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# Ground state of the two-dimensional antiferromagnetic Heisenberg model studied using an extended Wigner-Jordon transformation

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A two-dimensional (2D) Wigner-Jordon transformation which maps spin variables into spinless fermion variables is found and used to study the 2D spin-$\frac{1}{2}$ antiferromagnetic Heisenberg model. The transformation generates a fictitious gauge field in the $XY$ component of the Heisenberg model, and hence induces an in-phase orbital current in the Ising component flowing around each elementary plaquette of the underlying lattice. The ground state of the Heisenberg model in a 2D square lattice is found to be an in-phase Néel flux phase, i.e., a coexisting state of the flux phase with in-phase orbital currents and a long-range antiferromagnetic spin order. The zero-temperature mean-field energy of the in-phase Néel flux state, $E_0 = -0.33J$ per bond, is only 1% higher than the best-estimated ground-state energy, $-0.334J$ per bond.

The two-dimensional (2D) antiferromagnetic Heisenberg model has been extensively studied since the discovery of high-temperature superconductors due to the possibility of a magnetic mechanism[1] for high-temperature superconductivity. Various techniques have been used to study the model, e.g., variational calculations,[2-4] exact diagonalization of small systems,[5] and Monte Carlo simulations.[6-8] Many of the calculations seem to conclude that the spin-$\frac{1}{2}$ 2D Heisenberg antiferromagnetic model in a square lattice has a long-range spin order, with the zero-temperature sublattice magnetization reduced by quantum fluctuation to about 60% of its maximum value. Neutron-scattering experiments[9,10] on $La_2CuO_4$ indeed indicate an antiferromagnetic ordering in the $CuO_2$ plane, but the ordering is quickly destroyed by a small amount of doping, suggesting that the antiferromagnetic order is rather vulnerable to external perturbations. In a variational calculation, Liang, Doucot, and Anderson[2] noticed that a disordered spin state can have an energy very close to that of the ordered state, and thus could serve as a better starting point for discussing the doped copper oxides. An interesting disordered spin state is the flux phase discussed by Affleck and Marston[11] (or the $s+id$ phase by Kotliar[12]) in the large-$n$ limit of the SU($n$) generalized Hubbard-Heisenberg model, although the applicability of their results to the real situation ($n=2$) has not been clearly established.

In this Rapid Communication we present an approximate solution of the spin-$\frac{1}{2}$ antiferromagnetic Heisenberg model in a 2D square lattice using an extended Wigner-Jordon transformation. The spin variables in this representation are transformed into pure fermion variables. A fictitious gauge field is generated by the transformation in the $XY$ component of the Heisenberg model. In response to such a gauge field the Ising component of the model generates an in-phase orbital current flowing around each elementary plaquette. The ground state is determined by the competition between the formation of the orbital current, which is associated with the disordered spin component, and a staggered magnetization. The result is an in-phase Néel flux phase, i.e., a coexisting state of the flux phase with in-phase orbital currents and a commensurate spin-density wave-like long-range sublattice magnetization. The zero-temperature mean-field energy of the in-phase Néel flux state is found to be $-0.33J$ per bond, which is only 1% higher than the best-estimated value of the ground-state energy, $E_G = -0.334J$ per bond,[2] where $J$ is the Heisenberg exchange energy.

The one-dimensional (1D) Wigner-Jordon transformation has played an important role in understanding the 1D quantum-spin problems. It gives a complete solution of the 1D $XY$ model, and enables one to use the well-developed many-body techniques to study the 1D Heisenberg model. The 2D extension of the transformation has been discussed recently by Mele.[13] The discussion has focused on mapping the $XY$ model into a noninteracting fermion problem. Apparently such a mapping introduces complicated interactions in the Ising component of the Heisenberg model.[13] We present here a different approach to the transformation which successfully maps the spin variables into spinless fermion variables. The transformed $XY$ component remains interactive among the fermions. However, the interaction is shown to be in such a way that it corresponds to a gauge field.

As in the one-dimensional case,[14] we define a particle-annihilation operator $d_i$ at site $i$ by

$$d_i = e^{-i\phi_i} S_i^{(-)}, \tag{1}$$

where $S_i^{(-)} = S_i^x - iS_i^y$ is the spin-lowering operator. Using the 1D case as a guideline, the phase $\phi_i$ assumes the form $\phi_i = \sum_{j\neq i} d_j^\dagger d_j B_{ij}$. It can be shown that the $B_{ij}$'s must satisfy the relation $e^{iB_{ij}} = -e^{iB_{ji}}$ in order for the $d_i$'s to obey pure Fermi statistics. Obviously the relative angles of the spin coordinates satisfy such a relation. We therefore have

$$\phi_i = \sum_{j\neq i} d_j^\dagger d_j \,\mathrm{Im}\log(\tau_j - \tau_i)\,. \tag{2}$$

Here $\tau_i = x_i + iy_i$ is the complex coordinate of the $i$th spin. The Heisenberg Hamiltonian, $H = J\sum_{\langle i,j\rangle} \mathbf{S}_j \cdot \mathbf{S}_j$, in this representation is

$$H = J\sum_{\langle i,j\rangle} d_i^\dagger e^{i(\phi_i-\phi_j)} d_j + J\sum_{\langle i,j\rangle} d_i^\dagger d_i d_j^\dagger d_j - NJ/2\,, \tag{3}$$

where $N$ is the total number of spins and the summations are over pairs of nearest neighbors. The first term comes from the $XY$ part of the Hamiltonian, which now serves as a kinetic energy. The second term corresponds to the ising component of the model, which now acts as a nearest-neighbor repulsive interaction. It is interesting to compare Eq. (3) with the Heisenberg Hamiltonian in the hard-core boson representation, e.g., the one studied by Kalmeyer and Laughlin.[15] In the boson representation one must add an infinite repulsive on-site interaction to the Hamiltonian in order to prevent double occupation of the bosons. The advantage of working in the extended Wigner-Jordon representation is that the double occupation is automatically excluded by the Fermi statistics of the $d_i$'s.

The phase factor in the first term of Eq. (3) creates a gauge field, with the vector potential given by

$$\mathbf{A}(\mathbf{r}_i) = \sum_{l\neq i} n_l \frac{\hat{z}\times(\mathbf{r}_l-\mathbf{r}_i)}{(\mathbf{r}_l-\mathbf{r}_i)^2}\,, \tag{4}$$

where $n_j = d_j^\dagger d_j$ is the fermion number operator. Since $n_j = \frac{1}{2} + S_j^z$ each of the spinless fermions in the antiferromagnetic (or paramagnetic) state in this extended Wigner-Jordon transformation has a flux tube of one-half flux quantum on average attached. In the mean-field description of the phase factor, which we adopt following the same treatment of Laughlin[15] and Mele,[13] the dynamics of the particles are determined very much by the presence of the background gauge field.

We now describe various mean-field solutions of Eq. (3) in the gauge shown in Fig. 1 (which is the most convenient one for our discussion). The corresponding results in the usual asymmetric gauge, $\mathbf{A} = Hy\hat{\mathbf{x}}$, can be obtained by changing $\sin k_x$ to $\cos k_x$ in all the following equations.

*1. The uniform flux phase.* The uniform flux phase corresponds to a uniform density of the spinless fermions,

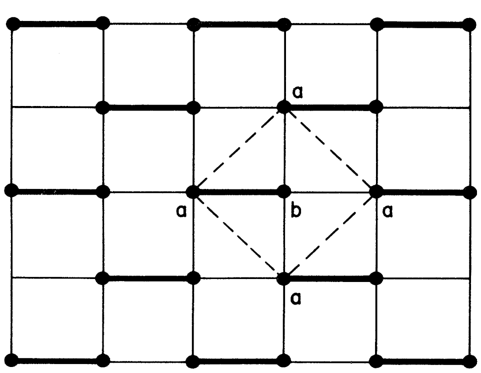


FIG. 1. The gauge used in the text. Since each of the elementary plaquettes encloses a net flux of $\pi$, the hopping energy across a heavy bond has a sign opposite to the ones across the light bonds. The dashed lines indicate the primitive unit cell.

$\langle d_i^\dagger d_i\rangle = \frac{1}{2}$. The energy spectrum of this phase is

$$E_{\mathbf{k}} = \pm J(\sin^2 k_x + \cos^2 k_y)^{1/2}\,. \tag{5}$$

It has a Fermi surface at isolated points, $\mathbf{k}_F = (0, \pm\pi/2)$, and a linear density of states near the Fermi surface. The excitation spectrum is gapless. The mean-field energy of this phase is entirely contributed from the $XY$ component and at $T=0$, $E_0 \approx -0.24J$ per bond. The physics of this flux phase is very much the same as the one discussed by Affleck and Marston.[11] Indeed the zero-temperature mean-field energy obtained by them is $-0.115nJ$, where $n=2$ for the spin-$\frac{1}{2}$ case.

*2. The in-phase flux phase.* In this phase the density of the spinless fermions is also uniform, but the Ising component generates an orbital current flowing around each elementary plaquette in response to the gauge field in the $XY$ component. The mean field in this phase is chosen to be

$$\Delta_{ij} = \Delta_1 e^{i\theta_{ij}} = \langle d_i d_j^\dagger\rangle\,, \tag{6}$$

where $i$ and $j$ are a pair of nearest neighbors. The phase $\theta_{ij}$, having the lowest energy, is found to be the one equal to the gauge phase, $\phi_{ij} = \phi_i - \phi_j$. The amplitude $\Delta_1$ is calculated self-consistently and is found to be $\Delta_1 = 0.2395$ at $T=0$. The energy spectrum of the in-phase flux phase has the same characteristics as that of the uniform flux phase,

$$E_{\mathbf{k}} = \pm J(1+2\Delta_1)(\sin^2 k_x + \cos^2 k_y)^{1/2}\,. \tag{7}$$

However, since $\Delta_1$ is temperature dependent, the bandwidth of the in-phase flux phase decreases with the increase of temperature. The zero-temperature mean-field energy of the in-phase flux phase is found to be $E_0 = -0.297J$ per bond. The mean-field energy does not include the corrections from the virtual transitions between the lower and the upper subbands. Such virtual transitions will further reduce the total energy. We have calculated the second-order correction from the Ising component alone, and the zero-temperature energy of the in-phase flux state including the correction is found to be $-0.324J$ per bond.

*3. The Néel flux phase.* In this phase a staggered magnetization is introduced, but not the in-phase orbital current. The energy spectrum of the Néel flux phase is

$$E_{\mathbf{k}} = \pm J(4\Delta_2^2 + \cos^2 k_y + \sin^2 k_x)^{1/2}\,, \tag{8}$$

where $\Delta_2$ is the amplitude of the sublattice magnetization (a value of $\Delta_2 = 1$ corresponds to a full sublattice magnetization). A value of $\Delta_2 = 0.875$ at $T=0$ is calculated through the self-consistent equation, and the zero-temperature mean-field energy of the Néel flux phase is found to be $E_0 = -0.311J$ per bond. This phase has been recently discussed by Hsu[16] and Zhang *et al.*[17] It is interesting to notice that the Néel flux phase can also have spin-wave excitations,[16] reminiscent of that in spin-density wave states.

*4. The in-phase Néel flux phase.* Both the in-phase flux state and the Néel flux phase have surprisingly low mean-field energy. The mean fields describing the two phases, therefore, are the major parameters that specify the ground state of the 2D spin-$\frac{1}{2}$ antiferromagnetic

Heisenberg model. It is important to see how the two mean fields compete with each other, and whether the ground state can be specified by one field or necessarily by both. We find that they coexist below the Néel temperature, resulting in the in-phase Néel flux phase. The self-consistent equations for the two mean fields are

$$\Delta_1 = \frac{1}{4N} \sum_{\mathbf{k}} \frac{J(1+2\Delta_1)}{E_{\mathbf{k}+}} [n_F(-E_{\mathbf{k}+}) - n_F(E_{\mathbf{k}+})] \times (\sin^2 k_x + \cos^2 k_y) \,, \tag{9}$$

and

$$\frac{1}{N} \sum_{\mathbf{k}} (2J/E_{\mathbf{k}+})[n_F(-E_{\mathbf{k}+}) - n_F(E_{\mathbf{k}+})] = 1 \,, \tag{10}$$

where $n_F(E_{\mathbf{k}})$ is the Fermi function, and $E_{\mathbf{K}+}$ is the upper-subband energy spectrum of the Néel flux phase,

$$E_{\mathbf{k}\pm} = \pm J[4\Delta_2^2 + (1+2\Delta_1)^2(\sin^2 k_x + \cos^2 k_y)]^{1/2} \,. \tag{11}$$

Equations (9) and (10) give $\Delta_1 = 0.155$ and $\Delta_2 = 0.778$ at $T=0$. The zero-temperature mean-field energy of the in-phase Néel flux phase is found to be $E_0 = -0.33J$ per bond, only slightly higher than the best-estimated ground-state energy. Because of the competition between $\Delta_1$ and $\Delta_2$ the staggered magnetization can vary within a wide range without causing significant changes in the ground-state energy. For example, a value of $\Delta_1 = 0.2$ and $\Delta_2 = 0.5$ gives the zero-temperature mean-field energy of the in-phase Néel flux state $E_0 = -0.321J$ per bond. This insensitivity of the ground-state energy to the staggered magnetization is apparently also implied in the calculation of Liang, Doucot, and Anderson.[2]

The two mean fields have very different temperature dependence. The staggered magnetization decreases with the increase of temperature, behaving the same way as the usual Weiss molecular field, whereas the in-phase current amplitude $\Delta_1$ is virtually a constant (but increases slightly) from zero temperature up to the Néel temperature. Above the Néel temperature $\Delta_1$ also decreases. These results show that the occurrence of the in-phase orbital current in the 2D antiferromagnetic Heisenberg model is rather robust.

The spinless-fermion excitation spectrum of both the Néel flux phase and the in-phase Néel flux state has a gap of $E_g = 4J\Delta_2$ at isolated points $(0, \pm\pi/2)$. The existence of such a gap has also been found by Kalmeyer and Laughlin[15] for the 2D antiferromagnetic Heisenberg model in a triangular lattice. In our case, however, the occurrence of the gap is associated with the staggered magnetization, not with the disordered spin state, i.e., the flux state. It is likely, therefore, that when the long-range antiferromagnetic spin order is destroyed by doping, for instance, the gap in the spinless-fermion excitation spectrum may also disappear.

The in-phase flux phase is a resonating-valence-bond state. It has strong short-range antiferromagnetic correlations, but lacks long-range spin order. Our result that the flux phase and the long-range antiferromagnetic spin order can coexist in the 2D Heisenberg model provides a reasonable interpolation between the 1D and 3D behavior of the Heisenberg antiferromagnets. In the 1D antiferromagnetic Heisenberg model the long-range spin order is completely suppressed, and the ground state can be described in terms of resonating-valence-bond states; whereas the 3D Heisenberg antiferromagnets favor a strong long-range antiferromagnetic spin order. The 2D Heisenberg antiferromagnet is more complex, since it has a large disordered-spin component coexisting and competing with the Néel order at zero temperature.

Finally we comment on the possible connections between our results and the magnetic behavior of $La_2CuO_4$. $La_2CuO_4$ is found to have an antiferromagnetic ordering below the Néel temperature, $T_N$. Above $T_N$ the spins are found in a state[9,10] which has strong spin correlations over a distance exceeding 200 Å, but has no time-averaged staggered magnetic moment. The spin-correlation length, which is determined by the long-wavelength fluctuations of this state, has been successfully interpreted by Chakravarty, Halperin, and Nelson,[18] by Auerbach and Arovas,[19] and also by Ding and Makivic.[20] All these calculations suggest that the 2D Heisenberg antiferromagnet in a square lattice is Néel ordered at $T=0$, and that the zero-temperature spin stiffness is significantly renormalized by the quantum fluctuations. In our calculation the in-phase flux state persists above the Néel temperature, and therefore it may also be relevant to this state. Indeed we have succeeded in calculating the Raman spectra of the in-phase flux phase, and found excellent agreement with the experimentally observed Raman spectra. More importantly, the exchange parameter, $J$, obtained from our calculation of the Raman spectra agrees very well with that obtained from the analysis of the spin-correlation length. This shows that the in-phase flux state is a good description for at least the short-wavelength excitation of this state, since the Raman spectrum is very sensitive to the short-wavelength excitations. The calculation will be discussed elsewhere.

In summary, we have found a 2D Wigner-Jordon transformation which maps the spin variables into pure fermion variables. The ground state of the 2D antiferromagnetic Heisenberg model was studied in the transformed representation and was found to be the in-phase Néel flux phase, i.e., a coexisting state of the flux phase with in-phase orbital currents and a long-range antiferromagnetic spin order.

*Note added.* After submitting the manuscript, we learned that a similar Wigner-Jordon transformation has been discussed by P. W. Anderson, S. John, G. Baskaran, B. Doucot, and S. D. Liang (unpublished), and also by J. Ambjorn and G. Semenoff, Phys. Lett. **B 226**, 107 (1989).

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