Equivalence of the Resonating-Valence-Bond and Fractional Quantum Hall States

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We present evidence that the ground state of the frustrated Heisenberg antiferromagnet in two dimensions is well described by a fractional quantum Hall wave function for bosons. This is compatible with the resonating-valence-bond concept of Anderson in being a liquid with neutral spin-$\frac{1}{2}$ excitations. Our results suggest strongly that the resonating-valence-bond and fractional quantum Hall states are the same thing. We also argue that the excitation spectrum has an energy gap.

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It was recently pointed out to us by Lee and Joannopoulos[1] that the physics of the fractional quantum Hall effect is very similar to that originally hypothesized by Anderson[2] to be operating in the two-dimensional Heisenberg antiferromagnet on a triangular lattice. In both cases, the ground state is understood to be a nondegenerate quantum liquid[2-4] with an energy gap. The existence of an energy gap is presently controversial. Anderson *et al.*[5] have recently claimed that the gap is zero, contrary to Anderson's original hypothesis, while Kivelson, Rokhsar, and Sethna[6] have argued that a gap exists. In this Letter we show that the fractional quantum Hall (FQH) state at $m=2$ confined to a triangular lattice has the same variational energy as the Anderson resonating valence-bond (RVB) wave function to within 2%. We see this as strong evidence that the ground state and excitation spectrum, in particular the energy gap, survive under adiabatic evolution of the FQH Hamiltonian into that of the antiferromagnet. If this is the case, it necessarily implies that the ground state is a nondegenerate singlet, and that the elementary excitations are spin-$\frac{1}{2}$ fermions with long-range interactions. The occurrence of FQH-type behavior in a system such as this is important because it shows that a magnetic field is not essential to the physics. It is also an indication that such behavior may be ubiquitous in nature.

We consider the antiferromagnetic Heisenberg Hamiltonian

$$\mathcal{H}_{\mathrm{AF}}=J\sum_{\langle ij\rangle}\mathbf{S}_i\cdot\mathbf{S}_j, \tag{1}$$

where $J>0$, the (unrestricted) sum is over all pairs of near-neighbor sites of the 2D triangular lattice, and $\mathbf{S}_j=\frac{1}{2}\hbar\boldsymbol{\sigma}_j$ is the spin operator at jth site. Following Lee and Joannopoulos, we now show that this Hamiltonian is equivalent to the FQH Hamiltonian for bosons on a lattice.

The first step in this procedure is the Holstein-Primakoff transformation[7]: One interprets the spin problem as a lattice gas by imagining an "atom" to be present on every site with an up spin. The atoms are then bosons with creation operators $a_j^\dagger=\hbar^{-1}(S_j^x+iS_j^y)$. Written in terms of these, (1) becomes

$$\mathcal{H}=T+V, \tag{2a}$$

where

$$T=\tfrac{1}{2}J\sum_{\langle ij\rangle}(a_j^\dagger a_i+a_i^\dagger a_j), \tag{2b}$$

and

$$V=J\sum_{\langle ij\rangle}a_j^\dagger a_i^\dagger a_i a_j+\tfrac{3}{2}JN_s-6J\sum_i a_i^\dagger a_i, \tag{2c}$$

where N_s is the number of spins or lattice sites. The boson kinetic energy operator T comes from the spin-exchange or XY part of the Heisenberg interaction. The potential energy, which is a near-neighbor repulsion of bosons, comes from the Ising part. This Hamiltonian also contains a *de facto* hard-core repulsion of the form

$$V_0=U_\infty\sum_{i=1}^{N_s}a_i^\dagger a_i^\dagger a_i a_i, \tag{2d}$$

with $U_\infty\to\infty$, due to the fact that configurations with more than one boson on a site do not exist. The Holstein-Primakoff transformation is completed by altering the Hamiltonian in the manner

$$\mathcal{H}\to\mathcal{H}+V_0,$$

and treating the lattice particles as ordinary bosons.

The second step is the identification in the Hamiltonian of a fictitious magnetic field. The kinetic energy T, as given by (2b), does not have the right free-particle form because the hopping matrix elements $J_{ij}=J$ are positive. This makes the boson energy bands disperse down as one moves away from the center of the Brillouin zone. To

remedy this problem, we consider J_{ij} to be matrix elements of the right sign, namely negative, in the presence of a fictitious vector potential. To make contact with the FQH problem, we change the signs of the kinetic energy couplings to produce the pattern shown in Fig. 1, where solid line segments are positive (wrong) bonds and dashed lines are negative (right) bonds. This is a gauge transformation and has no effect on the physics. In the original gauge all lines would have been solid. We now observe that one obtains just such a bond configuration by assigning an arbitrary charge e^* to the bosons and then coupling them to a fictitious vector potential

$$\mathbf{A} = \tfrac{1}{2} B(x\hat{\mathbf{y}} - y\hat{\mathbf{x}}), \tag{3}$$

with a particular value for B. This coupling introduces phases into the hopping matrix elements J_{ij} in (2b) according to

$$J_{ij} \rightarrow \tilde{J}_{ij} = -J \exp\left\{ \frac{2\pi i}{\phi_0} \int_i^j \mathbf{A} \cdot d\mathbf{s} \right\}, \tag{4}$$

where $\phi_0 = hc/e^*$ is the quantum of flux associated with bosons of charge e^*. If we fix the magnitude of the fictitious B field in (3) by

$$\sqrt{3} a_0^2 = 4\pi l_0^2, \tag{5}$$

where a_0 is the lattice constant and $l_0 = (e^* B/\hbar c)^{-1/2}$ is the magnetic length, then all phase factors in (4) are real, and we get the bond configuration of Fig. 1. This choice of B corresponds to one fictitious flux quantum per spin of the original problem.

Except for the presence of the lattice, this system is just a bosonic analog of the two-dimensional electron gas with short-range interactions in a real magnetic field. In light of our experience with the FQH effect, we expect this system either to crystallize or to form a nondegenerate quantum liquid. The former cannot be ruled out categorically, but we feel it is unlikely for the same reasons Anderson did.[2] If it is a liquid, it should be described approximately by the $m=2$ FQH wave function[3]

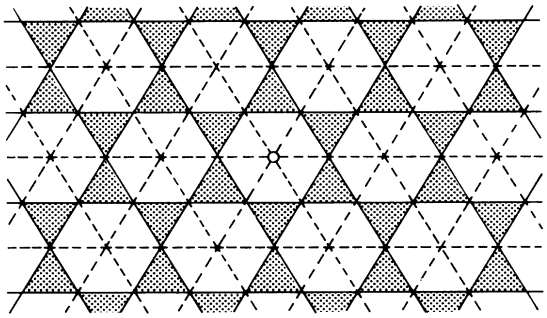

FIG. 1. Distribution of signs of the couplings $\tilde{J}_{ij} = \pm J$ defined by (3)–(5). Positive (negative) bonds are shown as solid (dashed) line segments. Open circle denotes the origin.

for N_b bosons:

$$\psi_{\rm gs}(z_1, \ldots, z_{N_b}) = \prod_{j<k} (z_j - z_k)^2 \exp\left\{ \frac{-1}{4l_0^2} \sum_{i=1}^{N_b} |z_i|^2 \right\}, \tag{6}$$

where $z_j = x_j + iy_j$ is the complex lattice coordinate of the jth particle. $\psi_{\rm gs}$ describes a state of density $\rho_2 = 4\pi l_0^2$, which corresponds to $\frac{1}{2}$ boson per unit cell. In other words, the number of up spins is equal to the number of down spins. We must emphasize that the only reason for considering such a wave function is the physical precedent of its success in describing the FQH states.

We have evaluated the energy of the system in the ground state (6) by a semiclassical Monte Carlo method.[4] For a half-filled lattice, the equivalent lattice-gas Hamiltonian is

$$\tilde{\mathcal{H}} = \tilde{T} + \tilde{V}, \tag{7a}$$

where the kinetic and potential terms are

$$\tilde{T} = \tfrac{1}{2} \sum_{\langle ij \rangle} \tilde{J}_{ij} (a_j^\dagger a_i + a_i^\dagger a_j), \tag{7b}$$

$$\tilde{V} = J \sum_{\langle ij \rangle} a_j^\dagger a_i^\dagger a_i a_j - 1.5 J N_s. \tag{7c}$$

We work in the cylindrical gauge (3), and so the hopping matrix elements $\tilde{J}_{ij}$ are as shown in Fig. 1. In Fig. 2 we have plotted the kinetic and potential terms in the ground-state energy $E_{\rm gs} = \langle \psi_{\rm gs} | \tilde{\mathcal{H}} | \psi_{\rm gs} \rangle / \langle \psi_{\rm gs} | \psi_{\rm gs} \rangle$ for lattices of different sizes. Since the wave function $\psi_{\rm gs}$ keeps the particles localized within a circular region of area $\rho_2 N_b$, we use free boundary conditions. The potential energy $\tilde{V}_{\rm gs}$ contains a negative surface term which scales like $(N_s)^{-1/2}$, since the bosons on the boundary have

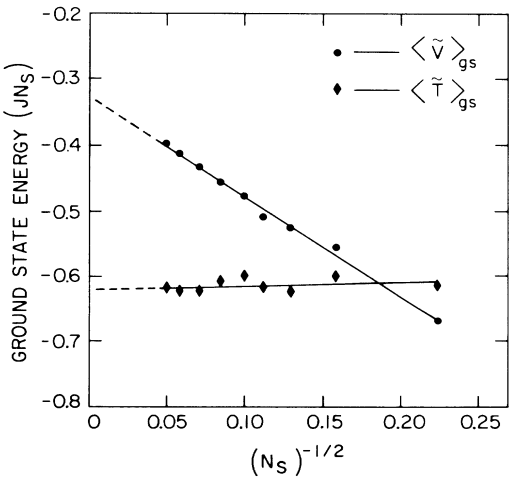

FIG. 2. Energy of the variational ground state (6), in units of $N_s J$, as a function of system size. $2N_b = N_s$ is the number of lattice sites. Kinetic energy (XY model), lozenges; potential energy (Ising term), circles.

fewer near neighbors than in the bulk. Our results for the kinetic (XY) and total (Heisenberg) ground-state energies are $\tilde{T}_{gs}=-0.62\pm0.01$ and $E_{gs}=-0.94\pm0.02$, in units of JN_s. These values are $\simeq 10\%$ higher than extrapolated finite-lattice results of Oguchi, Nishimori, and Taguchi[8] who get $\tilde{T}_{gs}=-0.74$, $E_{gs}=-1.05$, in the same units. The potential (Ising) contribution to the energy, $\tilde{V}_{gs}=-0.32JN_s$ agrees very well with finite-lattice calculations. The agreement is surprisingly good, in view of the fact that our trial wave function ψ_{gs} involves no free parameters.

For the resonating-valence-bond (RVB) state, Anderson[2] estimated $E_{RVB}=-0.98$ by extrapolation from lattices with 4, 8, 12, and 16 sites, while Oguchi, Nishimori, and Taguchi, working with lattices of up to 20 sites, obtain $E_{RVB}=-0.95\pm0.02$, in units of JN_s. It thus appears that the RVB and fractional quantum Hall wave functions are equivalent variationally.

We check the accuracy of the Monte Carlo calculations by computing the radial distribution function and the potential energy of the ground state (6) using the hypernetted chain (HNC) procedure.[4] The HNC result for the ground-state potential energy is $V_{gs}^{HNC}=-0.30JN_s$, in excellent agreement with the extrapolated Monte Carlo value shown in Fig. 2.

These numerical results strongly support the idea that the RVB and FQH states are in the following sense physically identical: One can imagine adiabatically transforming the FQH problem into the antiferromagnet problem. This might be accomplished, for example, by expressing the Hamiltonian in terms of the single-boson basis orbitals

$$\phi_\alpha(z)=(1/2\pi)^{1/2}\exp[-\tfrac{1}{4}|z|^2-\tfrac{1}{4}|z_\alpha|^2+\tfrac{1}{2}z_\alpha^* z], \tag{8}$$

where z_α is a lattice site, and then letting the off-diagonal matrix elements of the overlap matrix $S_{\alpha\beta}$, given by

$$S_{\alpha\beta}=\int \phi_\alpha^*(z)\phi_\beta(z)d^2z, \tag{9}$$

go to zero. On the basis of our experience with the FQH problem for fermions, we can say with some certainty that the adiabatic evolution starts from a system with a nondegenerate ground state described approximately by Eq. (6), an energy gap, and elementary excitations of "charge" $\frac{1}{2}$. Charge in this case means excess spin. If, during the evolution, the gap remains intact, which is not clear, the nondegeneracy of the ground state and fractional nature of the excitations almost certainly remain intact as well. If the gap collapses during the evolution, on the other hand, the situation is less certain. The excitation spectrum could conceivably survive. A more likely outcome, in our opinion, is that antiferromagnetic order would set in.[9] For this reason we believe that the RVB state possesses an energy gap, and that the assertion of Anderson *et al.*[5] that the state is gapless is incorrect. Our picture of the elementary excitation spectrum is in fact almost identical to that proposed by Kivelson, Rokhsar, and Sethna.[6]

We have obtained a numerical estimate of the gap Δ using the FQH quasihole wave function[3]

$$\psi_{z_0}=\prod_{i=1}^{N_b}(z_i-z_0)\prod_{j>k}(z_j-z_k)^2 \times\exp\left\{-\frac{1}{4l_0^2}\sum_{n=1}^{N_b}|z_n|^2\right\}, \tag{10}$$

where z_0 is a complex number locating the quasihole center. Since the real excitation is necessarily an eigenstate of linear momentum, this estimate is for the center of mass of the quasiparticle band. It is a good estimate for the gap only if the band disperses very little, which we believe to be the case. Calculations of this dispersion are under way and will be reported in a later publication.

We find that Δ is minimized when z_0 is on a lattice site. The potential energy contribution to Δ is calculated using the generalized HNC algorithm,[4] which is insensitive to boundary effects. The value we find is $\Delta V=0.21J$, independent of N_s. The kinetic energy cost ΔT to create a quasihole is estimated as the difference in kinetic energy between states (6) and (10). Figure 3 shows the results of Monte Carlo calculations of ΔT for lattices of up to 400 sites. Extrapolation to the thermodynamic limit $N_s\to\infty$ yields $\Delta T=-0.04\pm0.10$ in units of J. The total energy required to create a localized spin-$\frac{1}{2}$ excitation is thus finite and equal to $\Delta=(0.17\pm0.10)$ J.

Several remarks are in order. We believe that the *true* ground state is a nondegenerate singlet even though it is not evident that this is the case for the wave function of Eq. (6). We note particularly that the *true* ground state

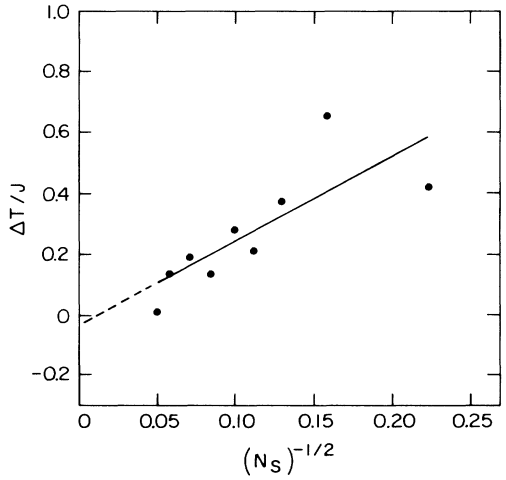

FIG. 3. Kinetic energy cost ΔT to create a quasihole excitation, as a function of system size. The HNC result for ΔV is $0.21J$.

must be real, while the wave function (6) is not, at least for some configurations. This does not mean that the time-reversal symmetry of the Hamiltonian is spontaneously broken. In fact, the correlation functions we have so far been able to calculate for the variational wave function (6) are real in the thermodynamic limit. We also have some preliminary evidence that the ground-state *Ansatz* (6) is a spin singlet. The identification of the state (6) with the true ground state of the frustrated antiferromagnet is, therefore, physically meaningful.

Adopting this picture of the ground state as a quantum spin liquid with an energy gap, we conclude that its elementary excitations are neutral spin-$\frac{1}{2}$ objects. Their spin is the charge of the elementary excitations of the equivalent FQH state, which, for a half-filled Landau level, is equal to $\pm\frac{1}{2}$. The fractional charge quantization is *exact* given the uniqueness of the ground state and the existence of a gap. The underlying rotational symmetry of the Heisenberg Hamiltonian also guarantees that the quasiparticle and quasihole, which are equivalent to the spin-up and spin-down states of the same excitation, are degenerate. Like the elementary excitations of the FQH system, these excitations may be thought of either as fermions or as particles obeying fractional statistics.[4,10] The former approach leads to an intriguing situation where the quasiparticles interact via long-range forces while all interactions in the original Hamiltonian are short-ranged.

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