RAPID COMMUNICATIONS

PHYSICAL REVIEW B VOLUME 37, NUMBER 7 1 MARCH 1988

Resonating-valence-bond state: Comments on the antiferromagnetic ordering of the two-dimensional Heisenberg model

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(Received 16 November 1987)

We consider a resonating-valence-bond state as a trial wave function for the ground state of the antiferromagnetic Heisenberg model on the square lattice. The energy and the staggered spin-spin correlation functions are calculated on a small lattice and are compared with the results of the exact diagonalization of Oitmaa and Betts. The trial energy is only about 4.7% different from the exact ground-state energy on a 4×4 lattice. The importance of the singlet pairs between the next-nearest antiferromagnetic sites is inferred. An argument against the previous interpretation of the numerical data as being evidence of long-range order is presented.

The ground-state properties of the antiferromagnetic Heisenberg model are not well-understood except in one dimension where the exact Bethe ansatz solution is available.[1,2] The model is gapless in one dimension; there is no long-range order and the correlation functions decay algebraically with respect to the distance.[3]

The two-dimensional problem seems to be rather important since, in the oxide high-T_c superconductors, the antiferromagnetism in the planes might play an important role. The Hubbard model which contains the electron-electron interaction can be mapped to the antiferromagnetic Heisenberg model in the strong repulsion limit at the half-filled case.[4] Anderson and co-workers[5] proposed that the resonating-valence-bond (RVB) state to be a basic ingredient of the new mechanism of superconductivity. This RVB state is based on various combinations of singlet pairing of spins and may be regarded as a spin liquid.

There is no exact result on the ground state of the two-dimensional Heisenberg antiferromagnet. However, based on numerical calculations and the spin-wave theory,[6] there is a tendency among condensed-matter physicists to believe in the existence of long-range order at $T=0$. If this is the case, the ground state is certainly not of a RVB type and one perhaps requires more special ingredients (e.g., next-nearest coupling, spin-Peierls phase) to have the RVB state if it exists at all.

One of the numerical calculations which is often referenced as a support of long-range order is that of Oitmaa and Betts[7] who diagonalize the Hamiltonian on a small lattice. On the other hand, there is more recent work[8] on related antiferromagnetic models such as the XY and the Heisenberg model on the triangular lattice which seem to show the absence of long-range order. Although these results do not directly imply the absence of long-range order in the Heisenberg model it is, however, rather natural to consider the absence of the long-range order in the Heisenberg model, if the XY model does not have any. The Heisenberg model has more spin degree of freedom which acts toward destroying long-range order.

In order to shed light on this confusing situation, we reexamine the numerical results of Oitmaa and Betts and also consider a special type of the RVB state as a trial wave function for the ground state. The Hamiltonian of the Heisenberg antiferromagnet is

$$H=J\sum_{\langle i,j\rangle}s(i)s(j)\,, \tag{1}$$

where J is a coupling constant which is set to unity for convenience and $s(i)$ is the usual spin-$\frac{1}{2}$ operator at site i. The summation is taken over the all nearest-neighbor sites of the square lattice. We take a special type of the RVB state as a trial wave function for the ground state. Consider a dimer covering of a square lattice [see Figs. 1(a) and 1(b) for examples]. For each dimer, associate a singlet coupling of the spins whose wave function is written as $|\uparrow\downarrow\rangle-|\downarrow\uparrow\rangle$ with obvious notation. Now each dimer covering corresponds to a wave function, say ψ_α, which is a product of these singlets. The trial wave function is a linear combination of all the wave functions of the dimer coverings, namely $\Psi=\sum_\alpha c_\alpha\psi_\alpha$. We choose all the coefficients to be unity.[9,10] A rationale for this choice is discussed later. The trial energy is given by

$$E_{\rm RVB}=\langle\Psi|H|\Psi\rangle/\langle\Psi|\Psi\rangle\,. \tag{2}$$

This gives an upper bound on the true ground-state energy and if it is close to the ground-state energy one can expect that the trial wave function has a large overlap with the true ground-state wave function. The integral $\langle\Psi|\Psi\rangle$ is a sum of terms involving $\langle\psi_\beta|\psi_\alpha\rangle$ for various α and β. This overlap integral is graphically represented by a covering of the square lattice by loops and (double) dimers [see

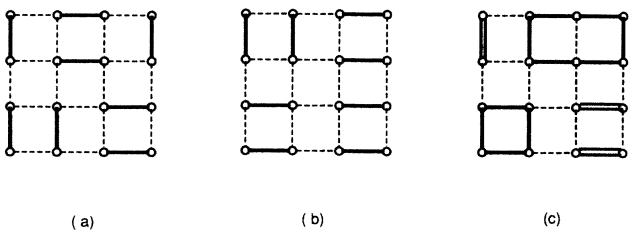

FIG. 1. (a) and (b) Examples of dimer covering. (c) The overlap of dimer coverings (a) and (b).

Fig. 1(c)]. It is possible to have a sign convention such that all the overlap integrals are positive. Divide the square lattice into two ordinate lattices A and B. A bond always connects a site on sublattice A and a site on sublattice B. Give a bond $+1$ for spin up for the site in A and spin down for the site in B. Consequently, the bond gets -1 in the other case where the spin is down for the site in A and the spin is up for the site in B. A loop has L sites in A and L sites in B. If spins on A are up, then the spin on B are down. In this case all the bonds have $+1$ and the overall sign is positive. The other case is that the spins on A are down and the spins on B are up. We then have -1 for all the bonds and get $(-1)^{2L}=1$ for the overall sign. Therefore, all the loops get the same sign. Each loop or dimer carries a weight of 2 since there is two ways of assigning spins antiferromagnetically on the sites on a loop or a dimer. On the other hand, the integral can be written as a sum over the coverings Γ. In a covering Γ, a dimer carries a weight of 2 as described above. However, a loop carries a weight 4 instead of 2. There is an extra multiplicative factor of 2 due to two ways to have a loop with assigned spin directions. In a loop, color every other bond red, and all the others black. One way to have the loop is that the red bonds comes from a bra state and the black bonds from a ket state. Another way is obviously obtained by exchanging the red and the black bonds. Note that a dimer does not have this extra factor of 2. Thus we have

$$\langle\Psi\,|\,\Psi\rangle=\sum_{\Gamma}x^{P_2}y^{P}, \tag{3}$$

where $x=2$, $y=4$, P_2 is the number of dimers, and P is the number of loops in a covering Γ. This expression can be thought as a partition function of a statistical mechanical model, and related statistical models for different values of x and y are discussed by Sutherland.[11] The energy integral $\langle\Psi\,|\,H\,|\,\Psi\rangle$ is also written in terms of a summation over the covering by examining how the Hamiltonian acts on those dimers and loops. The result is given by Sutherland[9]

$$\langle\Psi\,|\,H\,|\,\Psi\rangle=\sum_{\Gamma}\varepsilon(\Gamma)x^{P_2}y^{P}, \tag{4}$$

where $\varepsilon(\Gamma)$ is the singlet energy $\varepsilon_{\text{singlet}}$ $(=-\frac{3}{4})$ times the number of bonds in the loops and the dimers plus the number of additional bonds which are not on a loop, yet connect two sites of a loop. An example of this additional bond is in Fig. 1(c) as the middle broken line of the rectangle. If one chooses a single state, say ψ_a, as a trial wave function, there is only a single covering with (double) dimers. Then we have the trial energy per spin $E_{\text{dimer}}=\varepsilon_{\text{singlet}}/2=-\frac{3}{8}$ since each dimer associates with two sites. This is a rather poor trail energy since the Néel state without quantum correction already gives $E_{\text{Néel}}=-\frac{1}{2}$. As seen from (4) we can expect that the mixture of different dimer coverings will lower the energy since the number of bonds and sites are equal in a loop and also we have additional bonds connecting two sites in a loop which contribute to the energy. The above observation rationalizes our choice of the coefficients of the linear combinations ($c_\alpha=1$ for all α) which maximizes the overlap. It is, however, far from obvious how this simple choice of the coefficients is close to optimal. Note that we also must take into account the denominator of (2) for the energy estimate.

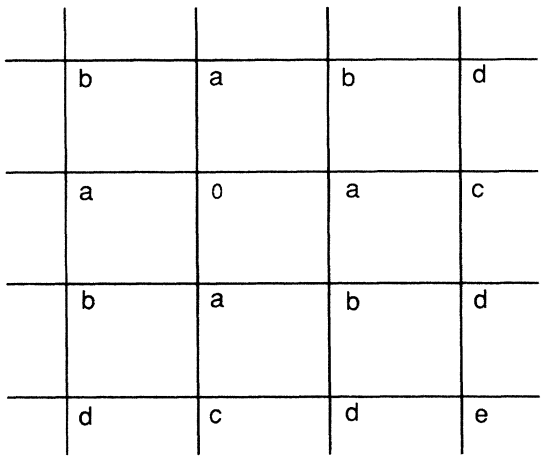

FIG. 2. A 4×4 square lattice. Note that this lattice is actually wrapped around a torus due to the periodic boundary condition.

We numerically determined the energy and the correlation function of Ψ_{RVB} on a 4×4 lattice with the periodic boundary condition. Denote the correlation function by

$$G_r=4\langle\Psi\,|\,s_z(0)s_z(r)\,|\,\Psi\rangle/\langle\Psi\,|\,\Psi\rangle. \tag{5}$$

There are five different values of the correlation function G_a, G_b, G_c, G_d, and G_e on the 4×4 lattice. The corresponding sites are marked in Fig. 2. The RVB trial state gives $G_a=-0.446$, $G_b=G_c=0.198$, $G_d=-0.125$, and $G_e=0.0937$. These are plotted in Fig. 2 together with the result of the numerical diagonalization of the Hamiltonian which gives $G_a=-0.0468$, $G_b=G_c=0.285$, $G_d=-0.270$, and $G_e=0.240$.[7] The energy per site E and the staggered magnetization $M=\sum_r(-1)^r\langle s_z(0)s_z(r)\rangle$ are given by

$$E=\tfrac{3}{2}G_a, \tag{6}$$

and

$$M=-G_a+G_b+G_c/2-G_d+G_e/4. \tag{7}$$

First note that the RVB trial energy is $E_{\text{RVB}}=-0.669$ which is only 4.7% different from the exact energy $E_{\text{exact}}=-0.702$. The Néel state without quantum fluctuation would give $E_{\text{Néel}}=-0.5$. Thus we see that the RVB state may be a much better starting choice of a variational wave function than the Néel state.

Another interesting feature is that G_b equals G_c in both data. This can be understood as a finite-size effect. Note that a site of type b has two sites of type a and two sites of type d at nearest neighbors, while a site of type c also has two sites of type a and two sites of type d at nearest neighbors due to the periodic boundary condition (see Fig. 1). For a larger lattice we would certainly expect to have $G_b>G_c$. Therefore G_c is enhanced by the finite-size effect. This enhancement is expected for all the correlation functions. For example, G_e must be much enhanced

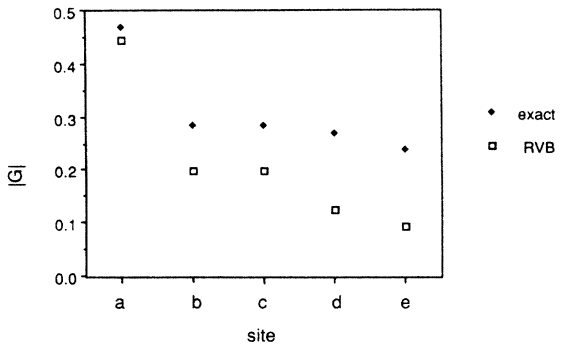

FIG. 3. Staggered correlations.

since there are four equivalent lines connecting 0 and e (note that the lattice is actually wrapped around a torus due to the periodic boundary condition).

Oitmaa and Betts claimed that the ground state has nonzero staggered magnetization in the infinite lattice based on the extrapolation of the finite-size data. As shown explicitly above, however, the finite-size effect is rather prominent even in their largest lattice of 4×4. Therefore we should not draw a definitive conclusion in regard to the existence of long-range order.

In conclusion, we calculated the energy and the correlation functions of the trial RVB state on a small lattice. The comparison to the exact energy shows that the ground state may have a large overlap with the RVB state. Probably one can improve the trial wave function by introducing singlet pairings between non-nearest-neighbor antiferromagnetic sites variationally. A sign of this may be seen in Fig. 3 where the correlation function at d of the exact diagonalization is rather large compared with that of the RVB state. We also exhibited the enhancement of the staggered magnetization in the finite lattice and warned that the previous prediction of the existence of long-range order cannot be accepted as it stands. We instead anticipate a possibility that the ground state of the antiferromagnetic Heisenberg model on the square lattice is of a resonating-valence-bond type. The correlation function of the RVB state treated in this paper decays exponentially with respect to the distance.[12] However, even in one dimension where the quantum fluctuation is expected to be larger than two dimension, the Heisenberg antiferromagnet has a power-law decaying correlation function. Therefore the true ground state in two dimension should have significant amount of singlet pairings between distant spins which probably gives the long-range power-law correlation.

I had very useful discussions with Bill Sutherland. This work was supported by a grant from the National Science Foundation, Grant No. DMR-8615609, and in part by the National Science Foundation under Grant No. PHY82-17853, supplemented by funds from the National Aeronautics and Space Administration, and the A. P. Sloan Foundation.

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