Two distinct spin liquid states in a layered cubic lattice

Jin Xu and K. S. D. Beach
Department of Physics, University of Alberta, Edmonton, Alberta, Canada T6G 2E1
(Dated: October 31, 2013)

We construct a family of short-range resonating-valence-bond wave functions on a layered cubic lattice, allowing for a tunable anisotropy in the amplitudes assigned to nearest-neighbour valence bonds along one axis. Monte Carlo simulations reveal that four phases are stabilized over the full range of the anisotropy parameter. They are separated from one another by a sequence of continuous quantum phase transitions. An antiferromagnetic phase, centred on the perfect isotropy point, intervenes between two distinct quantum spin liquid states. One of them is continuously deformable to the two-dimensional U(1) spin liquid, which is known to exhibit critical bond correlations. The other has both spin and bond correlations that decay exponentially. The existence of this second phase is proof that, contrary to expectations, neither a bipartite lattice structure nor a conventional Marshall rule is an impediment to realizing a fully gapped quantum spin liquid.

A quantum spin liquid [1] is an exotic insulator that breaks no symmetries down to zero temperature. The picture is that of a Mott phase [2] with quenched charge fluctuations, whose residual degrees of freedom are governed by a low-energy model of lattice spins coupled through local interactions. By some confluence of disruptive factors—quantum fluctuations, unfavourable geometry, exchange interactions that are at odds with one another—the system is unable to establish any kind of long-range order. Over the years, a large number of gapped and ungapped liquid states has been proposed [3–12], and there is sufficient evidence to believe that such states are found in real materials [13–15].

There has been a spate of recent numerical results supporting the existence of spin liquid ground states in simple frustrated Heisenberg models [16–20]. These are believed to be related to states with \( Z_2 \) topological order [10, 11, 21–24]. There are, however, serious practical difficulties in (convincingly) connecting spin models to their purported spin liquid ground states. In particular, obtaining unbiased, well-converged results is a challenge. Quantum Monte Carlo simulation is hindered by the infamous sign problem [25]; and beyond one spatial dimension (1D), the computational complexity for density-matrix renormalization group calculations scales exponentially in the lattice size [26]. So there remains some question about the reliability of numerical results and ongoing controversy as to whether some of these delicate liquid states might actually be unstable to valence bond crystal order [27–30].

A somewhat less fraught path is to dispense with the microscopic model entirely and simply to construct liquid states for study. Considerable analytical work has been done (using slave-particle approaches, gauge field theories, and the ideas of projective symmetries and cohomology groups) to develop classification schemes [31–34]. On the numerical side, there has been an active effort to construct and characterize trial wave functions that are designed to be featureless. These calculations have generally been carried out in the context of resonating-valence-bond (RVB) states [35, 36], which are total-spin-zero states built out of pairs of spins forming singlets. In a few cases, and with some success, the RVB states have been treated variationally [37–41]. But more often, the program is simply to consider particular RVB wave functions, either evaluated directly [42–45]; recast as Pfaffians [46]; or Gutzwiller-projected from a free Fermi sea [47] or a Bardeen-Cooper-Schrieffer (BCS) state [48].

What motivates our study is the conjecture by Yang and Yao that spin and bond correlations decay exponentially in all short-range, nonbipartite RVB states [48]. (This is suggested by the special role that a nonbipartite lattice plays in achieving the \( Z_2 \) topological state in quantum dimer models [23, 24].) What has been unclear until now is whether the converse also holds. In other words, is frustration at the level of the wavefunction a necessary condition for a gapped spin liquid? As it turns out, no—but there has been good reason to think it might. It is certainly true that on the square lattice the NN RVB state is understood to be a U(1) spin liquid with critical bond correlations [42, 43]; and the same state transplanted to the cubic and diamond lattices exhibits bond correlations with a dipolar form [45] characteristic of the Coulomb phase [49]. Indeed, in all the currently studied examples of a short-range RVB state on a bipartite lattice, there are remnants of critical correlations inherited from the underlying set of classical hardcore dimer tilings. The results reported here, however, provide a clear counterexample.

Model.—We consider a system of \( S = 1/2 \) spins, \( 2N = L^3 \) in number, living on a cubic lattice of linear size \( L \) with periodic boundary conditions. The wave function is taken to be a superposition of valence bond states, and we treat their coefficients (in the style of Liang, Doucot, and Anderson [50]) as a product of individual bond amplitudes

\[
h(x,y,z) = \delta_{x+y+z=1} (1 + (a-1) \delta_{z=1}). \tag{1}
\]

Equation (1) encodes a very simple rule: the amplitude is 1
asition at some critical value

and the isotropic 3D Néel state (a = 0) and the isotropic 3D Néel state (a = 1), there is a phase transition at some critical value $a_1$. Moreover, we are free to tune the anisotropy in the opposite direction. In the limit $a \to \infty$, the system consists of $L^2$ decoupled chains, each of them a perfectly ordered 1D bond crystal (as occurs in the Majumdar-Ghosh chain [59]). Hence, we anticipate an additional pair of critical points, $a_2$ and $a_3$, at which the Néel order is extinguished and the bond order emerges. What is so exciting is that these two points turn out not to be coincident, and an additional disordered phase occupies the region $a_2 < a < a_3$.

Numerical results.—The wave function is evaluated using Monte Carlo with worm-like updates [40]. Expectation values of observables

$$\langle \hat{O} \rangle = \frac{1}{Z} \sum_c w(c) O(c)$$

(3)

are sampled with respect to the probability distribution $w(c)/Z$, whose domain is the set of all (closed-loop-forming) short-range double bond coverings $c = (v_1, v_2)$. Here, the factor $Z = \langle \psi | \psi \rangle = \sum_c w(c)$ fixes the overall normalization. The weight $w(c) = w(v_1, v_2) = a^{n_z(v_1) + n_z(v_2)} |v_1 v_2\rangle$ is guaranteed to be positive definite, provided that $a > 0$; since the basis of nearest-neighbour bond states is bipartite on the cubic lattice, the overlap $\langle v_1 v_2\rangle$ is positive definite [60] and is given by a simple power of 2 as dictated by the transition graph [61]. Operator expectation values $O(c) = \langle v_1 | O | v_2\rangle / \langle v_1 v_2\rangle$ are computed according to the loop estimators given in Ref. 62.

In order to track the magnetism, we measure the spin correlation function $C_s(x, y, z) = \langle S(x, y, z) \cdot S(y, z, x) \rangle$, the square of the $(\pi, \pi, \pi)$ staggered moment

$$\langle \hat{m}_s^2 \rangle = \frac{1}{L^3} \sum_{x,y,z=1}^L C(x, y, z)(-1)^{(x+y+z)}$$

(4)

and $U = 1 - 3 \langle \hat{m}_s^4 \rangle / 5 \langle \hat{m}_s^2 \rangle^2$, the corresponding Binder cumulant. Within our simulations, the appearance of long-range antiferromagnetic correlations is signalled by the proliferation of system-spanning loops. In terms of our update algorithm, we expect Néel ordering to coincide with the worm head and tail (i.e., the end-points of the evolving open string that serves as the Monte Carlo walker) becoming deconfined and thus free to circumnavigate the periodic lattice independently. With that in mind, we also compute $\langle W^2 \rangle = \langle W_x^2 \rangle + \langle W_y^2 \rangle + \langle W_z^2 \rangle$, the average of the squared winding number of the worm path, summed over each of the three orthogonal directions.

As shown in Fig. 2, we observe a continuous transition from the easy-plane spin liquid to the Néel phase at $a_1 \approx 0.22$ and from the Néel phase to the easy-axis spin liquid at $a_2 \approx 3.9$. We estimate the critical points and exponents of the thermodynamic system from finite-size simulations on the $L^3$ cubic lattice, performed for increasing values of the linear size up to $L = 48$. In our analysis, we assume the conventional, leading-order scaling form for the staggered magnetization:

$$\langle n_s^{2k} \rangle = L^{-2k\beta/\nu} \mathcal{M}_{k\nu}([a - a_n] L^{1/\nu_s})$$

(5)

Furthermore, we suppose that the Binder cumulant and (by analogy) our winding measurement scale according to $U = \mathcal{U}_n([a - a_n] L^{1/\nu_s})$ and $\langle W^2 \rangle = \mathcal{W}_n([a - a_n] L^{1/\nu_s})$. Here, $a_n$ is

FIG. 1. A snapshot of the resonating short-bond-only state on a layered cubic lattice. Valence bonds lying in the $xy$ plane (dark purple) are distinguished from those aligned with the $z$ axis (light blue). Each $z$-oriented bond contributes an additional factor $a$, which encodes its probability relative to bonds of the other two orientations.

for any nearest-neighbour (NN) bond oriented along the $x$ or $y$ axes, $a > 0$ for any NN bond oriented along the $z$ axis, and zero otherwise.

Hence, as illustrated in Fig. 1, the wave function realizes a one-parameter family of short-range RVB states living on an effectively layered cubic lattice, with quite different easy-plane ($a \ll 1$) and easy-axis ($a \gg 1$) limits. The wave function can be expressed concisely as

$$|\psi\rangle = \sum_v a^{n_z(v)} |v\rangle,$$

(2)

where $|v\rangle$ is a valence bond state; the prime indicates a sum over all bipartite, short-bond-only configurations; and $n_z(v)$ counts the number of bonds parallel to the $z$ axis.

Including only NN valence bonds is a reasonable choice. Such a restriction emerges naturally in some exact solutions [51–53], and it is has been judged an excellent approximation in the case of many strongly frustrated antiferromagnets [54–57]. A crucial observation is that when long bonds are suppressed in two-dimensional (2D) systems, the accompanying Néel order is suppressed too, but this is not always the case in 3D. Specifically, the equal-amplitude NN RVB wave function on the square lattice turns out to be disordered [42, 43], whereas the same state on the cubic lattice has a substantial staggered moment $m_s = 0.1519(5)$ [45, 58].

Our trial wave function on a layered cubic lattice is designed to interpolate between these two limits. Therefore, it must be that, somewhere between the 2D spin liquid ($a = 0$) and the isotropic 3D Néel state ($a = 1$), there is a phase transition at some critical value $a_1$. Moreover, we are free to tune the anisotropy in the opposite direction. In the limit $a \to \infty$, the system consists of $L^2$ decoupled chains, each of them a perfectly ordered 1D bond crystal (as occurs in the Majumdar-Ghosh chain [59]). Hence, we anticipate an additional pair of critical points, $a_2$ and $a_3$, at which the Néel order is extinguished and the bond order emerges. What is so exciting is that these two points turn out not to be coincident, and an additional disordered phase occupies the region $a_2 < a < a_3$.

Numerical results.—The wave function is evaluated using Monte Carlo with worm-like updates [40]. Expectation values of observables

$$\langle \hat{O} \rangle = \frac{1}{Z} \sum_c w(c) O(c)$$

(3)

are sampled with respect to the probability distribution $w(c)/Z$, whose domain is the set of all (closed-loop-forming) short-range double bond coverings $c = (v_1, v_2)$. Here, the factor $Z = \langle \psi | \psi \rangle = \sum_c w(c)$ fixes the overall normalization. The weight $w(c) = w(v_1, v_2) = a^{n_z(v_1) + n_z(v_2)} |v_1 v_2\rangle$ is guaranteed to be positive definite, provided that $a > 0$; since the basis of nearest-neighbour bond states is bipartite on the cubic lattice, the overlap $\langle v_1 v_2\rangle$ is positive definite [60] and is given by a simple power of 2 as dictated by the transition graph [61]. Operator expectation values $O(c) = \langle v_1 | O | v_2\rangle / \langle v_1 v_2\rangle$ are computed according to the loop estimators given in Ref. 62.

In order to track the magnetism, we measure the spin correlation function $C_s(x, y, z) = \langle S(x, y, z) \cdot S(y, z, x) \rangle$, the square of the $(\pi, \pi, \pi)$ staggered moment

$$\langle \hat{m}_s^2 \rangle = \frac{1}{L^3} \sum_{x,y,z=1}^L C(x, y, z)(-1)^{(x+y+z)}$$

(4)

and $U = 1 - 3 \langle \hat{m}_s^4 \rangle / 5 \langle \hat{m}_s^2 \rangle^2$, the corresponding Binder cumulant. Within our simulations, the appearance of long-range antiferromagnetic correlations is signalled by the proliferation of system-spanning loops. In terms of our update algorithm, we expect Néel ordering to coincide with the worm head and tail (i.e., the end-points of the evolving open string that serves as the Monte Carlo walker) becoming deconfined and thus free to circumnavigate the periodic lattice independently. With that in mind, we also compute $\langle W^2 \rangle = \langle W_x^2 \rangle + \langle W_y^2 \rangle + \langle W_z^2 \rangle$, the average of the squared winding number of the worm path, summed over each of the three orthogonal directions.

As shown in Fig. 2, we observe a continuous transition from the easy-plane spin liquid to the Néel phase at $a_1 \approx 0.22$ and from the Néel phase to the easy-axis spin liquid at $a_2 \approx 3.9$. We estimate the critical points and exponents of the thermodynamic system from finite-size simulations on the $L^3$ cubic lattice, performed for increasing values of the linear size up to $L = 48$. In our analysis, we assume the conventional, leading-order scaling form for the staggered magnetization:

$$\langle n_s^{2k} \rangle = L^{-2k\beta/\nu} \mathcal{M}_{k\nu}([a - a_n] L^{1/\nu_s})$$

(5)

Furthermore, we suppose that the Binder cumulant and (by analogy) our winding measurement scale according to $U = \mathcal{U}_n([a - a_n] L^{1/\nu_s})$ and $\langle W^2 \rangle = \mathcal{W}_n([a - a_n] L^{1/\nu_s})$. Here, $a_n$ is
L simulations sizes (tilde marks the corresponding value extracted from the wind-
a

...a stand-in for one of the critical anisotropies \( a_1 \) or \( a_2 \). The tilde marks the corresponding value extracted from the winding data alone.

We make use of measurements from the largest three simulations sizes \( L = 32, 40, 48 \) to determine the critical anisotropies and critical exponents. We bootstrap [63] the underlying data and apply the fitting procedure to each resampled set in order to establish the spread. The resulting values with error estimates are listed in Table I. Note that the critical anisotropies extracted (independently) from the magnetic and winding number data disagree slightly for the first phase transition: \( a_1 \) and \( \tilde{a}_1 \) differ by about 4%. Nonetheless, it is likely

\[
\begin{array}{cccccc}
 n & a_n & v_n & \beta_n & \tilde{a}_n & \mu_n \\
 1 & 0.2157(4) & 0.768(3) & 0.85(1) & 0.2240(2) & 1.00(2) \\
 2 & 3.944(5) & 0.764(7) & 0.65(2) & 3.954(3) & 0.98(2) \\
\end{array}
\]

TABLE I. The critical points and exponents extrapolated from a finite-size scaling analysis of the simulation data for \( L = 32, 40, 48 \).

that \( a_n = \tilde{a}_n \) for both \( n = 1 \) and \( n = 2 \) and that our analysis simply underestimates the systematic error that accrues from neglecting subleading corrections to the scaling form.

The correlation length exponents at the opposite edges of the Néel-ordered region, \( v_1 \) and \( v_2 \), are consistent with one another, but the large difference between the magnetization exponents, \( \beta_1 \) and \( \beta_2 \), suggests that the two transitions are in different universality classes. A deconfinement transition is evident in the dynamics of the worm, with an (algorithm-
dependent) exponent that appears to be exactly \( \mu_1 = \mu_2 = 1 \).

Finally, we also consider spatially resolved measurements of the spin correlations \( C_s(x,y,z) \) and of the correlations

\[
C_s(x,y,z) = \langle P(0,0,0)P(x,y,z) \rangle - \langle P(0,0,0) \rangle \langle P(x,y,z) \rangle \tag{6}
\]

between \( z \)-directed valence bonds, as detected by the singlet projection operator \( P(x,y,z) = 1/4 - S(x,y,z) \cdot S(x,y,z+1) \). When \( 0 < a < a_1 \), we think of the system as consisting of \( L \) stacked copies of the U(1) spin liquid, weakly coupled. In

- FIG. 2. Various magnetization order parameters as a function of the anisotropy \( a \) on cubic lattices of linear size \( L = 24, 32, 40, 48 \). The quantities shown are (a) the square of the staggered magnetic moment, (b) the Binder cumulant, and (c) the worm winding order parameter.---We have investigated a family of positive-
definite, short-range RVB wave functions on a layered cubic lattice, where a controllable anisotropy allows us to interpolate between three points that are effectively 1D (\( a = \infty \), 2D (\( a = 0 \), and 3D (\( a = 1 \)). The phase diagram contains three continuous quantum phase transitions at critical points \( a_1 \approx 0.22, a_2 \approx 3.9, \) and \( a_3 \approx 10 \).
Alternating with the Néel antiferromagnet ($a_1 < a < a_2$) and the valence bond crystal ($a > a_3$) are two phases in which all long-range order is extinguished. The first is an easy-plane quantum spin liquid state ($0 < a < a_1$) that has short-range spin correlations but critical bond correlations. The second is an easy-axis spin liquid ($a_2 < a < a_3$) that is short-ranged with respect to both spins and bonds. The existence of this state is surprising, because its wave function is built from exclusively bipartite valence bonds (only connecting sites in opposite sublattices) and has a trivial Marshall sign structure [64, 65]—a state of affairs that usually leads to critical bond correlations.

There is some possibility that a cubic RVB state of the kind we describe could be realized in ultracold atomic gases in optical lattices [66]. Indeed, proof-of-concept realizations of short-range RVB states on a single, four-site plaquette [67, 68] have been achieved. Recently, even more elaborate short-range bond states have been demonstrated for fermionic cold atoms in a cubic lattice laser trap with the same anisotropy we consider here [69].

We do not have a good intuition for what kind of spin model might have this class of wave function as its ground state, but we imagine it must be a highly frustrated one. Models on the cubic lattice with competing, nonfrustrating interactions strong enough to kill the antiferromagnetism seem invariably to result in crystalline ground states [70]. Note that we make the distinction between frustration at the level of the model and frustration at the level of the wavefunction. The latter is simply a statement about a lack of bipartiteness and the impossibility of choosing bond amplitudes [such as Eq. (1)] that are real-valued and nonnegative.

There are some interesting future directions to consider. We expect the gapped RVB liquid to be a topological phase. Hence, its wave function should exhibit topological entanglement entropy and a degeneracy that depends on the genus of the lattice [71–73]. We also expect there to be topological invariants under local updates of the valence bond configurations [74], and so it should be straightforward to measure properties specific to each topological sector. It might also be interesting to extend our calculations to product states of SU($N$) singlets [75], in which case the loop fugacity would scale up with $N$. A likely outcome, as $N$ is increased from 2, is that the Néel ordered region would shrink. It would be worth checking to see if we are ever left with a direct transition between the two liquid states.

We emphasize that our results differ from the work reported in Ref. 76. Our wave function describes $S = 1/2$ spin degrees of freedom living in three spatial dimensions.

**Acknowledgements.**—This work was supported by a Discovery grant from NSERC of Canada. Simulations were performed on the computing facilities of WestGrid and on a local cluster generously made available to us by John P. Davis.

* kbeach@ualberta.ca

[1] L. Balents, Nature (London) 464, 199 (2010).
[2] N. F. Mott, Proc. Phys. Soc. A 62, 416 (1949).
[3] G. Baskaran, Z. Zou, and P. W. Anderson, Solid State Comm. 63, 973 (1987).
[4] P. W. Anderson, Science 235, 1196 (1987).
[5] I. Affleck and J. B. Marston, Phys. Rev. B 37, 3774 (1988).
