RAPID COMMUNICATIONS

PHYSICAL REVIEW B VOLUME 45, NUMBER 21 1 JUNE 1992-I

Spin-liquid state of Wigner-Jordan fermions of the quantum antiferromagnetic Heisenberg model on a triangular lattice

Y. R. Wang

Xerox Webster Research Center, 800 Phillips Road, 0114-41D, Webster, New York 14580

(Received 11 February 1992)

A disordered spin state, the nearest-neighbor virtual bonding state of Wigner-Jordan fermions, of the quantum antiferromagnetic Heisenberg model on a triangular lattice is found to have a zero-temperature energy $-1.106J$ per spin, lower than that calculated from spin-wave theories, and in excellent agreement with that from numerical calculations, $(-1.094\pm0.018)J$ per spin. The excitations of the state are Wigner-Jordan fermions with a gapless spectrum. The low-temperature specific heat is predicted to be proportional to T^{ν}, with ν between $\frac{2}{3}$ and 1, significantly deviating from the spin-wave prediction, T^2. At higher temperature, a broad peak in the specific heat near $T/2J\approx0.75$ is also predicted.

The possibility that the quantum antiferromagnetic (AFM) Heisenberg model on a triangular lattice may have a quantum ground state qualitatively different from the classical Néel state has made the system one of the most studied. It was first suggested by Anderson[1] that the ground state may be of the resonating-valence-bond (RVB) type based on the estimation that the zero-temperature energy of the RVB state is lower than that of the classical Néel state. Kalmeyer and Laughlin[2] suggested a different type of quantum ground state, the $m=2$ fractional quantum Hall (FQH) state. Similar applications of the fractional quantum Hall state to the quantum AFM spin problem have also been made by Mele.[3] Both the RVB state and the $m=2$ FQH state are quantum spin liquid states. The excitation spectrum is gapless in the RVB state, when long-range resonating valence bonds are included,[4] whereas that of the $m=2$ FQH state possesses a gap. The zero-temperature energy of the RVB state is estimated by Anderson to be $-0.98J$ per spin, and that of the $m=2$ fractional quantum Hall state $-0.94J$ per spin. While these energies are lower than that estimated from the variational spin-wave theory,[1] $-0.926J$ per spin, they are much higher than that calculated from the conventional spin-wave theories[5] based on the Holstein-Primakoff transformation, $-1.078J$ per spin, and that from a variational wave function,[6] $-1.073J$. The latter spin-wave theories and the variational wave function predict a long-range spin ordering with a reduced sublattice magnetization. So far no other quantum states have been reported to have a lower zero-temperature energy than that estimated from the conventional spin-wave theory.

Numerical calculations[7,8] for a finite number of spins give conflicting results with regard to the existence of the sublattice magnetization. Exact diagonalization of a 27-spin cluster[9] (which is, to our knowledge, the largest finite system for which calculations have even been performed) indicates the nonexistence of the sublattice magnetization. Large projections of the finite system wave function onto the RVB state were found, but the projection nevertheless decreases linearly with the system size.[10] Experimental realization[11] of the quantum AFM Heisenberg model on a triangular lattice has been reported, where neutron-scattering data of $NaTiO_2$ suggest a disordered spin ground state. It is therefore important to see if one could find a disordered quantum spin state which has a lower zero-temperature energy than that of the Néel ordered states. In this paper we show one such state, the nearest-neighbor virtual bonding (NNVB) state of Wigner-Jordan (WJ) fermions. The NNVB state has a pure imaginary bonding field, $\langle d_i^{\dagger}d_j\rangle=\pm i\Delta$, where i and j are nearest-neighbor sites, $d_i^{\dagger}$ is a creation operator of a WJ fermion at site i, and $\Delta>0$ at any temperature. The state has a zero-temperature energy $E_0=-1.106J$ per spin, in excellent agreement with that calculated from the 27-spin cluster extrapolated to infinite sizes, $(-1.094\pm0.018)J$ per spin. The excitations of the NNVB state are fermions and are gapless. The density of states of the WJ fermions has a divergence at zero excitation energy which is not the usual Van Hove type, but behaves as $1/E^{1/3}$. Such a density of states would predict, taking possible fluctuations into account, a temperature dependence of the low-temperature specific heat to be T^{ν}, with ν between $\frac{2}{3}$ and 1, significantly deviating from that predicted from spin-wave theories, T^2. At higher temperature, the specific heat shows a broad peak near $T/2J\approx0.75$. The above predictions may be examined by experiments and also by numerical calculations of finite systems.

We begin by summarizing the two-dimensional (2D) Wigner-Jordan (WJ) transformation[12,13] on which our analyses are based. The strategy of the WJ transformation is to transform the spin variables into spinless fermion operators. Thus a spinless fermion operator, d_i, for site i, is defined to be $d_i=e^{-i\phi_i}S_i^-$, where S_i^- is the spin lowering operator, and the phase ϕ_i is given by $\phi_i=\sum_{j\neq i}d_j^{\dagger}d_jB_{ij}$ [$B_{ij}\equiv\mathrm{Im}\log(\tau_j-\tau_i)$, where $\tau_j=x_j+iy_j$ is the complex coordinate of the jth spin]. The z component of the spin operator is related to the number operator of the WJ fermions, $S_i^z=d_i^{\dagger}d_i-\frac{1}{2}$. It can be shown that the above defined transformation preserves all spin commutation relations, as other transformations, such as the Holstein-Primakoff transformation, also do. The advantage of the WJ transformation is that it automatically satisfies N unique identities of the $S=\frac{1}{2}$ spin operators, $S_i^+S_i^-+S_i^-S_i^+\equiv1$, whereas for the Holstein-Primakoff

transformation the identities are satisfied only if infinite on-site repulsive interactions between the bosons are added. The 2D WJ transformation has been used in studying the quantum AFM Heisenberg model on a square lattice at finite temperatures, where one obtains the in-phase flux state[12] which has a complex bonding field, $\langle d_i^\dagger d_j\rangle = \Delta e^{i\theta_{ij}}$, with the phase given by a uniform gauge field of strength half flux quanta per spin. The in-phase flux state[12] has an energy $E_0 = -1.3J$ per spin in the $T \to 0$ limit, and a linear excitation spectrum with the velocity approximately equal to that of the spin waves. The Raman spectrum[14] calculated for the in-phase flux state shows significant improvement over that calculated from spin-wave theories compared with the experimental spectrum[15] of La_2CuO_4.

There is a local gauge invariance in the WJ transformation, namely that the phase ϕ_i can be replaced by $\phi_i + C_i$ as long as C_i is a c number. One therefore could take advantage of this invariance to simplify the spin problem. For the quantum Heisenberg model, a desired choice of the local gauge (i.e., the C_i's) is such that the fluctuations around a mean-field state in the XY part of the Hamiltonian maximally cancel those in the Z part. The possibility of such cancellation can be seen in the WJ representation of the Heisenberg Hamiltonian [Eq. (1) below]. For the Heisenberg model on a triangular lattice, we shall use $C_i = -\frac{1}{2}\sum_{j\neq i} B_{ij}$. (Since only the phase differences, $\phi_j - \phi_i$, come into play in the Heisenberg Hamiltonian, we actually only need to choose the differences, $C_j - C_i$.) As can be easily seen below, this choice is the simplest, and at least for the ground-state energy, the cancellation mentioned above appears rather complete with this choice.

The quantum AFM Heisenberg model, $H = J\sum_{ij} \mathbf{S}_i \cdot \mathbf{S}_j$, can be written in the WJ representation

$$H = J\sum_{ij} d_i^\dagger e^{i(\phi_j - \phi_i)} d_j + J\sum_{ij} (d_i^\dagger d_i - \tfrac{1}{2})(d_j^\dagger d_j - \tfrac{1}{2}) , \quad (1)$$

where the summations are over all nearest neighbors, and $\phi_i = \sum_{j\neq i} (d_j^\dagger d_j - \frac{1}{2}) B_{ij}$. The phase factor in the first term, in its present form, cannot be treated by a mean-field approximation, since it does not commute with the fermion operators $d_i^\dagger$ and d_j. However, we can rewrite it as

$$d_i^\dagger e^{i(\phi_j - \phi_i)} d_j \equiv e^{i\Phi_{ij}} d_i^\dagger d_j e^{-i(B_{ji} - B_{ij})/2} , \quad (2)$$

where $\Phi_{ij} = \sum_{l\neq i,j} (d_l^\dagger d_l - \frac{1}{2})(B_{lj} - B_{li})$, and we have used the identity $d_j^\dagger \exp(i d_j^\dagger d_j B_{ij}) = d_j^\dagger$. Φ_{ij} commutes with both $d_i^\dagger$ and d_j, since $d_i^\dagger d_i$ and $d_j^\dagger d_j$ are excluded from its summation. We notice that $B_{ji} - B_{ij} \equiv \pm\pi$, where the sign depends on the relative location of the site i and j. In a spin state where the z component of the spins is zero on average, which is indeed the case for the Heisenberg model on a triangular lattice, $\langle d_i^\dagger d_i\rangle = \frac{1}{2}$. Thus in the mean-field approximation, Φ_{ij} can be taken to be zero. This approximation can be viewed as the zeroth order of the expansion of $e^{i\Phi_{ij}}$ in terms of $(d_l^\dagger d_l - \frac{1}{2})$, and therefore is expected to be valid when the condition $\langle d_l^\dagger d_l\rangle = \frac{1}{2}$ is satisfied. We next define a nearest-neighbor bonding field, Δ_{ij}, for each nearest-neighbor pair of WJ fermions,

$$\Delta_{ij} \equiv \langle d_i d_j^\dagger\rangle = \Delta e^{i\theta_{ij}} . \quad (3)$$

The phase of the bonding field, θ_{ij}, can be shown self-consistently below to be $-(B_{ji} - B_{ij})/2$. The Heisenberg Hamiltonian, Eq. (1), is now readily reduced to the mean-field Hamiltonian,

$$H_{\rm MF} = J\sum_{ij} (1+2\Delta) e^{-i(B_{ji} - B_{ij})/2} d_i^\dagger d_j + 6NJ\Delta^2 . \quad (4)$$

This mean-field Hamiltonian is easily diagonalized in the momentum space. The single-particle energy of momentum $\mathbf{k}$ is

$$E_{\mathbf{k}} = -2J(1+2\Delta)[\sin(\mathbf{k}\cdot\boldsymbol{\delta}_1) + \sin(\mathbf{k}\cdot\boldsymbol{\delta}_2) + \sin(\mathbf{k}\cdot\boldsymbol{\delta}_3)] , \quad (5)$$

where $\boldsymbol{\delta}_1$, $\boldsymbol{\delta}_2$, and $\boldsymbol{\delta}_3$ are the three nearest-neighbor vectors. This energy spectrum can be viewed as a concise representation of the two spectra, $E_{\mathbf{k}}^+ = |E_{\mathbf{k}}|$, and $E_{\mathbf{k}}^- = -|E_{\mathbf{k}}|$. All states in $E_{\mathbf{k}}^-$ are filled by the WJ fermions, and all states in $E_{\mathbf{k}}^+$ are empty. The spectrum therefore possesses a particle-hole symmetry. This particle-hole symmetry is a reflection of the fact that in the original Heisenberg Hamiltonian the energies for two parallel and two antiparallel nearest-neighbor spins are equal in magnitude, but opposite in sign.

From the definition in Eq. (3), both the phase θ_{ij} and the amplitude Δ of the bond-order mean-field Δ_{ij} can be determined self-consistently,

$$\Delta = \frac{1}{6N}\sum_{\mathbf{k}} [-E_{\mathbf{k}}/J(1+2\Delta)] n_F(E_{\mathbf{k}}) , \quad (6)$$

where $n_F(E)$ is the Fermi function at energy E. At zero temperature, Eq. (6) gives $\Delta = 0.159$. The mean-field energy, from Eq. (4), is given by $E_{\rm MF} = -6NJ(1+\Delta)\Delta$, and at $T=0$, $E_{\rm MF} = -1.106J$ per spin. This energy is lower than that of the spin-wave theory, and is in excellent agreement with numerical calculations.

The solution given above describes a disordered (or liquid) state of the spins in the sense that no preferred direction of the spins is given in the solution. The expansion of $e^{i\Phi_{ij}}$ in terms of $(d_l^\dagger d_l - \frac{1}{2})$ thus can be understood as an expansion around the disordered state, in contrast to the $1/S$ expansion in the spin-wave theories which is around the Néel ordered state. Our results that a self-consistent solution can be obtained for $\langle d_i^\dagger d_i\rangle$, Δ and θ_{ij} indicate that the solution is a locally stable one. While the comparison of the energy of the NNVB state with that of the Néel state from spin-wave calculations suggests that the energy of the NNVB state also represents a global minimum, it would be useful to compare the energy of the NNVB state with that of the Néel ordered state calculated using the WJ transformation. For this purpose, we divide the triangular lattice into three sublattices, A, B, and C, and for each sublattice we carry out a WJ transformation which is related to the transformations in the other sublattices by a $2\pi/3$ (or $-2\pi/3$) rotation. Thus for the A sublattice, we have $S_{Ai}^+ = A_i^+ e^{i\phi_i}$, and $S_{Ai}^z = A_i^+ A_i - \frac{1}{2}$, where we have designated the x-z plane to be the plane of the lattice. The transformation in the B sublattice is related to that of the A sublattice by a $2\pi/3$ rotation around the y axis:

$$S^x_{Bl}=\tfrac{1}{2}\sqrt{3}(B_l^+B_l-\tfrac{1}{2})-\tfrac{1}{4}(B_l^+e^{i\phi_l}+B_le^{-i\phi_l}), \quad (7a)$$

$$S^y_{Bl}=(1/2i)(B_l^+e^{i\phi_l}-B_le^{-i\phi_l}), \quad (7b)$$

and

$$S^z_{Bl}=-\tfrac{1}{4}\sqrt{3}(B_l^+e^{i\phi_l}+B_le^{-i\phi_l})-\tfrac{1}{2}(B_l^+B_l-\tfrac{1}{2}). \quad (7c)$$

A similar transformation for the C sublattice can also be written down. The phase ϕ_i for the three sublattices is chosen to be

$$\phi_i=\sum_{j\neq i}(d_j^\dagger d_j-\tfrac{1}{2}-\Delta_1)B_{ij}, \quad (8)$$

where $\Delta_1=\langle S_i^z\rangle$, and $d_j=A_j$ (B_j, C_j) if j belongs to the sublattice A (B, C). Following the spin-wave calculation,[5] we next only retain the terms bilinear in the fermion operators in the Hamiltonian, using the usual mean-field approximation of breaking quartic terms into bilinear terms. The reduced mean-field Hamiltonian becomes

$$H_{MF}=J\sum_{\mathbf{k}}[-(\tfrac{3}{4}+\Delta_2)U_{\mathbf{k}}^*(A_{\mathbf{k}}^+B_{-\mathbf{k}}^++C_{\mathbf{k}}^+A_{-\mathbf{k}}^++B_{\mathbf{k}}^+C_{-\mathbf{k}}^+)+\tfrac{1}{4}U_{\mathbf{k}}(A_{\mathbf{k}}^+B_{\mathbf{k}}+C_{\mathbf{k}}^+A_{\mathbf{k}}+B_{\mathbf{k}}^+C_{\mathbf{k}})+\text{H.c.}$$
$$-6\Delta_1(A_{\mathbf{k}}^+A_{\mathbf{k}}+B_{\mathbf{k}}^+B_{\mathbf{k}}+C_{\mathbf{k}}^+C_{\mathbf{k}}-\tfrac{3}{2})]+3\Delta_1^2+3\Delta_2^2, \quad (9)$$

where $\Delta_2=\langle A_i^+B_{i+\delta}^+\rangle$ and

$$U_{\mathbf{k}}=e^{i\mathbf{k}\cdot\boldsymbol{\delta}_1}+e^{-i\mathbf{k}\cdot\boldsymbol{\delta}_2}+e^{i\mathbf{k}\cdot\boldsymbol{\delta}_3}.$$

The Hamiltonian can be diagonalized numerically using a 6×6 matrix, and the mean-field energy is minimized with respect to Δ_1 and Δ_2. The result is that at $T=0$ the sublattice magnetizations, which are 120° apart from each other, are about 53% of the maximum value, and the energy is $-0.863J$ per spin. The value of the sublattice magnetization is in excellent agreement with that calculated from spin-wave theories,[5] but the energy is substantially higher than that of the NNVB state, and also that of spin waves. The discrepancy in the energy of the Néel state calculated from the WJ transformation and that from spin-wave theories may be attributed to the relative simple approximation in our treatment, but may also be related to the fact that the energy from the spin-wave theory is only calculated up to the first order in the $1/S$ expansion.[5] While further studies are clearly needed to answer these questions, it is nevertheless demonstrated that at a comparable approximation level, the disordered spin state has a lower energy than that of the ordered state.

There are several interesting properties associated with the NNVB state. First, the excitations are WJ fermions without a gap, as can be seen from Eq. (5). The fermionic statistics of the excitations in the NNVB state agrees with that of both the RVB state[4] and the $m=2$ FQH state,[2] whereas the gaplessness of the excitation spectrum may have to do with the fact that $\langle d_id_j^\dagger\rangle$, when expressed in terms of spin operators, actually involves many spins. The elementary excitation process in a spin system is to flip a spin from down to up, or visa versa. In the WJ representation, this is described by adding (or subtracting) a WJ fermion with energy $E_{\mathbf{k}}^+$ (or $E_{\mathbf{k}}^-$) and momentum $\mathbf{k}$. The fermionic nature of the excitation arises from the phase change in the many-spin wave function because of the flipping. Second, the density of states, $\rho(E)$, of the WJ fermions in the NNVB state diverges at zero excitation energy. The divergence does not come from small wave vectors, but originates from the saddle points $(\pi,-\pi/\sqrt{3})$ and $(-\pi,\pi/\sqrt{3})$. the saddle points are not the usual Van Hove type (quadratic). Expanding $E_{\mathbf{k}}$ near the saddle points gives $E_{\mathbf{k}}\sim\delta k_x(\delta k_x^2-3\delta k_y^2)$, indicating that the divergence is stronger than logarithmic. We have analytically evaluated the density of states at low energies, and have shown that the divergence actually behaves as $\rho(E)\sim1/E^{1/3}$. Such a strong divergence would predict a temperature dependence of the low-temperature specific heat to be $T^{2/3}$. Since the NNVB state is a mean-field

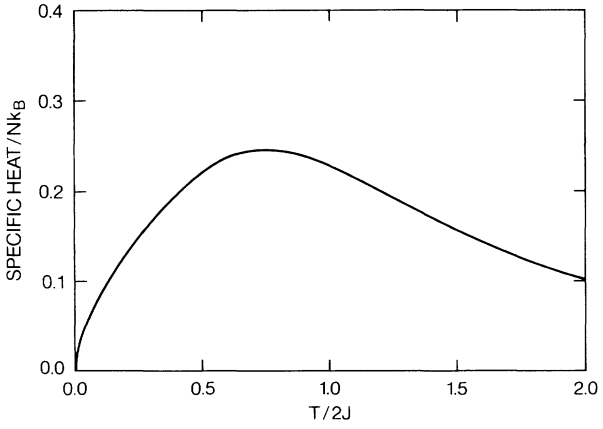

FIG. 1. The specific heat of the nearest-neighbor virtual bonding state. It is proportional to $T^{2/3}$ at low temperature, and has a broad peak located near $T/2J=0.75$.

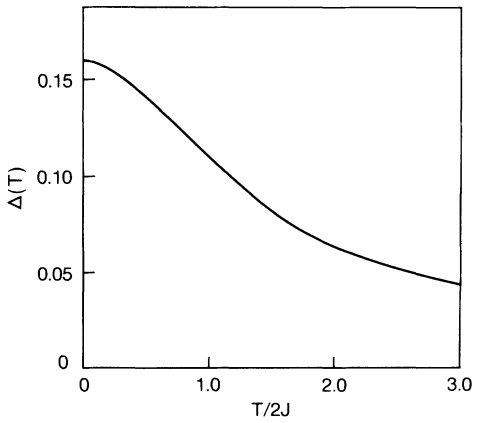

FIG. 2. The temperature dependence of the bonding amplitude, Δ, of the nearest-neighbor virtual bonding state.

solution, fluctuations might reduce the divergence to a cusp or slightly shift the peak position. Thus the temperature dependence of the low-temperature specific heat could vary from $T^{2/3}$ to T. This temperature dependence significantly deviates from the T^2 dependence predicted from spin-wave theories, and is also different from the temperature dependence of the specific heat of the quantum AFM Heisenberg model for a square lattice where both the spin-wave theories and the in-phase flux state of the WJ fermions predict the temperature dependence to be T^2. At higher temperature, the specific heat of the NNVB state shows a broad peak near $T/2J \approx 0.75$, as shown in Fig. 1. Finally, the above solution predicts no phase transition at any finite temperature. Unlike many other mean-field theories, where mean-field solutions exist only in a limited parameter space, Δ in Eq. (6) is nonvanishing and a smooth function at all temperatures, as shown in Fig. 2. The nonexistence of phase transitions has also been predicted by numerical calculations,[8-10] and is also in agreement with neutron-scattering data[11] of $NaTiO_2$.

Finally, we comment on the possible visualization of the NNBV state. A WJ fermion at site i, from its definition, is a vortexlike spin object with the "vortex core" at site i. The creation of a WJ fermion at site i, apart from a phase factor, can be approximately viewed as creating a spin with, say, up orientation. Thus the bonding field, $\langle d_i d_j^\dagger \rangle$, can be approximately viewed as the bonding amplitude between the nearest-neighbor spins with opposite orientations. The phase factors effectively introduce long-range correlations between the spins. Our picture of the NNVB state is therefore similar to that of the RVB state. Oppositely oriented nearest-neighbor spins are bonded, and the NNVB state is a liquid of vortexlike WJ fermions. However, the many-spin wave function is not the simple product of the wave function of each bond, as in the RVB state, but involves Wigner-Jordan phase factors which correlate between long-distance spins.

[1]P. W. Anderson, Mater. Res. Bull. **8**, 153 (1973); P. Fazekas and P. W. Anderson, Philos. Mag. **30**, 423 (1974).

[2]V. Kalmeyer and R. B. Laughlin, Phys. Rev. Lett. **59**, 2095 (1987).

[3]E. J. Mele, Phys. Scr. **T27**, 82 (1989).

[4]P. W. Anderson, G. Baskaran, Z. Zou, and T. Hsu, Phys. Rev. Lett. **58**, 2790 (1987).

[5]Th. Jolicoeur and J. C. Le Guillou, Phys. Rev. B **40**, 2727 (1989).

[6]D. A. Huse and V. Elser, Phys. Rev. Lett. **60**, 2531 (1988).

[7]Numerical calculations suggesting nonzero sublattice magnetization, see, for example, J. Ottmaa and D. D. Betts, Can. J. Phys. **56**, 897 (1978); G. B. Arnold and G. J. Mata, Phys. Rev. B **42**, 8638 (1991).

[8]Numerical calculations suggesting zero sublattice magnetization, see, for example, S. Fujiki, Can. J. Phys. **65**, 489 (1987); S. Fujiki and D. D. Betts, Prog. Theor. Phys. Suppl. **87**, 268 (1986).

[9]H. Nishimori and H. Nakanishi, J. Phys. Soc. Jpn. **57**, 626 (1987).

[10]T. Oguchi, H. Nishimori, and Y. Taguchi, J. Phys. Soc. Jpn. **55**, 323 (1986).

[11]K. Hirakawa, H. Kadowaki, and K. Ubukoshi, J. Phys. Soc. Jpn. **54**, 3536 (1985).

[12]Y. R. Wang, Phys. Rev. B **43**, 3786 (1991); Y. R. Wang, *ibid.* (to be published); Y. R. Wang, M. J. Rice, and H. Y. Choi, *ibid.* **94**, 9743 (1991).

[13]J. Ambjorn and G. Semenoff, Phys. Lett. B **226**, 107 (1989); E. Fradkin, Phys. Rev. Lett. **63**, 332 (1989); E. J. Mele, Phys. Scr. **T27**, 82 (1989).

[14]Y. R. Wang, Phys. Rev. B **43**, 13774 (1991).

[15]R. R. P. Singh, P. A. Fleury, K. B. Lyons, and P. E. Sulewski, Phys. Rev. Lett. **62**, 2736 (1989); S. L. Cooper, G. A. Thomas, A. J. Millis, P. E. Sulewski, J. Orenstein, D. H. Rapkine, S-W. Cheong, and P. L. Trevor, Phys. Rev. B **42**, 10785 (1990).