PHYSICAL REVIEW B **92**, 201105(R) (2015)

Variational Monte Carlo study of a gapless spin liquid in the spin-$\frac{1}{2}$ XXZ antiferromagnetic model on the kagome lattice

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(Received 31 May 2015; published 11 November 2015)

By using the variational Monte Carlo technique, we study the spin-$\frac{1}{2}$ XXZ antiferromagnetic model (with easy-plane anisotropy) on the kagome lattice. A class of Gutzwiller projected fermionic states with a spin Jastrow factor is considered to describe either spin liquids [with $U(1)$ or Z_2 symmetry] or magnetically ordered phases [with $\mathbf{q} = (0,0)$ or $\mathbf{q} = (4\pi/3,0)$]. We find that the magnetic states are not stable in the thermodynamic limit. Moreover, there is no energy gain to break the gauge symmetry from $U(1)$ to Z_2 within the spin-liquid states, as previously found in the Heisenberg model. The best variational wave function is therefore the $U(1)$ Dirac state, supplemented by the spin Jastrow factor. Furthermore, a vanishing $S = 2$ spin gap is obtained at the variational level, in the whole regime from the XY to the Heisenberg model.

DOI: 10.1103/PhysRevB.92.201105 PACS number(s): 75.10.Jm, 75.10.Kt, 75.40.Mg, 75.50.Ee

Introduction. Quantum spin liquids with topological order and fractional excitations are exotic states of matter that do not show any local order down to zero temperature [1]. Their importance for the field of correlated systems is directly related to the connection to unconventional electron pairing, thus giving a clue to explain the mechanism of high-temperature superconductivity [2,3]. In the last two decades there have been intensive studies suggesting that quantum spin liquids might be stabilized at low temperatures in realistic two-dimensional frustrated magnetic systems. The spin-$\frac{1}{2}$ Heisenberg antiferromagnetic model on the kagome lattice represents one of the most promising examples [4]. From the experimental side, the so-called Herbertsmithite shows very promising signatures for magnetically disordered phases down to extremely low temperatures [5–8]. Even more interestingly, many experimental probes suggested the existence of gapless spin excitations; in particular, neutron scattering measurements highlighted the presence of a broad continuum of excitations down to small energies [7,8].

For Herbertsmithite, it is widely believed that the gross features can be captured by the spin-$\frac{1}{2}$ Heisenberg antiferromagnet on the kagome lattice with the nearest-neighbor interactions only. This model has been studied by several analytical and numerical approaches in recent years, with contradicting outcomes [9–23]. In particular, accurate density-matrix renormalization group (DMRG) calculations highlighted the possibility that the ground state can be a fully gapped Z_2 topological spin liquid [16,17]. A different scenario has been put forward by using variational Monte Carlo approaches based upon a Gutzwiller projected fermionic state [10,11,24], which finds a gapless spin liquid with a competing ground-state energy [25,26].

In order to clarify the nature of the spin-liquid phase, several authors considered the effect of different "perturbations" to the nearest-neighbor Heisenberg model, the most obvious one being a second-neighbor superexchange [20,27–31]. However, given the lack of the consistent results [20,28,30,31], it is still not clear if this term helps the stabilization of the spin liquid or not. The inclusion of additional third-neighbor couplings [21,30,32,33] or three-spin chiral interactions [34] stabilizes a topological spin liquid with spontaneously time-reversal symmetry breaking [35,36], which has been identified as the $\nu = 1/2$ bosonic quantum Hall state [30,32,33]. Recent DMRG studies found that this chiral state can persist also by changing the magnetic anisotropy within the XXZ model [37,38]. In this respect, the XXZ model with the only nearest-neighbor interactions has not been thoroughly investigated. Some recent calculations have pointed out the possibility that different magnetic orders are favored for the XY and Heisenberg models, based upon order-by-disorder mechanisms [39,40]. This situation should take place for large enough spin S, while for $S = 1/2$ magnetically disordered states should be expected. Indeed, DMRG calculations have suggested the existence of a spin-liquid phase; however, it remains unclear if there is a phase transition between the XY and the Heisenberg models for $S = 1/2$ [37,38]. In particular, the XY model could have a vanishing small spin gap, which is compatible with a gapless quantum spin liquid in the thermodynamic limit [38]. Therefore, the spin anisotropy in the nearest-neighbor coupling represents a very promising way to unveil the nature of the spin-liquid phase of the Heisenberg model.

In this paper we consider the following Hamiltonian:

$$\mathcal{H} = J_{xy} \sum_{\langle ij \rangle} \left(S_i^x S_j^x + S_i^y S_j^y \right) + J_z \sum_{\langle ij \rangle} S_i^z S_j^z, \quad (1)$$

where $\langle ij \rangle$ denotes the sum over the nearest-neighbor pairs of sites, and $\mathbf{S}_i = (S_i^x, S_i^y, S_i^z)$ is a spin-$\frac{1}{2}$ operator at each site i. In the following we will set $J_{xy} = 1$ as the energy scale. When $J_z = 1$ ($J_z = 0$), Eq. (1) reduces to the Heisenberg (XY) model. Here we focus on the region with $0 \leqslant J_z < 1$, and study the stability of different variational wave functions including the $U(1)$ and Z_2 spin liquids, as well as the magnetic ordered states (the isotropic Heisenberg model with $J_z = 1$ has been thoroughly investigated in previous works [11,25,26]). The main results can be summarized as follows: by applying an energy optimization, there is no signal for the stabilization of a gapped spin liquid; also the inclusion of magnetic orders does not improve the $U(1)$ Dirac state. Instead, some energy gain can be obtained by including a (short-range) Jastrow factor. Then we construct the $S = 2$ state by exciting four spinons in the $U(1)$ Dirac spin liquid and calculate the $S = 2$ spin gap at different values of J_z. The variational results are compatible with the conclusion that the same gapless spin liquid persists from $J_z = 1$ to $J_z = 0$.

Method and variational wave functions. Our variational wave functions are defined as

$$|\Psi_v\rangle = \mathcal{J}_s \mathcal{P}_G |\Psi_0\rangle, \tag{2}$$

where $|\Psi_0\rangle$ is an uncorrelated wave function that is obtained as the ground state of an auxiliary Hamiltonian (see below); $\mathcal{P}_G = \prod_i (1 - n_{i\uparrow} n_{i\downarrow})$ is the Gutzwiller projector, which enforces no double occupation on each site; and $\mathcal{J}_s = \exp(1/2 \sum_{ij} v_{ij} S_i^z S_j^z)$ is the spin Jastrow factor, with v_{ij} being variational parameters that depend upon the distance between sites i and j. We would like to stress the fact that such a Jastrow term, which includes the z components of the spin operator, does not break any symmetry of the spin Hamiltonian in the easy-plane limit ($J_z < 1$), while it breaks the spin SU(2) symmetry for the Heisenberg model ($J_z = 1$). Here we consider two cases for the auxiliary (noninteracting) Hamiltonian that are suitable for magnetic and spin-liquid wave functions.

Magnetic states are defined from

$$\mathcal{H}_{\text{MAG}} = \sum_{(i,j),\sigma} t_{ij} c_{i,\sigma}^\dagger c_{j,\sigma} + h \sum_{i,\sigma} \mathbf{M}_i \cdot \mathbf{S}_i, \tag{3}$$

where $c_{i,\sigma}^\dagger$ ($c_{i,\sigma}$) creates (destroys) one electron at site i with spin σ. We find that the best projected state within this class of wave functions has nontrivial hopping amplitudes, which define a magnetic flux $\Phi = \pi$ across hexagons and $\Phi = 0$ across triangles, see Fig. 1 (they are exactly the ones that define the $U(1)$ Dirac spin liquid in Ref. [10]). The magnetic order is defined by the (variational) parameter h and the vector $\mathbf{M}_i$ that defines the periodicity; here we consider coplanar states and restrict $\mathbf{M}_i$ in the XY plane, i.e., $\mathbf{M}_i = [\cos(\mathbf{r}_i \cdot \mathbf{q} + \eta_i), \sin(\mathbf{r}_i \cdot \mathbf{q} + \eta_i), 0]$ ($\mathbf{q}$ is the pitch vector and η_i is the phase shift for sites within the same unit cell). In the following we consider two antiferromagnetic patterns with $\mathbf{q} = (0,0)$ and $\mathbf{q} = (4\pi/3,0)$ (corresponding to the $\sqrt{3} \times \sqrt{3}$ order), see the insets of Fig. 2. With $\mathbf{M}_i$ in the XY plane, the spin Jastrow factor correctly describes the relevant spin fluctuations around the classical spin state [41]. We would like to emphasize that the existence of magnetic long-range order is directly related to the presence of a finite parameter h in Eq. (3).

Instead, spin-liquid wave functions are defined from

$$\mathcal{H}_{\text{SL}} = \sum_{(i,j),\sigma} t_{ij} c_{i,\sigma}^\dagger c_{j,\sigma} + \sum_{(i,j)} [\Delta_{ij} c_{i,\uparrow}^\dagger c_{j,\downarrow}^\dagger + \text{H.c.}]$$
$$+ \mu \sum_{i\sigma} c_{i,\sigma}^\dagger c_{i,\sigma} + \Delta_0 \sum_i [c_{i,\uparrow}^\dagger c_{i,\downarrow}^\dagger + \text{H.c.}], \tag{4}$$

where, in addition to the hopping terms, there is also a singlet pairing ($\Delta_{ij} = \Delta_{ji}$); the on-site paring Δ_0 and the chemical potential μ are also considered. It is possible to show that many different spin liquids can be constructed, depending on the symmetries of t_{ij} and Δ_{ij}, which may have $U(1)$ or Z_2 gauge structure and gapped or gapless spinon spectrum [42].

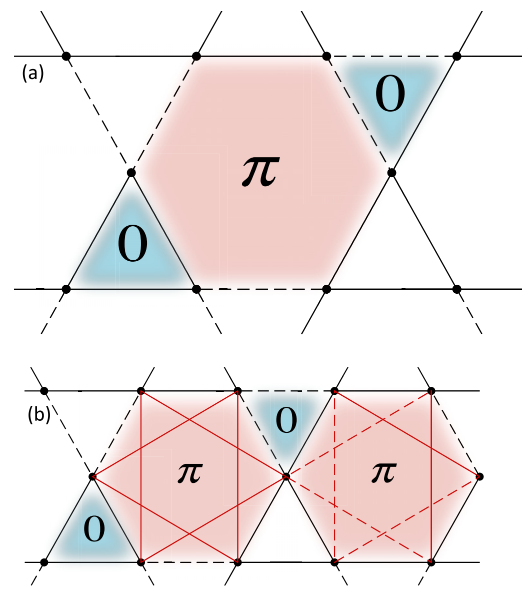

FIG. 1. (Color online) (a) The mean-field *ansatz* of the $U(1)$ Dirac state: black solid (dashed) bonds denote positive (negative) hoppings (t_1). The unit cell is doubled to accommodate a magnetic flux $\Phi = \pi$ across hexagons and $\Phi = 0$ across triangles. The same hopping amplitudes are also used to define the magnetic wave function obtained from Eq. (3). (b) The mean-field *ansatz* of the $Z_2[0,\pi]\beta$ state: red solid (dashed) lines indicate positive (negative) next-nearest-neighbor hoppings (t_2) and pairings (Δ_2).

In this paper we consider two kinds of spin liquids, namely the gapless $U(1)$ Dirac state and the gapped $Z_2[0,\pi]\beta$ state, as shown in Fig. 1. We emphasize that, for $J_z < 1$, a spin Jastrow factor can be also included, since the spin SU(2) symmetry is explicitly broken by the XXZ Hamiltonian (1).

In general, suitable boundary conditions in the auxiliary Hamiltonians are chosen, in order to have a unique mean-field ground state $|\Psi_0\rangle$. In order to fulfill the constraint of one electron per site (imposed by the Gutzwiller projector) and to take into account the spin Jastrow factor, a Monte Carlo sampling is needed. Along the Markov chain that defines the numerical simulation, only configurations belonging to the physical Hilbert space are proposed, so that the Gutzwiller

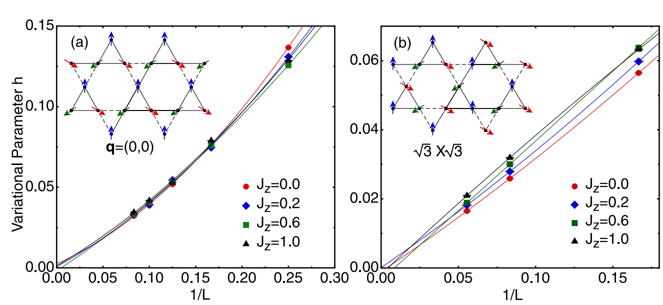

FIG. 2. (Color online) The finite size scaling of the variational parameter h as a function of the inverse geometrical diameter $1/L$ at different values of J_z for the magnetic order with $\mathbf{q} = (0,0)$ (a) and the $\sqrt{3} \times \sqrt{3}$ order (b). The quadratic fitting is used for all cases. The *ansatz* for the magnetic order with $\mathbf{q} = (0,0)$ and $\sqrt{3} \times \sqrt{3}$ are also shown.

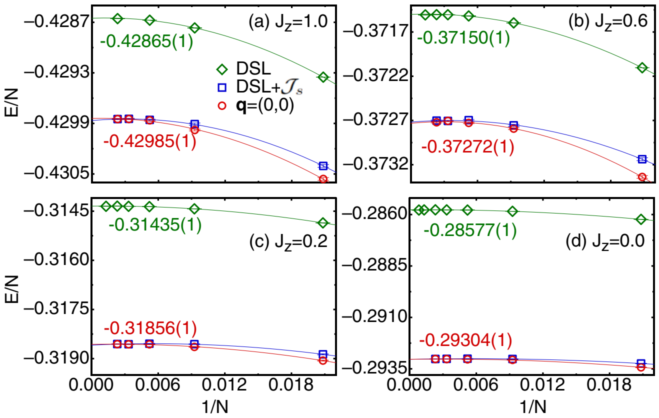

FIG. 3. (Color online) Energies per site of the $U(1)$ Dirac spin liquid (green diamonds) compared with the one of the magnetic state with $\mathbf{q} = (0,0)$ (red circles) for different values of J_z. The $U(1)$ Dirac state with spin Jastrow factor is also reported (blue squares), which corresponds to the magnetic state with a vanishing variational parameter h.

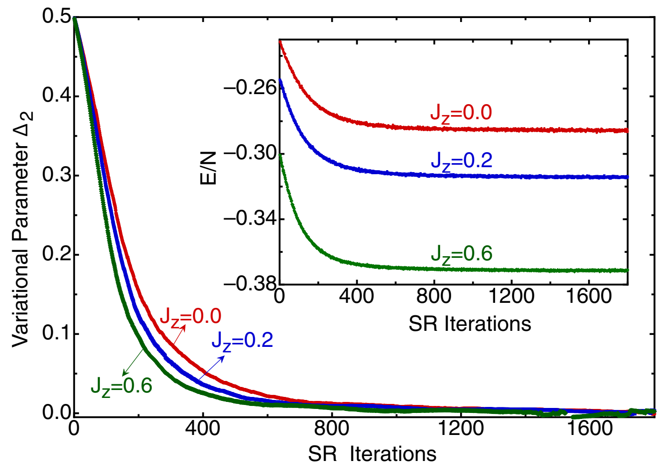

FIG. 4. (Color online) The variational parameter Δ_2 for the $Z_2[0,\pi]\beta$ spin liquid for $J_z = 0$, 0.2, and 0.6 on $L = 16$ cluster. The variational energy per site as function of the SR iterations is shown in the inset.

projector is exactly implemented. To optimize the variational parameters in both the auxiliary Hamiltonians and the spin Jastrow factor, we use the stochastic reconfiguration (SR) optimization method to find the energetically favored state in the variational Monte Carlo scheme [43]. The SR optimization method allows us to perform the optimization with many variational parameters, and to obtain an extremely accurate determination of variational parameters.

Results. We performed the variational Monte Carlo calculations on toric clusters with $L \times L \times 3$ sites and periodic boundary conditions. Let us start with magnetic states. In Fig. 2 we show the size scaling of the magnetic order parameter h of Eq. (3) for both the states with $\mathbf{q} = (0,0)$ and $\sqrt{3} \times \sqrt{3}$ order. The latter one is not frustrated by boundary conditions only when L is a multiple of 3. First of all, we find that a finite magnetic parameter h of Eq. (3) can be stabilized on finite clusters, and the two states have essentially the same energy within $10^{-4} J_{xy}$ for all the cases analyzed here. However, the most important outcome is that $h \to 0$ in the thermodynamic limit (for both antiferromagnetic states), indicating that no magnetic order can be stabilized in the XXZ model. Therefore, the auxiliary Hamiltonian from which the variational state is constructed reduces to the $U(1)$ Dirac state of Ref. [10]. Nevertheless, the parameters v_{ij} of the spin Jastrow factor remain finite, with sizable values at short-range distances. This fact gives a non-negligible energy gain with respect to the $U(1)$ Dirac state, especially close to the XY limit, see Fig. 3. We stress that the presence of the spin Jastrow factor is just relevant to improve short-range observables, such as the energy. We mention that the spin Jastrow factor gives a small energy gain of about $10^{-3} J_{xy}$ also in the Heisenberg case, see Fig. 3 [however, in this case, the spin Jastrow factor spoils the spin SU(2) invariance of the Dirac spin liquid].

We now move to study the possible stabilization of Z_2 spin-liquid states. According to the classification of Ref. [42], there is only one Z_2 gapped spin liquid that is directly connected to the $U(1)$ Dirac spin liquid, the so-called $Z_2[0,\pi]\beta$ state. In Ref. [11] the authors have shown that this gapped spin liquid cannot be stabilized in the Heisenberg model with $J_z = 1$. Here we would like to extend the analysis to the case of the XXZ model. The variational states is constructed from Eq. (4), and the noninteracting wave function that defines the $Z_2[0,\pi]\beta$ state includes the nearest-neighbor t_1, the next-nearest-neighbor t_2 hoppings, the next-nearest-neighbor paring Δ_2, which is responsible for the breaking from $U(1)$ to Z_2 symmetry, a chemical potential μ, and the on-site pairing Δ_0, see Fig. 1. In the following we do not consider the spin Jastrow factor, which may improve the energy but does not change the optimization of the variational parameter Δ_2. The optimization is shown in Fig. 4 for $J_z = 0$, 0.2, and 0.6 on the $L = 16$ cluster. The result is that, as for the Heisenberg case, both Δ_2 and Δ_0 (not shown here) go to zero for all the values of J_z considered, even on finite clusters. The vanishing Z_2 parameters indicates that, similar to what has been found in the Heisenberg model [11], the gapped $Z_2[0,\pi]\beta$ spin liquid is not stable in the XXZ model.

In summary, we obtain that the best variational state of the form (2) that can be constructed from Eqs. (3) and (4) is the $U(1)$ Dirac spin liquid, supplemented by a short-range spin Jastrow factor [44].

In the following we compute the $S = 2$ spin gap for the $U(1)$ Dirac state. The $S = 2$ state is constructed by changing boundary conditions, in order to have four spinons in an eightfold degenerate single-particle level at the chemical potential; a unique mean-field state is then obtained by taking all these spinons with the same spin. This $S = 2$ state can be written in terms of a single determinant, which is particularly easy to be treated within our Monte Carlo sampling. In the following we do not consider the spin Jastrow factor, since its inclusion does not modify the qualitative picture [44]. Similarly to what has been done on the Heisenberg model [26], we obtain the $S = 2$ spin gap by computing separately the energies of the $S = 0$ and $S = 2$ states. In Fig. 5 we report the results for $J_z = 0$, 0.2, and 0.6 (the case with $J_z = 1$ from Ref. [26] are also reported for comparison). First of all, we remark that, for each cluster size, the spin gap decreases by

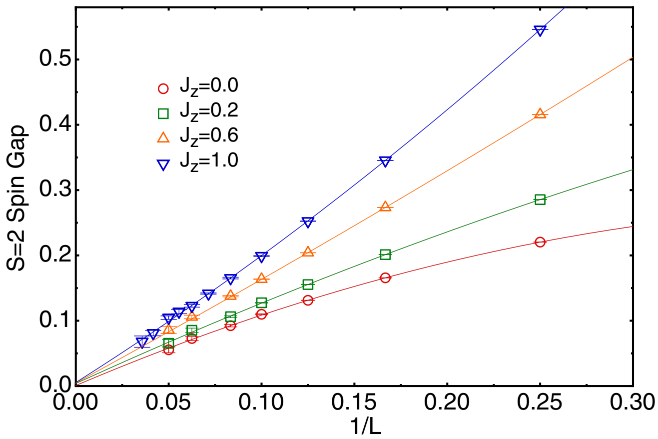

FIG. 5. (Color online) The finite size scaling of the $S = 2$ spin gap as a function of $1/L$ for different values of J_z. The results for $J_z = 1$ are from Ref. [26].

decreasing the value of J_z, indicating that the anisotropy in the spin superexchange tends to close the finite-size gap. This result is in agreement with DMRG calculations in Ref. [38]. Most importantly, the finite-size scaling with L up to 20 clearly indicates a vanishing spin gap for all values of J_z considered here. Therefore, our analysis based upon Gutzwiller-projected states suggests that the same $U(1)$ Dirac state with gapless spinon excitations can be stabilized from $J_z = 1$ to $J_z = 0$.

Conclusions. In summary, we investigated the XXZ model on the kagome lattice by using the variational Monte Carlo technique with the Gutzwiller projected fermionic states. We have studied different variational wave functions describing either magnetic states or spin-liquid phases. As previously obtained in the Heisenberg model [11], the gapped $Z_2[0,\pi]\beta$ spin liquid cannot be stabilized for $J_z < 1$, indicating a remarkable stability of the gapless $U(1)$ Dirac state. Moreover, the consideration of magnetic order does not give any energy gain in the thermodynamic limit, but a considerable energy gain can be obtained by the spin Jastrow factor. The $S = 2$ spin gap, on any finite-size clusters, decreases with decreasing the value of J_z, indicating that the best place to find a gapless spin liquid is most probably close to the XY limit. This outcome agrees with a recent DMRG study [38], which suggested that a critical state can be stabilized near the XY kagome model. In addition, we do not find any evidence for possible dimer states, as also suggested by DMRG calculations [37,38].

Finally, we would like to mention that the application of few Lanczos steps to the $U(1)$ Dirac spin liquid, as already done in recent works for the Heisenberg model [25,26], does not alter the results on the $S = 2$ gap, although the large statistical errors for $L = 8$ do not allow us to obtain as neat conclusions as in the Heisenberg model [44]. In fact, even though the $U(1)$ Dirac spin liquid remains the best variational state within the class of fermionic states that have been analyzed here, its accuracy slightly deteriorates when decreasing the value of J_z, which makes the zero-variance extrapolation harder than for the Heisenberg case.

Acknowledgments. We thank Y. Iqbal for providing us with the variational data for $J_z = 1$, and thank W. Zhu for providing the DMRG data. This research is supported by the National Science Foundation through Grants DMR-1408560 (W.-J.H, D.N.S) and PREM DMR-1205734 (S.S.G.), and by the Italian MIUR through PRIN 2010-11 (F.B.).

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