 16, E1, F-75252 Paris CEDEX 05, France*

(Received 22 March 1989)

We perform the standard spin-wave analysis of the triangular Heisenberg quantum antiferromagnet. Contrary to the variational calculation of Anderson, we diagonalize exactly the quadratic part of the spin-wave Hamiltonian and obtain results in a $1/S$ expansion. We compute the ground-state staggered magnetization per spin and the ground-state energy. For spin $\frac{1}{2}$, the agreement with the variational values of Huse and Elser suggests that the triangular lattice has long-range magnetic order.

The suggestion that a resonating-valence-bond (RVB) state is linked to high-temperature superconductivity[1] has prompted a reexamination of quantum antiferromagnetic spin systems. The spin-$\frac{1}{2}$ square-lattice Heisenberg antiferromagnet (HAF) has been studied within perturbation theory,[2] spin-wave theory,[3] exact diagonalization on small-size lattices,[4] and in quantum Monte Carlo simulations.[5] There is now convincing evidence that this system has a Néel-ordered ground state. At least two simple candidates remain for a quantum spin-liquid ground state. The first one is obtained by adding to the square-lattice HAF a frustrating next-to-nearest-neighbor exchange interaction.[6] The other one is the spin-$\frac{1}{2}$ triangular HAF as originally suggested by Anderson. In his work,[7] he gave an estimate of its ground-state energy using the variational spin-wave method of Kubo.[8] Calculations of only the ground-state energy have recently been performed in the context of two different spin-wave methods: the Villain method[9] and an extended version of the Holstein-Primakoff method.[10] However, the staggered magnetization has not been considered and so no conclusion about Anderson's proposal has been inferred from these calculations. In this Rapid Communication we use the conventional spin-wave theory[3] to obtain the first quantum corrections to the ground-state staggered magnetization and energy. For spin $\frac{1}{2}$, we obtain a value $E_0 = -0.1796J$/bond in agreement with previous results[9,10] and close to the variational value of Huse and Elser[11] $E_0 \simeq -0.1789$ and to the value coming from exact diagonalization of small clusters[12] $E_0 = -0.183 \pm 0.003$. We obtain a sublattice magnetization reduced from its classical value 0.5 to 0.239. All these numbers are quite different from the estimate $E_0 \sim -0.158$ from various RVB-type variational wave functions,[13,14] and also from the variational spin-wave value[7] $E_0 \cong -0.154$. This suggests that the situation of the frustrated triangular-lattice HAF is quite similar to that of the square lattice: a ground state with long-range Néel order exists in both cases.

We consider the triangular-lattice antiferromagnet. Only nearest-neighbor exchange is considered, so the Hamiltonian is

$$H = J \sum_{\langle i,j \rangle} \mathbf{S}_i \cdot \mathbf{S}_j , \tag{1}$$

with $\langle i,j \rangle$ denoting nearest-neighbor pairs of sites and $\mathbf{S}_i$ denoting quantum spins. The starting point of the spin-wave expansion[3] is a classical ground state of (1). It consists of three sublattices, $A$, $B$, and $C$, with spins on each sublattice at an angle of $2\pi/3$ to those on the other two sublattices. Nearest-neighbor pairs of spins are on different sublattices, while each spin is on the same sublattice as all of its second neighbors at distance $\sqrt{3}$ nearest-neighbor spacings. We choose a particular classical ground state with the spins on the $A$ sublattice oriented along the $z$ axis, and those on the $B$ and $C$ sublattices rotated $2\pi/3$ away from the $z$ axis in the $x$-$z$ plane (the sites are lying in the $x$-$z$ plane and the rotation between $A$ and $B$ is around the $y$ axis perpendicular to the plane). We then introduce three kinds of Holstein-Primakoff bosons, $a$, $b$, and $c$, on sublattices $A$, $B$, and $C$, respectively to parametrize the spin operators. The species $a$ describes the quantum fluctuations of the spin away from its classical direction $z$: $S_z = S - a^+ a$, $S^+ = a\sqrt{2S}$, and $S^- = a^+\sqrt{2S}$ (at leading order). On the other sublattices we have to take into account the $2\pi/3$ rotation so that on the $C$ sublattice:

$$\begin{aligned} S_x &= \frac{\sqrt{3}}{2}(S - c^+ c) + \sqrt{2S}\left(-\frac{1}{2}\frac{c+c^+}{2}\right), \\ S_z &= -\tfrac{1}{2}(S - c^+ c) + \sqrt{2S}\left(-\frac{\sqrt{3}}{2}\frac{c+c^+}{2}\right), \\ S_y &= \sqrt{2S}\frac{c-c^+}{2i}, \end{aligned} \tag{2}$$

at the order we need in the $1/S$ expansion. On the $B$ sublattice, we just rotate by $-2\pi/3$. We then substitute in

 

the Hamiltonian (1) and expand, keeping only the quadratic part in the $H$-$P$ oscillators.

It is then necessary to introduce the Fourier transforms of the bosonic operators $a,b,c$. Each sublattice is itself triangular so that all $k$ vectors are living in a hexagonal Brillouin zone. This leads to the following formula:

$$\frac{H}{J}=-\frac{S^2}{2}(B)+\frac{3S}{2}\sum_k\left[(\alpha_k^+\beta_k)H_0(k)\begin{pmatrix}\alpha_k\\ \beta_k^+\end{pmatrix}-3\right], \tag{3}$$

where

$$\alpha_k=\begin{pmatrix}a_k\\ b_k\\ c_k\end{pmatrix} \quad \text{and} \quad \alpha_k=\beta_{-k} \tag{4}$$

and $B$ represents the number of bonds. The new Hamiltonian to be diagonalized is $H_0(k)$, a $6\times6$ matrix of the form

$$H_0(k)=\begin{pmatrix}1+M & -3M\\ -3M & 1+M\end{pmatrix}, \tag{5}$$

where

$$M=\begin{pmatrix}0 & z & z^*\\ z^* & 0 & z\\ z & z^* & 0\end{pmatrix}. \tag{6}$$

In this formula, the complex number $z$ is given by

$$z=\tfrac{1}{12}\sum_L e^{i\mathbf{k}\cdot\delta_L}, \tag{7}$$

where $L=1,2,3$ and the two-dimensional vectors $\delta_L$ are pointing towards half of the neighbors of a site. We made use of the set

$$\delta_1=(1,0),\quad \delta_2=\left(-\frac{1}{2},\frac{\sqrt{3}}{2}\right),\quad \delta_3=\left(-\frac{1}{2},-\frac{\sqrt{3}}{2}\right). \tag{8}$$

The key observation is that all the $3\times3$ blocks building $H_0(k)$ are permutation matrices and thus can be diagonalized simultaneously in the basis

$$u_1=(1,1,1),\quad u_2=(1,j,j^2),$$
$$u_3=(1,j^2,j) \quad \text{with } j=\exp(2i\pi/3). \tag{9}$$

The appearance of the cubic roots of the unity is the manifestation of the ternary symmetry of the problem. We perform a generalized Bogolyubov transformation:

$$\begin{pmatrix}\mathcal{A}\\ \mathcal{B}^+\end{pmatrix}=T\begin{pmatrix}\alpha\\ \beta^+\end{pmatrix}. \tag{10}$$

This has to preserve the boson commutation relations and map $H_0$ onto a diagonal matrix. This can be achieved by taking the column vectors of $T^{-1}$ as

$$\begin{pmatrix}\lambda_i u_i\\ \mu_i u_i\end{pmatrix}, \tag{11}$$

where the coefficients $\lambda_i$ and $\mu_i$ satisfy hyperbolic orthonormalization conditions: $|\lambda_i|^2-|\mu_i|^2=1$, etc. Once three column vectors are found, the three remaining ones ($T$ is $6\times6$) are obtained by the action of $-\sigma_x$. The construction of $T$ is indeed the nontrivial part of the problem. One then has to take into account the inversion symmetry which relates $\alpha$ and $\beta$ to keep only the $\mathcal{A}$ modes over the entire Brillouin zone. The Hamiltonian is then

$$\frac{H}{J}=-\frac{S^2}{2}(B)+3S\sum_k\sum_{L=1}^{3}\omega_L\mathcal{A}_L^+\mathcal{A}_L+\frac{3S}{2}\sum_k(\omega_1+\omega_2+\omega_3-3). \tag{12}$$

The eigenfrequencies for a mode of wave number $k$ are given by

$$\omega_L(k)=\sqrt{(1-2\rho_L)(1+4\rho_L)}, \tag{13}$$

where $\rho_1=z+z^*$, $\rho_2=zj+z^*j^2$, and $\rho_3=zj^2+z^*j$.

The ground-state energy including the zero-point motion of the quantum spins can then be written as

$$E_0=-\frac{S}{2}\left[S+c+O\left(\frac{1}{S}\right)\right](J/\text{bond}),$$
$$c=1-\frac{1}{N}\sum_k(\omega_1+\omega_2+\omega_3). \tag{14}$$

If $N$ stands for the total number of sites, the sum over $k$ extends over the Brillouin zone corresponding to a single sublattice. The ground-state staggered magnetization per spin at the same order is given by

$$\langle S_z\rangle=S-\Delta+O\left(\frac{1}{S}\right),$$
$$\Delta=-\frac{1}{2}+\frac{1}{2N}\sum_k\sum_i\frac{1+\rho_i(k)}{\omega_i(k)}. \tag{15}$$

We find $c=0.2184$ and $\Delta=0.261$, leading to $E_0=-0.1796J/\text{bond}$ and $\langle S_z\rangle=0.239$, i.e., a reduction of the spin of more than 50% from its classical value. The values of $c$ and $\Delta$ are higher than those for the square-lattice HAF which are[3] $c=0.158$ and $\Delta=0.197$. This is in agreement with the naive expectation that the frustrated lattice has a more pronounced zero-point motion, the frustrated lattice being closer to the disorder than the square lattice.

It is interesting to note that this value for $E_0$ is much lower than the $E_0\cong-0.154$ estimated from the variational spin-wave theory.[7,8] It is worth stressing the differences between the two methods. We have used the conventional spin-wave theory[3] which leads to an expansion of the various quantities of interest in powers of $1/S$. The relevance of this method in the spin-$\frac{1}{2}$ cases is of course questionable, especially when one knows only the first quantum correction. However, the case of the square-lattice HAF shows that this can be a sensible procedure since the estimate $\langle S_z\rangle=0.303$ is very close to the values obtained through series analysis[2] and quantum Monte Carlo.[5] Perhaps we are helped by some inverse power of the coordination number. On the other hand, the variational spin-wave method of Kubo involves the choice of a trial

Hamiltonian that can be diagonalized in a particular basis. One then computes the diagonal elements of the true Hamiltonian in this basis. The vector minimizing the expectation value is then considered as an approximation to the true ground state. This is in essence a variational procedure which is difficult to improve systematically. The other variational methods that have been applied to the frustrated HAF gave ground-state energies most probably well above the true value. The original RVB proposal[7] has been refined by Oguchi, Nishimori, and Taguchi.[13] They extrapolated finite-lattice results from systems including up to 20 sites and found $E_0 = -0.158 \pm 0.003$. A very similar value is quoted by Kalmeyer and Laughlin.[14] They used a variational wave function inspired from that of the fractional quantum Hall effect.

The spin-wave results of Nishimori and Miyake[9,10] lead to $E_0 = -0.182$ when contributions up to $1/S^2$ are taken into account, but with no information on the staggered magnetization. Since they expressed the Hamiltonian in terms of spin operators, each quantized in the direction of the classical orientation, their spin-wave modes are related by a nontrivial transformation to our physical modes, the ones which are relevant to an actual experiment.

The diagonalization of small clusters[12] has led to an estimate for the ground-state energy which is $E_0 = -0.183 \pm 0.003$, but with no information on $\langle S_z \rangle$. Huse and Elser[11] have performed a variational calculation with an ordered trial function including three parameters. They deduce a strict upper bound on $E_0 \leq -0.1789$. This value is reached with a sublattice magnetization of about 0.34. These numbers are very close to our spin-wave values. The whole picture strongly suggests that the spin-$\frac{1}{2}$ triangular HAF has a Néel-ordered ground state. Of course, a spin-wave argument is circular: One can only prove that one is dealing with a local minimum. For this expansion to be safe, one has to check by another completely different means (e.g., quantum Monte Carlo) that the ground state is ordered.

Service de Physique Theorique is "Unite associeé au Laboratoire de l'Institut de Recherche Fondamentale du Commissariat à l'Énergie Atomique."

[1]P. W. Anderson, Science **235**, 1196 (1987).
[2]D. A. Huse, Phys. Rev. B **37**, 2380 (1988); M. Parrinello and T. Arai, *ibid.* **10**, 265 (1974).
[3]P. W. Anderson, Phys. Rev. **86**, 694 (1952); R. Kubo, *ibid.* **87**, 568 (1952); T. Oguchi, *ibid.* **117**, 117 (1960).
[4]J. Oitmaa and D. D. Betts, Can. J. Phys. **56**, 897 (1978).
[5]M. Gross, E. Sanchez-Velasco, and E. Siggia, Phys. Rev. B **39**, 2484 (1989).
[6]P. Chandra and B. Douçot, Phys. Rev. B **38**, 9335 (1988).
[7]P. W. Anderson, Mater. Res. Bull. **8**, 153 (1973).
[8]R. Kubo, Rev. Mod. Phys. **25**, 344 (1953).
[9]H. Nishimori and S. J. Miyake, Prog. Theor. Phys. **73**, 18 (1985).
[10]S. J. Miyake, Prog. Theor. Phys. **74**, 468 (1985).
[11]D. A. Huse and V. Elser, Phys Rev. Lett. **60**, 2531 (1988).
[12]H. Nishimori and H. Nakanishi, J. Phys. Soc. Jpn. **57**, 626 (1988); S. Fujiki, Can. J. Phys. **65**, 489 (1987).
[13]T. Oguchi, H. Nishimori, and Y. Taguchi, J. Phys. Soc. Jpn. **55**, 323 (1986).
[14]V. Kalmeyer and R. B. Laughlin, Phys. Rev. Lett. **59**, 2095 (1987), and references therein.