Hardcore bosons on checkerboard lattices near half filling: geometric frustration, vanishing charge order and 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 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 (±e/2). For 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, equals to V/2t when V ≫ t. Moreover, we argue that these fractional defects may propagate independently when the concentration of holes (or defects) is large enough.

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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 of 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 firstly stated explicitly by Anderson [4] to explain the metal-insulator transition in the spinel Fe₃O₄ [4], 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)^N/4 for checkerboard lattices [5]. 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 [6]. 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. [8] 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 [9]. The ground state was identified as a non-magnetic 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 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 section 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 section 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 checkerboard lattices, where the intra-site interaction has been assumed to be a higher energy scale and ignored. Then the extended Hubbard Hamiltonian is of the form

$$H = -t \sum_{\langle ij \rangle} (b_i^\dagger b_j + h.c.) + V \sum_{\langle ij \rangle} n_in_j + U \sum_i n_i^2,$$  \eqno(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 neighbors. We shall assume that $U \gg V, t$ is large enough to ensure the non-double occupancy condition, only empty and singly occupied sites are 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,

$$\sum_{i \in \Box} n_i = 2,$$ \eqno(2)$$

where $i$ belongs to a same crisscrossed plaquette. In this way, the inter-site 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 \cite{2},

$$H_f = -J \sum_{\square} b_{i_1}^\dagger b_{i_2}^\dagger b_{i_3} b_{i_4} + h.c.,$$ \eqno(3)$$

where $J = 2t^2/V$, and $\square$ denotes a four-site loop without crisscross, formed by sites $i_1i_2i_3i_4$. 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,

$$\sum_{i \in \Box} n_i \leq 2,$$ \eqno(4)$$

and the effective Hamiltonian in this subspace is given by

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

It means that if we take one particle from the half filling system, there will emerge two defects where $\sum_{i \in \Box} n_i = 1$ and $\sum_{i \notin \Box} n_i = 2$ elsewhere. The hopping terms (proportional to $t$) of (3) will change the defects position but $H_f$ 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 \cite{2, 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 confuse 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 $S_i^+ + \frac{1}{2}$, 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 can not be mapped to a positive one by an unitary transformation on a frustrated lattice. The related effective Hamiltonian in the Ising limit is a cyclic exchange which was studied by Shannon \cite{8} through ED on small lattices. The authors argued that spinons (defects) in the above XXZ model will respond to the spin component $S_i^+$ and $S_i^-$, and motion is driven by the hopping Hamiltonian.

III. GROUND STATE WAVE FUNCTION AND GFMC APPROACH

Note that both Hamiltonians (4) and (5) have only non-positive off-diagonal matrix elements in the Fock representation $|n_{11}n_{12} \cdots \rangle$. It implies that the many-body boson wave function can be chosen to be non-negative everywhere in the ground state. This prop-
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 density-density correlation function, which does not share eigenstates with the Hamiltonian, we use the "forward-walking" technique, well known in many-body theory [10, 11, 12, 13, 14], to measure the expectation values. In this way, at the \( n \)th step of iteration, \( O (R_n) \) is evaluated for each configuration \( R_n \) in the ensemble \( \{R_n\} \). For the remaining \( m \) steps of the random walk, a record is kept of the configuration of \( \{R_n\} \) 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 \([11]\)

\[
\langle O \rangle = \frac{\sum_i \psi_T \left( R_{m+n}^j \right) O \left( R_{n}^{(j)} \right) \sum_j \psi_T \left( R_{m+n}^j \right)}{\sum_j \psi_T \left( R_{m+n}^j \right)},
\]

where the notation \( i \langle j \rangle \) 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, 16, 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.

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

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       | -22.29225 | -22.9310(16) |

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 Table 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 III: Density-density correlaton \( D(i_x, i_y) \) on 6×6 lattice calculated by ED.

| \( i_x \) | \( i_y \) | \( d(i_x, i_y) \) |
|----------|----------|-----------------|
| 0.25     | -0.13170 | 0.01933         |
| -0.13170 | 0.07083  | -0.01509        |
| 0.01933  | -0.01590 | 0.01584         |
| -0.02527 | 0.02185  | -0.01920        |
| -0.01920 | 0.01998  |                |

TABLE IV: Density-density correlaton \( D(i_x, i_y) \) on 6×6 lattice calculated by GFMC.

| \( i_x \) | \( i_y \) | \( d(i_x, i_y) \) |
|----------|----------|-----------------|
| 0.25     | -0.1319(7) | 0.0196(12)       |
| -0.1319(7) | 0.0711(9)  | -0.0161(10)      |
| 0.0196(12) | -0.0161(10) | 0.0160(10)       |
| -0.0254(11) | 0.0220(8)  | -0.0193(7)       |
| -0.0193(7) | 0.0200(7)  |                |

The staggered pseudospin magnetization \([11]\) 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 100\( L^2 \) generations to reach the ground state distribution, then iterate about 1000\( L^2 \) 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

Firstly, 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. Fig. 2 shows ground state energies per site up to $28 \times 28$ lattice. We extrapolated it to the thermodynamic limit through the following formula,

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

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

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 $(\pi, \pi)$ 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

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

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 $24 \times 24$ lattice and extrapolated it to the thermodynamic limit by the following formula,

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

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 $(\pi, \pi)$ in the thermodynamic limit. This result agrees with the claim of non-magnetic phase in Ref. [8]. Similar conclusion was found for spinless fermion [3].

![FIG. 2: Ground state energy per site at half filling and extrapolation to thermodynamic limit. Values are shown for $L \times L$ lattices, $L = 8, 10, \ldots, 28$.](image1)

![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, $L = 8, 10, \ldots, 28$. Zero result for $m_0$ means charge order is absent here.](image2)

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 [9]. 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 can not move away by hopping terms, so that we should calculate the ground state energy with fixed defects. Fig. 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 distance 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:

\[
C(p, q) = \left\langle (2 - \sum_{ip} n_i)(2 - \sum_{jq} n_j) \right\rangle, \tag{9}
\]

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, 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 \(\delta = 2N_{\text{hole}}/N\) is large enough as to satisfy

\[
\delta \geq \frac{a^2}{\pi R^2(t/J)}, \tag{10}
\]

when the average area occupied by one defect, \(N\alpha^2/(2N_{\text{hole}})\), is smaller than the confinement area, \(\pi R^2\), the defects will have a homogeneous distribution on the infinite lattice instead of to be confined together in couples. It implies that it is possible to treat these defects as independent point like excitations.

\section{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 \((\pi, \pi)\) 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 de-
fects, while the hopping term as kinetic energy is tending
to separate them away. Moreover, we argue that these
defects may propagate independently when the concen-
tration of holes (or defects) is large enough.

Finally, confinement (deconfinement) is a subtle issue,
although we have presented some evidences for the pos-
sibility of the existence of defects which may carry frac-
tional charge ($\pm e/2$) in this system, a lots of work remain
to be done. This issue should be treated by other analyti-
cal 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 con-
fident conclusion for confinement/deconfinement will
be achieved.

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