Hardcore bosons on checkerboard lattices near half filling: Geometric frustration, vanishing charge order, and a fractional phase

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We study a spinless hardcore boson model on checkerboard lattices by Green function Monte Carlo method. At half filling, the ground state energy is obtained up to a 28×28 lattice and extrapolated to infinite size; the staggered pseudospin magnetization is found to vanish in the thermodynamic limit. Thus the (π, π) charge order is absent in this system. Away from half filling, two defects induced by each hole (particle) may carry fractional charge $(\pm e/2)$. For the one hole case, we study how the defect-defect correlation changes with t/J, which is the ratio between the hopping integral and cyclic exchange, and is equal to $V/2t$ when $V \gg t$. Moreover, we argue that these fractional defects may propagate independently when the concentration of holes (or defects) is large enough.

I. INTRODUCTION

During the past decade materials experiencing geometric frustration has been a topic of much interest, both on experimental and theoretical sides.[1] The rich behavior in such systems is due to a large ground-state degeneracy, which renders them highly unstable to perturbations. A well known 3D frustrated structure is the pyrochlore lattice which is the backbone structure shared by many physically realistic materials. One may think of checkerboard lattices as a 2D analog of pyrochlore lattices. This is the reason why a checkerboard lattice is often considered in theoretical studies instead of the more realistic pyrochlore structure.

Up to now most work has been devoted to an understanding of the magnetic properties of such frustrated lattices, while the charge degrees of freedom is waiting for more attention. Actually, the charge degrees of freedom may exhibit fascinating physical properties in frustrated systems such as pyrochlore and checkerboard lattices.[2,3] Recently, one of the fascinating predictions on charge degrees of freedom has been proposed: say, the geometric frustration present on the pyrochlore lattices may give rise to fractional charges in two or three dimensions based on strong nearest neighbor repulsion close to half-integer filling. This proposal comes from the so-called "tetrahedron rule" which is first stated explicitly by Anderson[4] to explain the metal-insulator transition in the spinel Fe_3O_4,[5] where the observed entropy reduction is much less than expected from electrons without the strong short range correlation. Both pyrochlore and checkerboard lattices are made up of corner sharing units which are tetrahedron or crisscrossed plaquettes. The nearest neighbor repulsion will be minimized when each of the corner sharing units contains only two particles. If the kinetic energy can be neglected, the system will possess a large ground-state degeneracy, $(4/3)^{(3N/4)}$ for checkerboard lattices.[6] Taking (putting) one particle from (into) the system, two tetrahedra (plaquettes) will emerge, each of them contains an extra particle (or hole). We will call this kind of tetrahedra (plaquettes) "defects." A demonstration of the configuration subject to "tetrahedron rule" and the formation

of "defects" is shown in Fig. 1. Provided that the perturbation such as kinetic energy can be neglected, these two defects induced by one particle (hole) will propagate independently. If a particle carries charge e, one of the defects will carry charge $e/2$. Thus, such defects are "fractional." Note that the above argument is valid for both hardcore bosons and fermions as well as spinless and spin-S system. On the other hand, current laser cooling and cold atom technique make it possible to realize these systems on some artificial optical lattices.[7]

However, the virtual processes induced by kinetic energy will lift the high degeneracy and lead to different ground states. Because of high degeneracy, any small perturbation may change the low energy states violently. To study this kind of quantum effects in spinless fermionic system on checkerboard lattices, Ref. 3 used exact diagonalization (ED) technique up to 32 sites. As a related problem to hardcore bosons, *XXZ* Heisenberg model in the Ising limit was studied by ED on small size lattices too.[8] The ground state was identified as a nonmagnetic state of resonating square plaquettes. Due to the limit of small size, there is lack of direct evidence to address the issue of confinement or deconfinement.

In this paper, we will study spinless hardcore bosons by the Green function Monte Carlo (GFMC) method which can give precise results on larger lattices (up to 28×28). The ground state energy is obtained with high accuracy and defect-defect correlation is present, which makes sense only on larger lattices. Also, we will inspect the issue of charge order. The outline of the paper follows. In Sec. II, we introduce the extended Hubbard model and derive its effective Hamiltonian subjected to tetrahedron rule in the strong repulsion limit. The relations between this model and *XXZ* Heisenberg model is discussed. In Sec. III, a brief discussion of GFMC method is present, we also compare some results on small lattices with exact diagonalization. Section IV contains the main numerical results. The final section is devoted to conclusions.

II. THE EFFECTIVE HAMILTONIAN

We consider strong on-site repulsion U and nearest-neighbor repulsion V between spinless hardcore bosons on
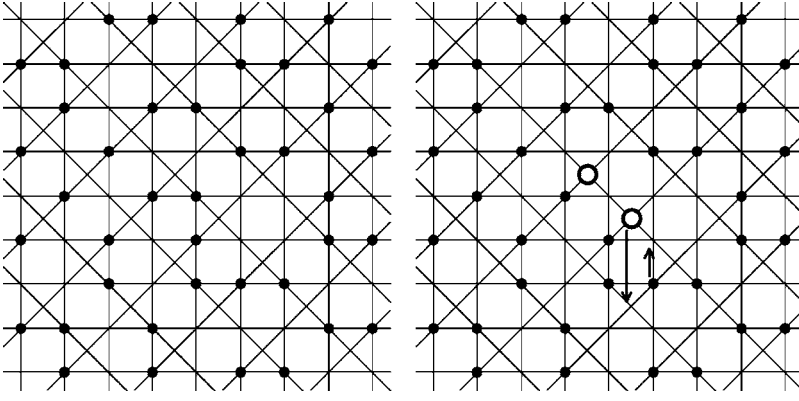
FIG. 1. Left: A typical configuration subject to the tetrahedron rule at half filling. Right: Two defects induced by one hole may be considered as pointlike fractional excitations, whose motion is driven by hopping Hamiltonian.

checkerboard lattices, where the intrasite interaction has been assumed to be a higher energy scale and ignored (see Fig. 1). Then the extended Hubbard Hamiltonian is of the form

$$H = -t\sum_{\langle ij \rangle} (b_i^\dagger b_j + \text{H.c.}) + V\sum_{\langle ij \rangle} n_i n_j + U\sum_i n_i^2, \qquad (1)$$

where $b_i(b_i^\dagger)$ denote annihilation (creation) operators at site i, $n_i = b_i^\dagger b_i$, and $\langle ij \rangle$ refers to a pair of nearest neighbor. We shall assume that $U \gg V, t$ is large enough to ensure the non-double occupancy condition, only empty and singly occupied sites ar considered. Then we will focus on the strong interaction regime $V \gg t > 0$ around half filling where the average occupation number per site is $\langle n_i \rangle = 1/2$, more precisely, half of the sites are occupied and the other half of the sites are empty. In that case the tetrahedron rule is imposed by the strong nearest neighbor repulsion,

$$\sum_{i \in \boxtimes} n_i = 2, \qquad (2)$$

where i belongs to a same crisscrossed plaquette. In this way, the intersite repulsion will be minimized. Thus, in the limit $V \gg t$, we obtain the effective low energy Hamiltonian in the subspace restricted by the condition (2),

$$H_J = -J\sum_{\square} b_{i_1}^\dagger b_{i_2} b_{i_3}^\dagger b_{i_4} + \text{H.c.}, \qquad (3)$$

where $J = 2t^2/V$, and $\square$ denotes a four-site loop without crisscross, formed by sites $i_1 i_2 i_3 i_4$. Away from half filling, we consider the hole doping only, due to the particle-hole symmetry at half-filling. Then the tetrahedron rule has to be modified as the following,

$$\sum_{i \in \boxtimes} n_i \leq 2, \qquad (4)$$

and the effective Hamiltonian in this subspace is given by

$$H_{eff} = -t\sum_{\langle ij \rangle} (b_i^\dagger b_j + \text{H.c.}) + H_J. \qquad (5)$$

It means that if we take one particle from the half filling system, there will emerge two defects where $\Sigma_{i \in \boxtimes} n_i = 1$ and $\Sigma_{i \in \boxtimes} n_i = 2$ elsewhere. The hopping terms (proportional to t) of (5) will change the defects position but H_J will not. Although $t/J = V/2t \gg 1/2$, we can generally consider an effective model in which the ratio t/J ranges from zero to positive

infinity. As pointed out in the former references,[2,3,8] if the virtual process at order J can be neglected, these two defects will propagate as independent fractional objects. However, quantum effects such as the cyclic exchange of the order of J may or may not confine these fractional defects.

A hardcore boson model can be mapped onto a spin-1/2 model in general. The occupation number n_i corresponds to the spin component $S_i^z + \frac{1}{2}$, and creation (annihilation) operators $b_i^\dagger(b_i)$ correspond to $S_i^+(S_i^-)$. The according spin-1/2 model of (1) is an *XXZ* Heisenberg model. It is noted that this *XXZ* Hamiltonian is *different* from an usual *XXZ* model by the *minus* sign before spin flip terms, which *cannot* be mapped to a positive one by an unitary transformation on a *frustrated* lattices. The related effective Hamiltonian in the Ising limit is a cyclic exchange which was studied by Shannon *et al.*[8] through ED on small lattices. The authors argued that spinons (defects) in the above *XXZ* model will be confined due to the ground state correlation.[9] In this paper we confirm this argument through calculating the defect-defect correlation directly by GFMC method up to 24×24 lattices which are large enough to suppress the size effect. If only one hole is present the two induced defects will be confined together. However, as concentration of holes and the ratio $t/J = V/2t$ increase these defects may behave as independent pointlike objects.

III. GROUND STATE WAVE FUNCTION AND GFMC APPROACH

Note that both Hamiltonians (3) and (5) have only nonpositive off-diagonal matrix elements in the Fock representation $|n_{i1} n_{i2} \cdots \rangle$. It implies that the many-body boson wave function can be chosen to be non-negative everywhere in the ground state. This property of the wave function will be crucial in applying the GFMC method to this system.

GFMC is a general scheme for finding the lowest eigenvalue of an operator. A trial eigenvector is subjected to a time evolution whose effect is to enhance those components of the solution with the lower eigenvalues of the operator. The ground state energy can be obtained as a mixed estimate. We choose the trial state $|\psi_T\rangle$ as an equal amplitude superposition in an invariant subspace of Hamiltonian which contains the ground state. For a local operator O whose matrix elements satisfy $\langle R|O|R'\rangle = \delta(R - R')O(R)$, such as densitydensity correlation function, which does not share eigen-

TABLE I. The ground state energy E/J at half filling.

Size	4×4	4×6	6×6
ED	−4.47214	−6.46995	−9.47393
GFMC	−4.4717(12)	−6.4695(19)	−9.4739(22)

states with the Hamiltonian, we use the "forward-walking" technique, well known in many-body theory,[10–14] to measure the expectation values. In this way, at the nth step of iteration, $O(R_n^i)$ is evaluated for each configuration R_n^i in the ensemble $\{R_n\}$. For the remaining m steps of the random walk, a record is kept of the configuration of $\{R_n^i\}$ from which each subsequent ensemble member has evolved. At the end of the $(m+n)$th step, $\langle O \rangle$ is evaluated by forming the weighted summation[11]

$$\langle O \rangle = \frac{\sum_j \psi_T(R_{m+n}^j) O(R_n^{i(j)})}{\sum_j \psi_T(R_{m+n}^j)},$$

where the notation $i(j)$ indicates that i is the progenitor of j. In this paper, we will calculate density-density correlation and defect-defect correlation, both of them are local operators and this method can be applied.

A. Comparison with exact diagonalization

GFMC is a very accurate method to obtain the ground state and low-lying excited state property of many-body interacting systems. In the past it has been applied successfully to the ground state properties of helium, interacting electron gas, small molecules, Heisenberg model on 2D square lattices, and lattice gauge theories.[10,11,15–17] To check the precision of the GFMC method in our system, we will compare some results from the ED with those from GFMC at small lattices with periodic boundary condition (PBC). Hereafter we will use PBC in this paper.

The ground state energy at half filling and at one hole doped lattice are given in Tables I and II, respectively. The digits in the bracket are statistics error bars.

Density-density correlation $D(i,j)=D(i-j)\equiv\langle n_i n_j\rangle-\frac{1}{4}$ at half filling on 6×6 lattice have been examined too. The results from ED and GFMC are present in Tables III and IV, respectively. Each of the two tables contains a matrix $D(i_x,i_y)$ whose column and row indices $i_x,i_y=0,1,2,3$ correspond to the displacements along two directions, respectively.

TABLE II. The ground state energy E/J of one hole doped 4×4 lattice.

t/J	ED	GFMC
0.02	−3.52850	−3.5290(9)
0.2	−4.91215	−4.9119(16)
2.0	−22.92923	−22.9310(16)

TABLE III. Density-density correlatoin $D(i_x,i_y)$ on 6×6 lattice calculated by ED.

0.25	−0.13170	0.01933	−0.02527
−0.13170	0.07083	−0.01590	0.02185
0.01933	−0.01590	0.01584	−0.01920
−0.02527	0.02185	−0.01920	0.01998

The staggered pseudospin magnetization (7) on a half filled 6×6 lattice given by GFMC is 0.1038(8), while the result from ED is 0.10417.

From the above, one sees that GFMC algorithm is an effective method to deal with spinless hardcore bosons on checkerboard lattices.

IV. RESULTS

Simulations were carried out for $L \times L$ lattices up to $L =28$ ($L=24$ for correlations). Time steps from 0.003 to 0.05 were used, depending on lattice size and the ratio t/J; here we set $J=1$. In practice, we use about $100L^2$ generations to reach the ground state distribution, then iterate about $1000L^2$ generations to measure the physical quantities. To avoid self-correlation and improve the efficiency, we make an expectation value measurement only after every L^2 iterations. It is not advantageous to perform measurements at still larger intervals, since the measured generations are already nearly statistically independent. For ergodicity we should control the population of random walkers large enough. Otherwise they will be trapped in a higher energy state instead of the ground state. According to our experience, keeping L^3 random walkers in each generation is enough to ensure ergodicity on $L \times L$ lattice.

A. Half filling: ground state energy and staggered pseudospin magnetization

First, we calculate the ground state energy at half filling which may serve as a standard to compare with other analytical or numerical study in this system. Figure 2 shows ground state energies per site up to 28×28 lattice. We extrapolated it to the thermodynamic limit through the following formula,

$$\frac{E(L)}{J} = E_0 + \frac{E_1}{L} + \frac{E_2}{L^2} + O\left(\frac{1}{L^3}\right), \tag{6}$$

where $E_0=-0.2591(4)$, $E_1=0.008(9)$, $E_2=-0.12(6)$, and L is the linear size of lattices.

TABLE IV. Density-density correlatoin $D(i_x,i_y)$ on 6×6 lattice calculated by GFMC.

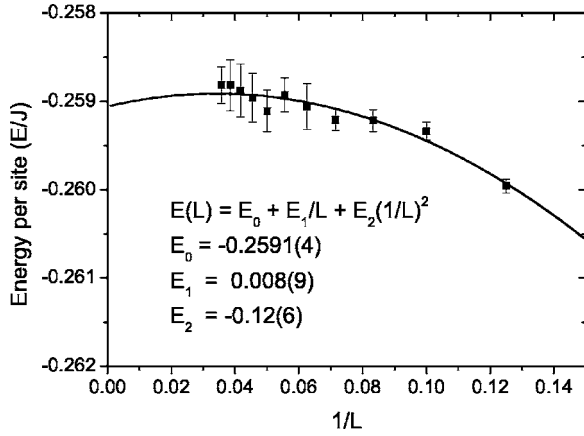| 0.25	−0.1319(7)	0.0196(12)	−0.0254(11)
−0.1319(7)	0.0711(9)	−0.0161(10)	0.0220(8)
0.0196(12)	−0.0161(10)	0.0160(10)	−0.0193(7)
−0.0254(11)	0.0220(8)	−0.0193(7)	0.0200(7)

FIG. 2. Ground state energy per site at half filling and extrapolation to thermodynamic limit. Values are shown for $L \times L$ lattices, $L = 8, 10, \ldots, 28$.
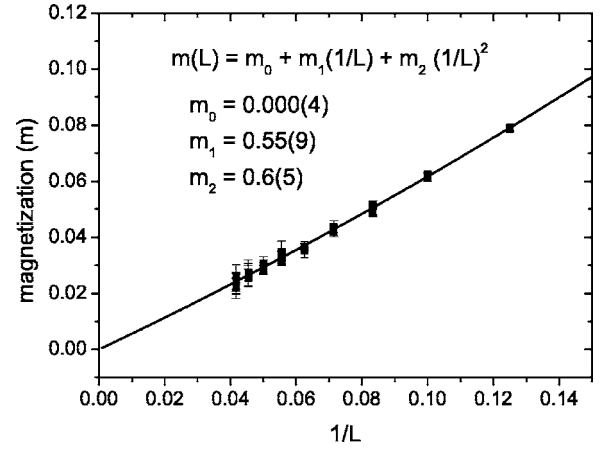

FIG. 3. Staggered pseudospin magnetization, Eq. (7), on finite size lattices at half filling and extrapolation to thermodynamic limit. Values are shown for $L \times L$ lattices, $L = 8, 10, \ldots, 24$. Zero result for m_0 means charge order is absent here.

Another issue that we shall address is whether there exists charge density order in the thermodynamic limit. Although density-density correlation $D(i,j)$ exhibits (π, π) charge-modulation patterns on small lattices with PBC, as it behaves in fermionic system,[3] it may vanish in the thermodynamic limit. To answer this question, we introduce the staggered pseudospin magnetization m, which is defined as

$$m = \frac{1}{2N} \sqrt{\left\langle \left(\sum_i (-1)^i n_i \right)^2 \right\rangle},\tag{7}$$

where N is the number of sites on checkerboard lattices. The staggered pseudospin magnetization has its name because if we map a hardcore boson model to a spin-1/2 model this quantity is nothing but the staggered magnetization. If the system is charge ordered, m will not vanish in the thermodynamic limit. By "forward walking" technique, we calculate the pseudospin magnetization up to 24×24 lattice and extrapolated it to the thermodynamic limit by the following formula,

$$m(L) = m_0 + \frac{m_1}{L} + \frac{m_2}{L^2} + O\left(\frac{1}{L^3}\right),\tag{8}$$

with $m_0 = 0.000(4)$, $m_1 = 0.55(9)$ and $m_2 = 0.6(5)$. As shown in Fig. 3, it results in a vanishing charge order at (π, π) in the thermodynamic limit. This result agrees with the claim of nonmagnetic phase in Ref. 8. Similar conclusion was found for spinless fermion.[3]

B. One hole doping: ground state energy and defect-defect correlation

One of the central questions is whether or not the defects will be confined by the Hamiltonian (5). To answer this question, we calculate the ground state energy at one hole doping and $t = 0$ at first. When $t = 0$, the two defects cannot move away by hopping terms, so that we should calculate the ground state energy with fixed defects. Figure 4 shows the numerical results for $L \times L$ lattice, $L = 16, 20, 24$. It turns out that the ground state energy will increase linearly as the dis-

tance between two defects increases. The distance between two defects is defined as the distance from one plaquette center to another in units of the lattice constant a, say, it is $\sqrt{2}$ for two nearest neighbor plaquettes.

Even though we turn on the hopping term, the upper bound of the gained kinetic energy is less than $2zt$, $z = 6$ for checkerboard lattices is the coordination number. Since the confinement potential increases linearly with the distance between the two defects, the two defects will be confined with an average distance R.

Now we turn to $t > 0$ case and study how the defect-defect correlation will change as the ratio t/J varies. The defect-defect correlation $C(p,q) = C(p-q)$ can be defined as

$$C(p,q) = \left\langle \left(2 - \sum_{i \epsilon p} n_i \right) \left(2 - \sum_{j \epsilon q} n_j \right) \right\rangle,\tag{9}$$

where p, q denote the crisscrossed plaquettes. The numerical result is present in Fig. 5. One notices that when t/J is small, the two defects will be linearly bounded. As t/J increasing,
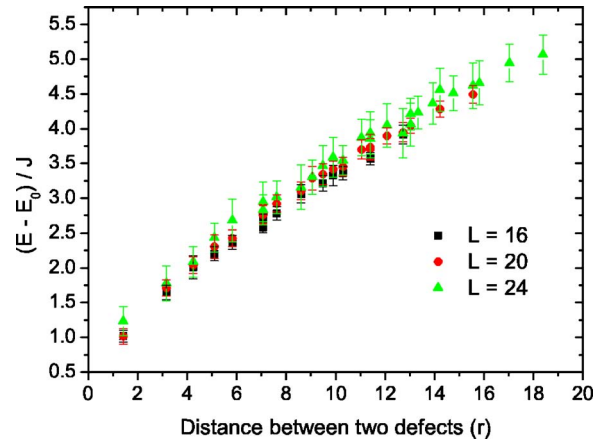

FIG. 4. (Color online) Cyclic exchange energy H_J will increase linearly when the distance between two defects increases in the case of $t = 0$. Here E_0 is the ground state energy at half filling.
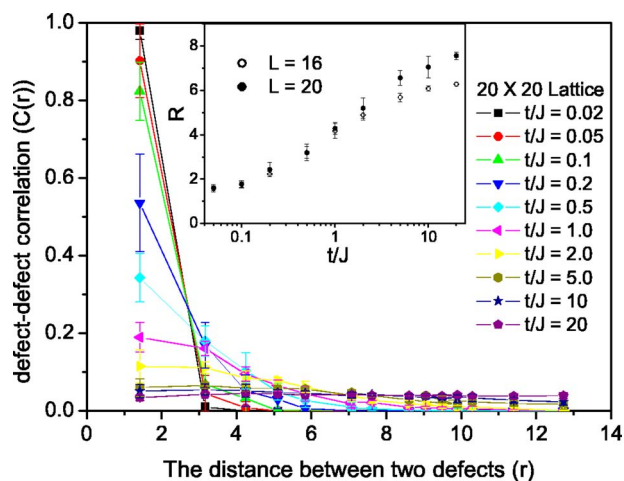
FIG. 5. (Color online) The defect-defect correlation on 20×20 lattice. As the ratio t/J increases, it will become more and more uniform. Inset: The average distance R between the two defects increases monotonically with t/J. The saturation is due to the size effect; for a homogeneous distribution, the maximum R will be 0.3826L. Solid dots are plotted for 20×20 lattice and circles for 16×16 lattice.

the defect-defect correlation will be more and more uniform in a finite size lattice with periodic boundary condition. Hence we expect that the average distance $R(t/J)$ between the two defects in the infinite lattice will increase monotonically with t/J. However, as shown in the inset of Fig. 5, it will reach the saturation on a finite lattice due to the size effect, the maximum will be $[\sqrt{2}+\ln(1+\sqrt{2})]L/6 = 0.3826L$ on $L \times L$ lattice for a homogeneous distribution.

From the above we can conclude that the cyclic exchange H_J provides a linear confinement potential between two defects but the hopping term tends to increase this average distance. If the concentration of defects $\delta = 2N_{hole}/N$ is large enough as to satisfy

$$\delta \geqslant \frac{a^2}{\pi R^2(t/J)}, \tag{10}$$

when the average area occupied by one defect, $Na^2/(2N_{hole})$, is smaller than the confinement area, πR^2, the defects will

have a homogeneous distribution on the infinity lattice instead of to be confined together in couples. It implies that it is possible to treat these defects as independent pointlike excitations.

V. CONCLUSION

In summary, we apply the GFMC algorithm to a spinless hardcore boson model with strong nearest neighbor repulsion on checkerboard lattices near half filling. To avoid any variational bias from the trial wave function, a "forward walking" technique has been used to compute density-density correlation and defect-defect correlations. At half filling, the ground state energy is obtained and extrapolated to infinity size. It turns out that the staggered pseudospin magnetization vanishes in the thermodynamic limit, thus charge order at (π, π) is absent in this system. Away from half filling, two defects induced by each hole (particle) may carry fractional charge ($\pm e/2$). In the case of one hole doping, we study how the defect-defect correlation changes with the parameter t/J, which equals to $V/2t$ when $V \gg t$. The cyclic exchange is found to provide a linear confinement potential between two defects, while the hopping term as kinetic energy is tending to separate them away. Moreover, we argue that these defects may propagate independently when the concentration of holes (or defects) is large enough.

Finally, confinement (deconfinement) is a subtle issue, although we have presented some evidences for the possibility of the existence of defects which may carry fractional charge ($\pm e/2$) in this system, a lots of work remain to be done. This issue should be treated by other analytical and numerical methods. Especially, the effective field theories for the present system are expected to describe the ground state and low lying excitations well, thus a confident conclusion for confinement or deconfinement will be achieved.

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[1] *Proceedings of the Conference on Highly Frustrated Magnetism, 2003*, August 2003, Grenoble, France [special issue, J. Phys.: Condens. Matter **16**, 11 (2004)].

[2] P. Fulde, K. Penc, and N. Shannon, Ann. Phys. **11**, 892 (2002).

[3] E. Runge and P. Fulde, Phys. Rev. B **70**, 245113 (2004).

[4] P. W. Anderson, Phys. Rev. **102**, 1008 (1956).

[5] E. J. W. Verwey and P. W. Haaymann, Physica (Amsterdam) **8**, 979 (1941).

[6] E. Lieb, Phys. Rev. Lett. **18**, 692 (1967).

[7] For a review on optical lattices, see D. Jaksch and P. Zoller, Ann.

Phys. (N.Y.) **315**, 52 (2005).

[8] N. Shannon, G. Misguich, and K. Penc, Phys. Rev. B **69**, 220403(R) (2004).

[9] Although the original *XXZ* Hamiltonian and cyclic spin exchange may confine spinons, adding a term by hand, they can be tuned to a deconfined phase through a RK point; see details in Ref. 8.

[10] D. M. Ceperley and M. H. Kalos, in *Monte Carlo Methods in Statistical Mechanics*, edited by K. Binder (Springer-Verlag, New York, 1979).

[11] S. A. Chin, J. W. Negele, and S. E. Koonin, Ann. Phys. (N.Y.) **157**, 140 (1984).

[12] M. H. Kalos, J. Comput. Phys. **1**, 257 (1966).

[13] K. S. Liu, M. H. Kalos, and G. V. Chester, Phys. Rev. B **10**, 303 (1974).

[14] P. A. Whitlock, D. M. Ceperley, G. V. Chester, and M. H. Kalos, Phys. Rev. B **19**, 5598 (1979).

[15] M. Gross and E. Sáncheze-Velasco, Phys. Rev. B **39**, 2484 (1989).

[16] J. Carlson, Phys. Rev. B **40**, 846 (1989).

[17] N. Trivedi and D. M. Ceperley, Phys. Rev. B **41**, 4552 (1990).