Spin-Liquid Phase in a Spin-1/2 Quantum Magnet on the Kagome Lattice

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(Received 28 July 2006; published 15 November 2006)

We study a model of hard-core bosons with short-range repulsive interactions at half filling on the kagome lattice. Using quantum Monte Carlo numerics, we find that this model shows a continuous superfluid-insulator quantum phase transition, with exponents $z = 1$ and $\nu \approx 0.67(5)$. The insulator, $\mathcal{I}^*$, exhibits short-ranged density and bond correlations, topological order, and exponentially decaying spatial vison correlations, all of which point to a Z_2 fractionalized phase. We estimate the vison gap in $\mathcal{I}^*$ from the temperature dependence of the energy. Our results, together with the equivalence between hard-core bosons and $S = 1/2$ spins, provide compelling evidence for a spin-liquid phase in an easy-axis spin-1/2 model with no special conservation laws.

DOI: 10.1103/PhysRevLett.97.207204 PACS numbers: 75.10.Jm, 05.30.Jp, 71.27.+a, 75.40.Mg

Spin-liquid states, or strongly correlated quantum paramagnets that preserve all lattice symmetries, were proposed long ago as plausible candidates for the ground state of frustrated quantum magnets [1]. In recent years, several frustrated antiferromagnets have been discovered which appear to either have a spin-liquid ground state (such as the $S = 1$ kagome lattice system $Nd_3Ga_5SiO_{14}$ [2] or the $S = 1/2$ triangular lattice Mott insulator κ-$(ET)_2Cu_2(CN)_3$ [3]) or are proximate to a spin-liquid phase (such as the $S = 1/2$ stacked triangular magnet Cs_2CuCl_4 [4]), thus lending support to this paradigm. On the theoretical front, there has been considerable progress in understanding the effective field theories and properties of such spin-liquid phases [5–8], showing that the excitations in this phase carry fractional quantum numbers and interact with emergent gauge fields. However, there is the pressing issue that most microscopic models which can be shown to have a spin-liquid phase have either very unusual interactions [9] or local Hilbert space constraints. An example of the latter are particular triangular [10] and kagome lattice [11] quantum dimer models which have dimer-liquid ground states but are not directly related to any microscopic spin Hamiltonians.

In a significant development, Balents *et al.* [12] proposed a model of $S = 1/2$ spins on the kagome lattice

$$H_{XXZ} = -J_\perp \sum_{\hexagon} [(S^x_{\hexagon})^2 + (S^y_{\hexagon})^2 - 3] + J_z \sum_{\hexagon} (S^z_{\hexagon})^2, \quad (1)$$

where $S^a_{\hexagon} = \sum_{i \in \hexagon} S^a_i$ is a sum over the six spins on each hexagon of the kagome lattice unit cell, $\sum_{\hexagon}$ denotes a sum over all hexagons on the lattice. This model is easily seen to be a short-range anisotropic XXZ model, with only the first, second, and third neighbor interactions being nonzero and equal to each other. Analyzing this model [12] for $J_\perp < 0$ and $J_z/|J_\perp| \gg 1$, they showed that it directly *maps* onto an effective triangular lattice quantum dimer model with three dimers touching each site. In spin language, this effective model takes the form of a ring-exchange model, with an exchange scale $J_{\text{ring}} = J_\perp^2/J_z$, which describes quantum dynamics in the Hilbert space with $S^a_{\hexagon} = 0$ on each hexagon, the local constraint arising from energetic considerations at large $J_z/J_\perp$. Supplementing this model with an additional four-site [Rokhsar-Kivelson (RK) [13]] potential term of strength v_4 was shown to lead to a spin-liquid for $v_4 = J_{\text{ring}}$, which was argued to be stable for small deviations $v_4 < J_{\text{ring}}$. Later exact diagonalization (ED) numerics [14] showed that the ring-exchange model appears to be in this spin-liquid phase down to $v_4 = 0$, but only system sizes up to 20 unit cells could be explored. A numerical study of a related rotor model on a decorated square lattice [15] also led to a Z_2 spin liquid, but the corresponding $S = 1/2$ model was not studied.

In this Letter, we show the presence of a spin-liquid phase in a $S = 1/2$ model on the kagome lattice, by studying numerically the Hamiltonian (1) with $J_\perp > 0$, $J_z > 0$. Since the ring-exchange model is independent of the sign of $J_\perp$, we expect to recover the physics of the ring-exchange model at large J_z, but without imposing Hilbert space restrictions by hand. On the technical side, the choice of $J_\perp > 0$ eliminates the quantum Monte Carlo (QMC) sign problem. This permits us to study very large systems at very low temperature using a generalized stochastic series expansion QMC algorithm [16,17] and, thus, to go significantly beyond earlier work on this class of models.

By the mapping between $S = 1/2$ spins and hard-core bosons, model (1) is equivalent to a hard-core boson model with short-range repulsion at half filling

$$H_b = -t \sum_{(i,j)} (b_i^\dagger b_j + \text{H.c.}) + V \sum_{\hexagon} (n_{\hexagon})^2 - \mu \sum_i n_i, \quad (2)$$

where $b_i^\dagger (b_j)$ is the boson creation (annihilation) operator, $t = J_\perp > 0$ is the hopping amplitude, $V = J_z > 0$ is the repulsion strength, $n_i = b_i^\dagger b_i$ is the number operator, and $\mu = 12 J_z$ is the chemical potential. The hopping term connects only the first, second, and third neighbors. We begin by showing that model (2) exhibits a superfluid-insulator transition at $(V/t)_c \approx 19.8$. We then turn to the

nature of the insulating phase and show that it is a topologically ordered Z_2 Mott insulator. We thus arrive at the result that for $J_\perp > 0$, model (1) exhibits a ferromagnetic phase at small J_z and a Z_2 fractionalized spin-liquid at large J_z, separated by a continuous quantum phase transition (QPT) at $(J_z/J_\perp)_c \approx 19.8$.

Superfluid-insulator transition.—For small values of V/t, we expect the ground state of (2) to be a superfluid ($\mathcal{SF}$). We confirm this by measuring the superfluid density ρ_s through winding number fluctuations $W_{a_{1,2}}$ [18] in each of the two lattice directions, with $\rho_s = (1/2\beta t)(\langle W_{a_1}^2\rangle + \langle W_{a_2}^2\rangle)$, where β is the inverse temperature. As seen from Fig. 1, for small V/t, ρ_s is large (its value agrees with mean field estimates [19]). ρ_s decreases with increasing V/t, eventually vanishing for $V/t \gtrsim 20$, suggesting a phase transition to an insulating phase ($\mathcal{I}^*$). This behavior is in sharp contrast to a nearly identical model where the hopping and repulsive interactions are restricted to the nearest neighbor only—in that case a uniform superfluid persists for arbitrarily large V/t [20]. The absence of a jump in ρ_s in Fig. 1 suggests that the $\mathcal{SF} - \mathcal{I}^*$ transition is continuous.

In the vicinity of a continuous QPT, we expect $\rho_s = L^{-z} F_{\rho_s}(L^{1/\nu}(K_c - K), \beta/L^z)$, where F_{ρ_s} is the scaling function, L is the linear system size, z the dynamical critical exponent, ν the correlation length exponent, and $(K_c - K) \propto (V_c - V)/t$ is the distance to the critical point. Thus if we plot $\rho_s L^z$ as a function of V/t at fixed aspect ratio β/L^z, the curves for different system sizes should intersect at the critical point. The inset of Fig. 2 shows such a plot for $z = 1$ and $\beta/L = 3/(4t)$ with a clear crossing point at $(V/t)_c \approx 19.8$. To obtain the correlation length exponent ν, we plot $\rho_s L$ as a function of $[(V/t)_c - V/t]L^{1/\nu}$ for different system sizes. It follows from the above scaling relation that the curves for different system sizes should collapse onto a universal curve F_{ρ_s} for a properly chosen $(V/t)_c$ and ν. In Fig. 2, we show such a data collapse for $(V/t)_c = 19.80(2)$ and $\nu = 0.67(5)$. The error bars are estimated from the stability of the collapse towards varying the parameters. To summarize, we find a continuous $\mathcal{SF} - \mathcal{I}^*$ transition with exponents $z = 1$ and $\nu = 0.67(5)$. We next examine the nature of the insulator $\mathcal{I}^*$.

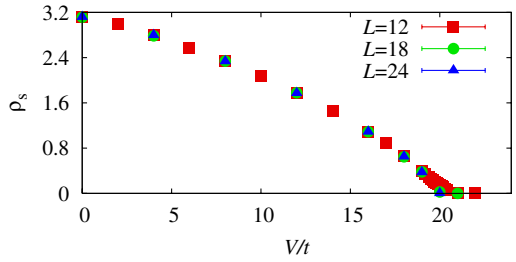

FIG. 1 (color online). The superfluid density ρ_s versus V/t, at $T = t/9$ for different linear system sizes L.

$\mathcal{I}^*$ does not break lattice symmetries.—For a system of bosons, flux-threading arguments [21,22] show that an insulating state at half filling could either be a conventional state with broken lattice symmetries or must *necessarily* have topological order (which means the ground state degeneracy depends on the topology of the system). We rule out the first possibility here by studying correlation functions in the insulating state. We look for signatures of diagonal (density) ordering by studying the equal-time density structure factor $S(\mathbf{q})/N = \langle \rho_{\mathbf{q}\tau}^\dagger \rho_{\mathbf{q}\tau}\rangle$, where $\rho_{\mathbf{q}\tau} = (1/N)\sum_i \rho_{i\tau} \exp(i\mathbf{q}\mathbf{r}_i)$ and $\rho_{i\tau}$ is the boson density at site i and imaginary time τ. Figure 3 compares a contour plot of the equal-time structure factor to that of the classical model (with $J_\perp = 0$), which is known to have short-range correlations [23]. The striking similarity between the two suggests short-ranged density correlations in the full quantum ground state of the insulator. We confirm this via a careful examination of the equal-time structure factor on large system sizes. Up to $L = 48$ we do not find any Bragg peaks, which rules out the possibility of density ordering even with moderately large unit cells. We also examine for possible bond ordering in $\mathcal{I}^*$ by computing the bond-bond structure factor $S_b(\mathbf{q})/N = \langle B_{\mathbf{q}\tau}^\dagger B_{\mathbf{q}\tau}\rangle$, where $B_{\mathbf{q}\tau} = (1/N)\sum_\alpha B_{\alpha\tau} \exp(i\mathbf{q}\mathbf{r}_\alpha)$ is summed over the bond index α connecting spins i and j, and $B_{\alpha(i,j),\tau} = t(b_i^\dagger b_j + b_i b_j^\dagger)$ is the off-diagonal bond operator. Again, we find no signatures of ordering from the bond-bond structure factor.

Finally, the $\mathcal{SF} - \mathcal{I}^*$ transition appears to be continuous, rather than first order which would be expected if we had a conventional transition between a superfluid and a broken symmetry insulator. This argument, together with the correlation function results, strongly favor a non-broken-symmetry ground state for $\mathcal{I}^*$. Therefore, we next examine the second possibility, that $\mathcal{I}^*$ is a featureless topologically ordered Mott insulator (a "spin liquid" in magnetic language).

Topological order in $\mathcal{I}^*$.—On a lattice with periodic boundary conditions in both lattice directions, the subspace

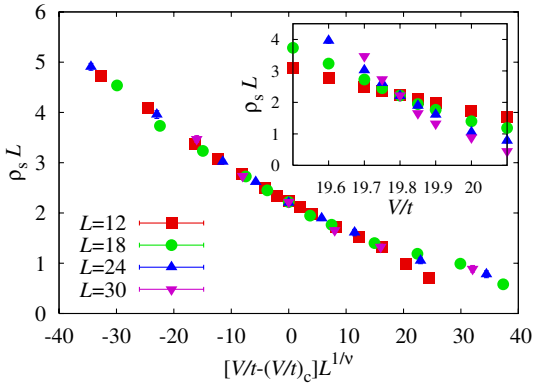

FIG. 2 (color online). Data collapse of the superfluid density ρ_s for $\beta/L = 4/(3t)$, $(V/t)_c = 19.80(2)$, and $\nu = 0.67(5)$. Inset: Finite size scaling of ρ_s for $\beta/L = 4/(3t)$.

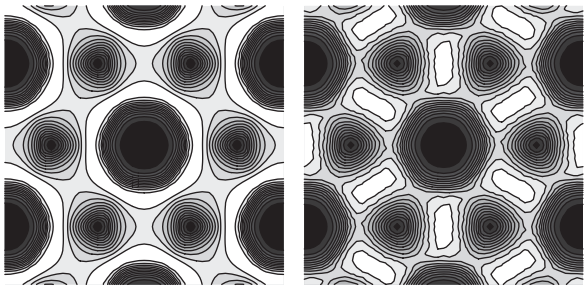

FIG. 3. Contour plots of the equal-time density structure factor ($L = 24$) for the classical model (with $t = 0$) [23] (left panel) at $T = 0$ and in the quantum insulator (right panel) for $V/t = 20$, $T = t/12$. Axes range from -2π to 2π.

of configurations with $n_{\bigcirc} = 3$ on every kagome hexagon, i.e., the "dimer subspace" which dominates the boson wave function for $V \to \infty$, has topological sectors defined by having, for each lattice direction $a_{1,2}$, an odd (or even) number of bosons on each row ("parity sectors"). In this torus geometry and in the restricted Hilbert space, we thus find four topological sectors labeled by row and column parity, such that any local move which obeys the local constraint $n_{\bigcirc} = 3$ leaves the sector unchanged. In order to change from one sector to another, one needs to make highly nonlocal boson moves over loops which wind around the lattice.

The row-column parities are however not well defined in model (2) since at any finite V; no matter how large, there will be a small density of hexagons with $n_{\bigcirc} \neq 3$ [24]. We have checked in our numerics, where we start from a configuration in the dimer subspace with a certain row-column parity, that the QMC algorithm generates a small density of particle-hole pair defects in equilibrium, so that the quantum ground state no longer lies in the "dimer subspace". However, for a large enough system size at a given value of V/t ($L \gtrsim 10$ at $V/t = 26$), we find that our simulations with the longest accessible MC steps do not lead to any nonlocal boson moves which wind around the lattice. Thus the winding number identically vanishes, and each configuration in the simulation which lies in the dimer subspace belongs to the same parity sector as the initial configuration. The full ground state accessed by the QMC algorithm is, in this sense, perturbatively connected to the initial parity sector. This means that four topological sectors continue to exist, and we can label them simply by the row-column parity of that component of the ground state wave function which lies in the dimer subspace.

For a *topologically ordered* insulator, the ground state energy should be *identical* in each of the four topological sectors (on a torus) leading to a ground state degeneracy of four. We have computed the energy of the four ground states by starting our simulations from configurations in the dimer subspace lying in four different parity sectors. We find that they are equal within statistical errors, which is strong evidence for topological order [25].

Spatial vison correlations in $\mathcal{I}^*$.—A second signature of Z_2 fractionalization is that visons, which are gapped Z_2 vortices in the effective field theory description, should have exponentially decaying spatial correlations. The spatial vison-vison (vv) correlation function is the expectation value of a string operator in terms of the spins. For the ring-exchange model (valid for $V/t \to \infty$), it takes the form [12]: $C_{\rm vv}(r_{ij}) = |\langle 0| \prod_{k=i}^{j} e^{i\pi n_k} |0\rangle|$, where $|0\rangle$ denotes the ground state and the product is along some path on the kagome lattice that contains an even number of sites, starts at site i, and ends at site j, making only "$\pm 60°$" turns to the left or right. $n_k = 0, 1$ is the number of bosons at site k. The absolute value of the product is *path independent* in the dimer subspace, and it is expected to decay exponentially in the topologically ordered phase. In model (1) at finite V/t, the ground state no longer lies entirely in the dimer subspace, but will mix in configurations with particle-hole defects. Correspondingly, the vison operator must include correction terms to the above definition since it otherwise becomes path dependent in the presence of such defects. Both the corrected ground state wave function and the vison operator may be determined order by order in a perturbation expansion [19], undoing the unitary transformation that leads from model (2) to a ring-exchange Hamiltonian.

Here, evaluate the leading term, correct to $\mathcal{O}(t/V)$, of $C_{\rm vv}(r_{ij})$ by computing the above string expectation value in the true ground state *projected into the dimer subspace* [19]. As seen from Fig. 4, $C_{\rm vv}(r_{ij})$ decays exponentially in $\mathcal{I}^*$, again signaling topological order in $\mathcal{I}^*$. At $V/t = 20.5$, we estimate a "decay length", $\xi = 1.43(5)$, which is comparable to its value at the RK point of the ring-exchange model [12], $\xi \approx 1$, and to that found by ED [14], $\xi \approx 1.7$, in the ring-exchange model with $v_4 = 0$.

Vison gap.—To provide further evidence for gapped vison excitations, we display the temperature dependence of the system energy per site and compressibility $\kappa = \frac{\beta}{N} \times \langle (\sum_i n_i)^2 \rangle$ in Fig. 5. The energy exhibits a two-step decrease upon lowering temperature, with a distinct intermediate plateau, before vanishing exponentially at a very low temperature. We identify the first drop in energy with a freez-

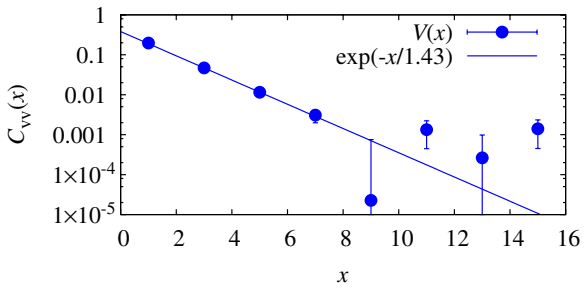

FIG. 4 (color online). Equal-time vison-vison correlation function for $L = 24$ and $T = t/18$ in the insulator at $V/t = 20.5$, showing exponential decay with a length scale $\xi = 1.43(5)$.

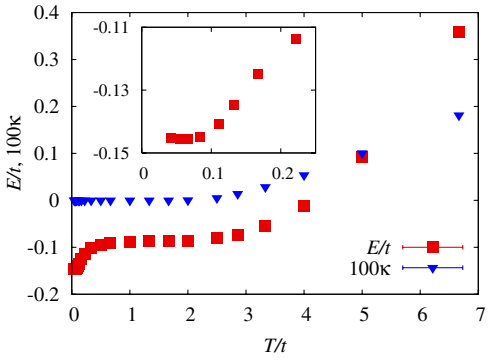

FIG. 5 (color online). Energy per site E and compressibility κ versus temperature for $L = 24$ ($V/t = 20.5$). The energy rises exponentially at very low T (see inset) with a wide intermediate plateau from $T/t \sim 0.5 - 3$ (see text). The compressibility is zero (within error bar) at low T, rising only at $T \sim 3t$ once gapped charge (spinon) excitations become relevant.

ing out of charge fluctuations below a charge gap scale, which we confirm by the sharp decrease in κ at this temperature (also shown in Fig. 5). The plateau then corresponds to a regime where the system dominantly explores configurations with $n_{\hexagon} = 3$ on each hexagon. (The large difference between the total energy of the ground state and that in the plateau regime can be explained by the macroscopic entropy density of multiple vison excitations [19]). Finally, at the lowest temperature, the system begins evolving into the spin-liquid ground state. Heating up from $T = 0$, we therefore identify the lowest energy excitations out of the ground state as vison-pair excitations (since the charge gap is much larger). The temperature dependence of the energy then leads to a rough estimate of the single vison gap; for $V/t = 20.5$, we find $E_v/t \sim 0.35(15)$.

Conclusions.—We have studied the $T = 0$ phase diagram of a hard-core boson model with short-range repulsion on the kagome lattice using QMC calculations. We find a continuous QPT from a superfluid phase to a featureless Mott insulator with increasing repulsion. In magnetic language, this corresponds to a ferromagnet-paramagnet QPT with the paramagnet being a correlated quantum spin liquid. This spin liquid supports gapped visons and exhibits topological order characteristic of a Z_2 fractionalized phase. The apparently 3D XY exponents at the $\mathcal{I}^* - \mathcal{SF}$ transition, $z = 1$ and $\nu = 0.67(5)$, are consistent with the QPT arising from condensation of fractionalized charge-1/2 bosons [15]. We have estimated the vison gap in the spin liquid from the temperature dependence of the energy. Finally, the spin-liquid phase is fully gapped and thus stable to weak perturbations away from the special choice of exchange couplings in our model. Although our model is not of direct relevance to known kagome magnets, our work represents significant progress towards understanding realistic Hamiltonians by showing a spin-liquid phase in a model with only local interactions and no special conserved quantities.

We acknowledge support from NSERC (S. V. I., Y. B. K., A. P.), CRC, CIAR, and No. KRF-2005-070-C00044 (S. V. I., Y. B. K.), and the Alfred. P. Sloan Foundation (A. P.). We thank L. Balents and D.-N. Sheng for useful discussions.

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[24] Such defects correspond to particle-hole pairs in real space, which are necessarily bound to each other since the system is insulating and charges cannot propagate freely in the ground state.
[25] For a finite size system which becomes a topologically ordered insulator in the thermodynamic limit, we expect four *nearly* degenerate ground states with an energy splitting which is exponentially small L. Evaluating this splitting is beyond the scope of our simulations.