Possible Spin-Liquid States on the Triangular and Kagomé Lattices

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The frustrated quantum spin-one-half Heisenberg model on the triangular and kagomé lattices is mapped onto a single species of fermion carrying statistical flux $\theta = \pi$. The corresponding Chern-Simons gauge theory is analyzed at the Gaussian level and found to be massive. This provides a new motivation for the spin-liquid Kalmeyer-Laughlin wave function. Good overlap of this wave function with the numerical ground state is found for small clusters.

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The 2D spin-$\frac{1}{2}$ antiferromagnetic Heisenberg model has attracted a lot of interest over the last few years. It is widely believed that the ground state has long-range Néel order on the square lattice [1]. On the triangular and kagomé lattices, the situation is much less clear due to the geometric frustration. In the case of the triangular lattice, Huse and Elser have constructed variational wave functions with long-range order and low energies [2]. Numerical and analytical evidence were found supporting this scenario [3]. Recently, however, Singh and Huse [4] have calculated the sublattice magnetization using a series expansion method, which is believed to be accurate, and found that the ground state is nearly disordered for the triangular lattice and strongly disordered for the kagomé lattice due to the large degeneracy of classical ground state configurations [5]. The large N calculation of Sachdev [6] has also found disordered ground states on both lattices for small enough spin.

Recently a two-dimensional extension of the Jordan-Wigner transformation, which essentially treats hard-core bosons (see below) as fermions with flux tubes, or equivalently, fermions coupled to a Chern-Simons gauge field, was developed [7]. The advantage of this approach is that the unwanted hard-core condition in the boson picture is taken care of by the Pauli principle, but as a price one has to introduce gauge interactions to fix the statistics. We applied this method to both triangular and kagomé lattices. At mean field level, the flux carried by the fermions is smeared out to form a uniform background magnetic field. If we neglect the Ising part of the Hamiltonian (which becomes a nearest-neighbor repulsive interaction between fermions after the transformation) for the moment, we have noninteracting fermions moving in a constant magnetic field. Numerical diagonalization yields two and six Landau subbands, with large excitation gaps [8] at the Fermi level of $2\sqrt{3}J$ and $1.46J$ for the triangular and kagomé lattices, respectively (J is the coupling between neighboring spins). The Hall conductance is quantized in such cases, in the form $\sigma_{xy} = \frac{e^2}{h}\nu$. In the continuum ν is just the Landau level filling factor $\nu = \frac{\pi}{\theta}$, where θ is the statistics angle which is π in this case. However, on a lattice, ν is one of the TKNN [9] integers, not necessarily equal to $\frac{\pi}{\theta}$. If one examines Gaussian fluctuations of the gauge field about its saddle point (mean field), one can integrate out the fermion degrees of freedom (which are quadratic in the action) and expand the effective action for the gauge field about its saddle point to second order to obtain [10]

$$S[A_\mu] = S_0 + \int d^2x dt \left[\frac{\epsilon}{2}E^2(\vec{x},t) - \frac{\chi}{2}B^2(\vec{x},t)\right] + \frac{1}{4}\int d^2x dt \left(\nu - \frac{\pi}{\theta}\right)\epsilon_{\mu\nu\lambda}A^\mu F^{\nu\lambda} + \cdots,$$

where S_0 is the mean field action, and ϵ and χ are the mean field values of the long-wavelength, low-frequency dielectric constant and diamagnetic susceptibility, respectively. As noted by Fradkin [10], the fluctuation is massless if and only if the Chern-Simons term in the action is canceled, i.e., $\nu = \frac{\pi}{\theta}$. This is easy to understand in terms of self-consistent linear response. Assume there is a long-wavelength, low-frequency fluctuation of the density of the fermions. Since the fermions carry flux, there should be a fluctuation of magnetic field in the same mode. According to Maxwell's equations, there will be a nonzero line integral of electric field around any region Γ:

$$\oint_\Gamma \vec{E}\cdot d\vec{l} = -\frac{1}{c}\frac{d\Phi}{dt} = -\frac{h}{e}\frac{\theta}{\pi}\frac{dN}{dt},$$

where Φ and N are the flux and number of particles in that region, respectively. Now look at the response of N to this electric field:

$$\frac{dQ}{dt} = e\frac{dN}{dt} = -\oint_\Gamma \sigma_{xy}\vec{E}\cdot d\vec{l} = -\frac{\sigma_{xy}}{c}\frac{d\Phi}{dt}.$$

The above equations are consistent if and only if $\nu = \frac{\pi}{\theta}$. This is guaranteed in the continuum, where Fetter *et al.* did find a gapless collective mode [11]. We have computed the TKNN integer for the triangular and kagomé lattices using the method of MacDonald [12] and found in both cases $\nu = -1 \neq \frac{\pi}{\theta} = 1$. Hence we expect the Chern-Simons field to be massive and the quantum XY model is therefore likely to have a gap assuming no broken translation symmetry. This gap may be stable against the Ising perturbation causing the Heisenberg model to have a spin-liquid ground state on these lattices [13].

By making analogy to the fractional quantum Hall effect (FQHE), Kalmeyer and Laughlin (KL) suggested a very interesting spin-liquid wave function for the Heisenberg model on the triangular lattice [14]. It was found to have reasonably good energy (about 10% higher than the best numerical estimate). We believe the massiveness of the Chern-Simons theory demonstrated here provides a more fundamental motivation for quantum Hall physics in frustrated spin systems. Furthermore, within the single-mode approximation [15] an excitation gap in a 2D system *requires* a Jastrow-like wave function whose square is a 2D one-component plasma in order for the structure factor to vanish at small q: $S(q) \sim q^2$. SU(2) symmetry uniquely restricts the coefficient of the plasma charge to be that given by the KL wave function ($m = 2$). The spin-$\frac{1}{2}$ excitations argued by Laughlin [16] similarly require $m = 2$ in the Bose representation. These arguments strongly suggest that a spin-liquid wave function should be of the Kalmeyer-Laughlin type.

In the rest of this paper we first briefly review the KL wave function, and prove that it is equivalent to a projected underlying fermion wave function. We apply this new wave function to the kagomé net, and calculate its energy using the Monte Carlo method. Then we calculate the overlap between this wave function and the exact wave functions on small clusters. Finally we summarize and discuss our results.

The Hamiltonian for the antiferromagnetic Heisenberg model is

$$H = J\sum_{\langle ij\rangle} \vec{S}_i \cdot \vec{S}_j, \tag{1}$$

where $J > 0$, $\vec{S}_i$ is the spin operator at site i, and the sum is over nearest neighbors. Following Ref. [14], we map the spin operators to hard-core boson operators. The Hamiltonian in this representation is

$$\begin{aligned} H &= T + V, \\ T &= \frac{J}{2}\sum_{\langle ij\rangle}(a_i^\dagger a_j + a_j^\dagger a_i), \\ V &= J\sum_{\langle ij\rangle} n_i n_j + \text{const} . \end{aligned}$$

The notation is the same as in Ref. [14]. As was shown by KL [14], on the triangular lattice, this new Hamiltonian describes hard-core bosons moving in a uniform magnetic field with field strength one flux quantum per unit cell. The bosons have a nearest-neighbor repulsive interaction. In the ground state, the lattice is half filled, which means the Landau level filling factor is one-half. By making analogy to the FHQE, they suggested the trial wave function for the bosons:

$$\Psi(z_1, \ldots, z_N) = \prod_{i<j}(z_i - z_j)^2 \prod_{k\leq N} G(z_k) e^{-\frac{1}{4}|z_k|^2/l_0^2}, \tag{2}$$

where G is a gauge phase factor [14]. From experience with the FQHE we know this is a liquid state with hidden off-diagonal long-range order (ODLRO) due to the binding of vortices to charges [17]. Since ODLRO corresponds to chiral order in the present spin problem [18], (2) actually describes a chiral spin liquid that breaks T reversal symmetry.

The state (2) has some nice features, including being a singlet in the thermodynamic limit, but it cannot be generalized to non-Bravais lattices, such as the kagomé lattice. Also it becomes a singlet only when the system is infinitely large, so it is not suitable for finite size studies. For these reasons, we want to find a more general wave function that reduces to (2) on the triangular lattice in the thermodynamic limit, and has better finite size properties. To do that, we assume the spins are carried by spin-$\frac{1}{2}$ fermions trapped on lattice sites, and try to describe state (2) in terms of them. We can express the spin operators in terms of these fermion operators:

$$\begin{aligned} a_j^\dagger &= S_j^+ = c_{j\uparrow}^\dagger c_{j\downarrow} , \\ a_j &= S_j^- = c_{j\downarrow}^\dagger c_{j\uparrow} , \end{aligned}$$

where $c_{j\uparrow,\downarrow}^\dagger$ are creation operators of up (down) spin fermions at the jth site. Just as for the bosons, there is a hard-core condition on the fermions: $n_{j\uparrow} + n_{j\downarrow} = 1$.

In the second quantized representation, the state (2) is

$$|\Psi\rangle = \sum_{\{z_1,\ldots,z_N\}} \Psi(z_1, \ldots, z_N) a_{z_1}^\dagger \cdots a_{z_N}^\dagger |0_b\rangle.$$

Here the sum is over all possible boson configurations. $|0_b\rangle$ is the boson vacuum state. Since it corresponds to the state that all spins are down, we have

$$|0_b\rangle = \prod_{j=1}^{N_s} c_{j\downarrow}^\dagger |0_f\rangle ,$$

where $|0_f\rangle$ is the fermion vacuum state and N_s is the number of sites. So we get

$$|\Psi\rangle = \frac{1}{N!}\sum_{\{z_1,\ldots,z_N;z_{[1]},\ldots,z_{[N]}\}} \Psi(z_1, \ldots, z_N) c_{z_1\uparrow}^\dagger c_{z_1\downarrow} \cdots c_{z_N\uparrow}^\dagger c_{z_N\downarrow} \prod_{k=1}^{N_s} c_{k\downarrow}^\dagger |0_f\rangle.$$

Here $z_{[j]} = z_{N+j}$ denotes the coordinate of jth down spin fermion. The sum is over all possible fermion configurations satisfying the hard-core condition. We do not distinguish between c_j and c_z, a_j and a_z, etc., if z is the complex coordinate of the jth site. Rearranging the order of fermion operators and neglecting constant factors, we have

$$|\Psi\rangle = \sum_{\{z_1,\ldots,z_N;z_{[1]},\ldots,z_{[N]}\}} \Psi(z_1, \ldots, z_N) F(z_1, \ldots, z_N; z_{[1]}, \ldots, z_{[N]}) \prod_{k=1}^{N} c_{z_k\uparrow}^\dagger \prod_{l=1}^{N} c_{z_l\downarrow}^\dagger |0_f\rangle.$$

Here $F(z_1,\ldots,z_{[N]})$ is a totally antisymmetric factor:

$$|F(z_1,\ldots,z_{2N})| = \text{const}, \quad F(\ldots,z_j,\cdots,z_k,\ldots,z_{2N}) = -F(\ldots,z_k,\ldots,z_j,\ldots).$$

We can take F to be

$$F = \prod_{i<j}(z_i - z_j)^{-1}(z_{[i]} - z_{[j]})^{-1} \prod_{k,l\leq N}(z_k - z_{[l]})^{-1}.$$

If we go back to the first quantization, the wave function that describes the underlying fermions is just

$$\Psi_f(z_1,\ldots,z_{[N]}) = \prod_{i<j\leq N}(z_i - z_j)(z_{[i]} - z_{[j]})^{-1} \prod_{k,l\leq N}(z_k - z_{[l]})^{-1} \prod_{m=1}^{N} G(z_m)e^{-\frac{1}{4}|z_m|^2}. \tag{3}$$

Obviously a fermion wave function should be antisymmetric under exchange (including spin variables), but here we neglect spin variables in the wave function and treat up and down spin particles as if they were distinguishable, so the above wave function is legal. Since we have the hard-core condition on fermions, what we really mean by (3) is the state that is projected to the subspace with no double occupancy. Hence it is a well defined wave function for the original quantum spins.

Now we can use a theorem proved by KL [14]:

$$\prod_{j\neq k}(\xi_k - \xi_j) = C_0 G(\xi_k)e^{\frac{1}{4}|\xi_k|^2},$$

where ξ_j is the complex coordinate of the jth site, C_0 is a constant, and $G(\xi_k)$ are the gauge phases [14]. This theorem holds only on the triangular lattice in the thermodynamic limit. Using it in (3) we get

$$\Psi_f(z_1,\ldots,z_{[N]}) = \prod_{i<j\leq N}(z_i - z_j)(z_{[i]} - z_{[j]}). \tag{4}$$

The right-hand side of Eq. (4) is just the product of two Vandermonde determinants [19], which is what one gets when both spin states of the first Landau level are fully occupied. Since up and down spin particles occupy the same spatial Slater determinant, the resulting state must be a spin singlet, even after projection. This provides another way to prove that the state (2) is a singlet in the thermodynamic limit. The advantage of (4) is it gives a singlet even on finite size systems, and it can be generalized directly to non-Bravais lattices.

As a test of the equivalence between (2) and (4), we calculated the energy of (4) on a triangular lattice. The calculation of the Ising part of the energy is straightforward using Monte Carlo, and the total energy is exactly 3 times that (for any system size). The extrapolated result is $-(0.48 \pm 0.01)J$ per site, which agrees with the KL result [14]. We have found that in our case the data converge much faster, i.e., the finite size results are much closer to the extrapolated result. This tells us that (4) is better for finite size study. The energy we get for the kagomé is $-(0.399 \pm 0.001)J$ per site, about 8% higher than the best numerical estimate [20].

We have also studied the overlap between (4) and the exact ground state on small clusters, where we need to minimize the finite size effect by applying periodic boundary conditions (PB). The wave function (4) satisfies open boundary conditions, so we need to solve the wave functions with PB:

$$t(\vec{L_j})\psi(z) = e^{i\phi_j}\psi(z); \quad j = 1,2,\ldots . \tag{5}$$

Here $t(\vec{L_j})$ is a magnetic translation operator [21]. This problem was solved for the torus geometry by Haldane and Rezayi [21]. The result is (up to a constant factor)

$$\Psi_f = \prod_{i,j\leq N}\left[\theta_1\left(\frac{\pi}{L_1}(z_i - z_j)\middle|\tau\right)\theta_1\left(\frac{\pi}{L_1}(z_{[i]} - z_{[j]})\middle|\tau\right)\right]\theta_1\left(\frac{\pi}{L_1}\left(\sum_k z_k - Z_0\right)\middle|\tau\right)\theta_1\left(\frac{\pi}{L_1}\left(\sum_k z_{[k]} - Z_0\right)\middle|\tau\right). \tag{6}$$

Here $\theta_1(z|\tau)$ is the elliptic theta function [21], $\tau = L_2 e^{i\delta}/L_1$, $\vec{L_1}$ and $\vec{L_2}$ are the vectors that determine the shape of the parallelogram, and δ is the angle between them. Z_0 is the center-of-mass coordinate determined by ϕ_1 and ϕ_2. In most cases we are interested in, it should be set to zero [22]. Like Eq. (4), Eq. (6) also describes a singlet state. A truly nondegenerate ground state wave function must be real [14]. So instead of using the complex wave function (6) directly, we use $\Psi_f e^{i\phi} + \Psi_f^* e^{-i\phi}$ in the overlap calculation and use ϕ as a variational parameter. We applied it to several clusters of the triangular lattice containing an even number of spins and having the shape of a parallelogram (torus geometry [21]) and also one with the shape of a hexagon (twelve spins). The results are listed in Table I. We find that the square of the overlap remains large in systems with up to twenty spins (4×5). The energies we get are close to the Monte Carlo result, which means the change of boundary condition does not change the short distance correlations. For reasons we do not understand yet, the overlap is *exactly*

TABLE I. Overlaps and variational energies on small clusters of the triangular lattice. Energies are in unit J per site; E_v is the variational energy.

Cluster	$\lvert\text{Overlap}\rvert^2$	E_v	Exact energy
Hexagon (12)	0.966	−0.591	−0.6103
3×4	0.821	−0.519	−0.5776
4×4	0.000	−0.459	−0.5347
6×3	0.554	−0.491	−0.5811
4×5	0.493	−0.481	−0.5581

zero in the 4×4 cluster. We have verified that Ψ_f has the correct symmetries (spin rotation, translation, 180^0 rotation and mirror reflection of space). Apparently there is some additional hidden symmetry which does not match that of the numerical ground state. We have done the same calculations on kagomé clusters [20] with twelve and eighteen spins. Again we got zero overlaps, probably for similar reasons. The energies, $-0.420J$ and $-0.418J$ per site, respectively, are close to the Monte Carlo result.

If the ground state of the triangular lattice has three sublattice order, such order is suppressed on clusters 3×4, 4×4, and 4×5 due to incommensurability, but is not on 6×3 and the hexagon with twelve spins. Our data suggest this commensurability is a weak effect. Both state (6) and the true ground states have a lot of symmetries (rotation, translation, etc.). It could happen that there are so few states of the right symmetries available that an arbitrary combination of them will have a decent overlap with the ground state. By assuming singlet states are uniformly distributed in the momentum space, we find the number of states with the right symmetry is of order 1000 in the case of twenty spins, and yet the square of the overlap is rather large: 0.493. The twelve-spin hexagon has additional symmetries, so the significance of the remarkably large squared overlap of 0.966 is unclear.

Sachdev [6] has an alternative proposal for spin-liquid ground states where no symmetry including T reversal is broken. His state shares the features of having an excitation gap and spinon excitations with the present one, and has the advantage of connecting smoothly to Néel ordered states at large S. The spinons are bosonic in his picture. Laughlin [16] argued that the spinons should be semions, but this issue remains controversial. The large overlaps we obtain suggest chiral order might be present in the exact ground states of the clusters [23], although Chalker and Eastmond found no obvious symmetry breaking in their finite size study on kagomé [5].

The central result of this paper is the demonstration that treating spins as fermions carrying flux tubes leads to a massive Chern-Simons theory on frustrated lattices. This provides a new and fundamental motivation for quantum Hall types of spin-liquid physics. We have developed the formalism needed to compute the overlap between these wave functions and the exact ground state and we have obtained large overlaps for small clusters. It would be highly desirable to see these calculations extended to large lattices, although this will require considerable numerical effort.

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