Bose-Fermi mixture in one-dimensional optical lattices with hard-core interactions

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We study a mixture of \( N_b \) bosons with point hard-core boson-boson interactions and \( N_f \) non-interacting spinless fermions with point hard-core boson-fermion interactions in 1D optical lattice with external harmonic confine potential. Using an extended Jordan-Wigner transformation (JWT) which maps the hard-core Bose-Fermi mixture into two component noninteracting spinless fermions with hard-core interactions between them, we get the ground states of the system. Then we determine in details the one particle density matrix, density profile, momentum distribution, the natural orbitals and their occupations based on the constructed ground state wavefunctions. We also discuss the ground state properties of the system with large but finite interactions which lead to the lift of ground degeneracy. Our results show that, although the total density profile is almost not affected, the distributions for bosons and fermions strongly depend on the relative strengths of boson-boson interactions and boson-fermion interactions.

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I. INTRODUCTION

Recently, strongly interacting gases of bosons in one dimension have been experimentally realized1, 2, 3, by loading a Bose-Einstein condensate into a deep two dimensional optical lattice to create arrays of one-dimensional (1D) atomic systems. The achievement of the Tonks-Girardeau (TG) regime4 in an optical lattice has stimulated extensive theoretical interest in the study of many-body physics of 1D quantum gases5, 6, 7, 8. With the increase in the interaction strength, the 1D Bose gas evolves from a Bose-Einstein condensate to “fermionized” TG9, 10, 11, 12, 13, 14, 15. The microscopic mechanisms of the evolution has been recently studied by both analytical methods10, 11 and various numerical methods12, 13, 14, 15. In the limit of the infinitely repulsive interaction, the many-body state of a TG gas has been shown to correspond to the states of a noninteracting Fermi gas via a Bose-Fermi mapping4. For the lattice model of TG gas, the Hamiltonian in a periodic lattice can be mapped onto the 1D XY model of Lieb, Schulz, and Mattis, which has been extensively studied in the literature16. With an additional confining potential, the lattice TG gas has been studied by means of an exact numerical approach by Rigol and Muramatsu18, 19, 20. Very recently, Girardeau’s Bose-Fermi mapping method has also been generalized to deal with mixtures of multi-component quantum gases21, 22, 23, 24.

On the other hand, mixtures of bosonic and fermionic atoms have been studied extensively as they initially provided a convenient way to achieve degenerate fermionic gas by means of sympathetic cooling25, 26. Due to their rich phase diagram, the Bose-Fermi mixtures have attracted many theoretical studies27, 28, 29, 30, 31, 32, 33, 34, 35, 36, 37, 38, 39, 40, 41, 42, 43. Among those works, particular attention has been paid to the 1D model of mixed bosons and polarized fermions27, 28, 29, 30, 31, 32, 33, 34, 35, 36, 37, 38, 39, 40, 41, 42, 43, in which there are only s-wave scattering for boson-boson and boson-fermion interactions present. While most of these investigations relied on the mean-field approximations or the Luttinger liquid theory, there is rarely exact result except for the homogenous model with equal boson-boson and boson-fermion interactions, which is exactly solved by the Bethe-ansatz method33, 34, 35, 36, 37, 38, 39, 40, 41, 42. However, for a lattice system, there is no exact result even for the lattice correspondence of the integrable continuum Bose-Fermi system44. In this work we mainly study the lattice Bose-Fermi gas in the hard-core limit where both the boson-boson and boson-fermion interactions are infinitely strong. In this limit, we can apply an extended Jordan-Wigner transformation and an exact numerical approach, which can be viewed as an extension of the method by Rigol and Muramatsu18, to treat the hard-core Bose-Fermi mixture exactly. We focus on the ground state properties and analyze the behaviors of the one-particle correlations, the momentum distribution function, the natural orbitals and their occupations. The properties of the system with large but finite interactions are also discussed. Since the interaction can be tuned in principle within a large range of regime by exploiting Fesbach resonance, our results might be experimentally relevant.

The content of the paper is as follows. In the next section we describe the model system first and then the approach used to calculate the ground state one particle density matrix exactly. In Sec. III, we discuss the properties of hard-core Bose-Fermi mixture confined in harmonic traps. In the Sec. IV, we discuss the proper-
ties of the system with large but finite interactions. The paper is concluded in Sec. V.

II. SYSTEM AND METHOD

We consider a mixture of \(N_b\) bosons with point hard-core boson-boson interactions and \(N_f\) noninteracting spinless fermions with point hard-core boson-fermion interactions and assume that the boson and fermion particles have the same masses \(m_b = m_f\), which could be realized by choosing an isotope of a given alkali element. Let \(X_b = (x_{1b}, ..., x_{N_b})\) and \(X_f = (x_{1f}, ..., x_{N_f})\) indicate the boson and fermion coordinates respectively. For the system trapped in the potentials including the optical lattice and an additional harmonic trap, the Hamiltonian of the system is

\[
H = H_B + H_F + H_{BB} + H_{BF}
\]  

with

\[
H_B = \sum_{j=1}^{N_b} -\hbar^2 \frac{\partial^2}{2m_b \partial x_{jb}^2} + V(x_{jb})
\]

\[
H_F = \sum_{j=1}^{N_f} -\hbar^2 \frac{\partial^2}{2m_f \partial x_{jf}^2} + V(x_{jf})
\]

\[
H_{BB} = \frac{g_{BB}}{2} \sum_{i,j}^{N_b} \delta(x_{ib} - x_{jb})
\]

\[
H_{BF} = g_{BF} \sum_{i,j}^{N_b,N_f} \delta(x_{ib} - x_{jf})
\]

where \(g_{BB}, g_{BF} \rightarrow \infty\) under the hard-core condition which means that the many-body wave function \(\Psi(X_b, X_f)\) of the system vanishes at all boson-boson (BB) and boson-fermion (BF) collision points. Explicitly, the potentials take the form

\[
v_{b,f}(x) = V_{b,f}^0 \sin^2(\pi x/a) + \frac{1}{2} m_{b,f} \omega_{b,f}^2 x^2
\]

where \(a\) is the lattice spacing associated with wave vector \(k_L = \pi/a\) of the standing laser light. In this work, we consider only the case with the trap acting on bosons and fermions being the same, i.e., \(v_b(x) = v_f(x) = v(x)\) with \(V_{b,f}^0 = V^0\) and \(\omega_b = \omega_f\).

We use the Wannier function (only consider the lowest Bloch band) of the optical lattice to expand \(\Psi(X_b, X_f)\) and get the second quantized Hamiltonian of \(H\), which is the standard Hubbard model of Bose-Fermi mixture \cite{31} with the from of

\[
H_{Hub} = -i \sum_{i=1}^{L-1} (b_i^\dagger b_{i+1} + f_i^\dagger f_{i+1} + H.c.)
\]

\[
+ V a^2 \sum_{i=1}^{L} \sum_{l=1}^{L} i^2 n_i^l + V a^2 \sum_{i=1}^{L} i^2 n_f^l
\]

\[
+ \frac{U_{bb}}{2} \sum_{i=1}^{L} n_i^b (n_i^b - 1) + U_{bf} \sum_{i=1}^{L} n_i^b n_i^f
\]

where \(b_i^\dagger (f_i^\dagger)\) and \(b_i (f_i)\) denote the bosonic (fermionic) creation and annihilation operators at site \(i\), respectively, and they satisfy the standard (anti-) commutation relations, i.e., \([b_i, b_j^\dagger] = \delta_{ij}, \{f_i, f_j^\dagger\} = \delta_{ij}\), and \([b_i, f_j] = 0\). In the hard-core limit, the Hamiltonian is simplified to

\[
H = H_b + H_f
\]

with

\[
H_b = -t \sum_{i=1}^{L-1} (b_i^\dagger b_{i+1} + H.c.) + V a^2 \sum_{i=1}^{L} i^2 n_i^b
\]

\[
H_f = -t \sum_{i=1}^{L-1} (f_i^\dagger f_{i+1} + H.c.) + V a^2 \sum_{i=1}^{L} i^2 n_i^f
\]

where additional on-site constraint

\[
b_i^\dagger b_i + f_i^\dagger f_i \leq 1
\]

is assigned to avoid double or higher occupancy \cite{43}. Here \(t\) is the hopping parameter to be decided by the optical lattice; \(L\) is the number of the sites; \(V(i) = V a^2 i^2\) is the harmonic confined potential with \(a\) is the lattice space and \(V\) is the strength; \(n_i^b = b_i^\dagger b_i\) and \(n_i^f = f_i^\dagger f_i\) are the boson and fermion particle number operators respectively. Given the local Hilbert space at \(i\)-th site composed of a set of \(\{0\}, b_i^\dagger b_i^\dagger |0\rangle, f_i^\dagger f_i^\dagger |0\rangle\) under the single occupied on-site constraint, the on-site constraint can be written in the follow forms

\[
\{b_i, b_i^\dagger\} = 1 - f_i^\dagger f_i
\]

\[
\{f_i, f_i^\dagger\} = 1 - b_i^\dagger b_i,
\]

and the following equations are also valid

\[
b_i^{12} = b_i^2 = f_i^{12} = f_i^2 = 0,
\]

\[
b_i^1 f_i^1 = f_i b_i = f_i b_i^1 = b_i f_i = 0.
\]

In order to get the ground state properties of the system, we extend the general Jordan-Wigner transforma-
tion (JWT)\textsuperscript{17} and get the following transformations:

\[ f_j^\dagger = \prod_{\beta=1}^{j-1} e^{-i\pi c_{j\beta}^\dagger c_{j\beta}}, \]

\[ f_j = c_{j\dagger} \prod_{\beta=1}^{j-1} e^{i\pi c_{j\beta}^\dagger c_{j\beta}}, \]

\[ b_j^\dagger = \prod_{\beta=1}^{j-1} e^{-i\pi (c_{j\beta}^\dagger c_{j\beta} + c_{j\beta} c_{j\beta}^\dagger)}, \]

\[ b_j = c_{j\dagger} \prod_{\beta=1}^{j-1} e^{i\pi (c_{j\beta}^\dagger c_{j\beta} + c_{j\beta} c_{j\beta}^\dagger)}, \]

which map the Hamiltonian of the bosons into noninteracting spinless fermions Hamiltonian. Using the JWT we can change the Hamiltonian of the system into

\[ H_1 = H_{c\uparrow} + H_{c\downarrow} \]

with

\[ H_{c\sigma} = -t \sum_{i=1}^{L-1} (c_{i\sigma}^\dagger c_{i+1,\sigma} + H.c.) + V a^2 \sum_{i=1}^{L} i^2 n_{i\sigma}^c, \]

(9)

where \( \sigma = \uparrow, \downarrow \), and

\[ \{c_{i\uparrow}, c_{j\dagger\downarrow}\} = \{c_{i\dagger\uparrow}, c_{j\downarrow}\} = \{c_{i\uparrow}, c_{j\dagger}\} = 0 \]

for \( i \neq j \), else

\[ \{c_{i\uparrow}, c_{j\downarrow}\} = 1 - c_{i\uparrow}^\dagger c_{i\downarrow}, \quad \{c_{i\dagger\uparrow}, c_{j\dagger\downarrow}\} = 1 - c_{i\dagger\uparrow}^\dagger c_{i\dagger\downarrow}, \]

\[ c_{i\uparrow}^\dagger c_{i\downarrow} = c_{i\dagger\uparrow}^\dagger c_{i\dagger\downarrow} = c_{i\uparrow}^\dagger c_{i\dagger\uparrow} = c_{i\dagger\uparrow}^\dagger c_{i\dagger\downarrow} = 0 \]

(10)

for the on-site constraints. Here \( n_{i\sigma}^c = c_{i\sigma}^\dagger c_{i\sigma} \) is the \( \sigma \)-kind (we note the spinless fermions from the boson by \( \downarrow \)-kind and the original fermions by \( \uparrow \)-kind) fermion number operator, and \( N_{l_1(1)} = N_b(l) \). The Hamiltonian \( H_1 \) describes a mixture of two component fermions with point hard-core interactions between two kinds. Notice that the operators anticommute between two kinds.

Next we construct the ground state of the Hamiltonian \( H_1 \) under the constraints Eq. (10) with the method proposed by Batista et al.\textsuperscript{17}. We consider a set of parent states, labeled by the string configuration \( \sigma \), with \( N = N_\uparrow + N_\downarrow \) particles and \( L - N \) holes, \( \{\Phi_0(\sigma)\} \), and the form is:

\[ \Phi_0(\sigma) = |\sigma_1\sigma_2\sigma_3 \cdots \sigma_N \bigcirc \bigcirc \bigcirc \cdots \bigcirc \rangle, \]

(11)

where \( \sigma_i \) indicates the kind (\( \uparrow \) or \( \downarrow \)) of the fermion particle at site \( i \), \( L \) is the number of sites. Notice that the number of the configuration \( \sigma \) is \( C_{N_i}^N \). Then we rewrite the Hamiltonian \( H_1 \) with \( H_1 = T + H_V \), and

\[ T = -t \sum_{i,\sigma} T_{i\sigma}, \quad T_{i\sigma} = c_{i\sigma}^\dagger c_{i+1,\sigma} + H.c., \]

\[ H_V = V a^2 \sum_{i,\sigma} i^2 n_{i\sigma}^c, \]

(12)

The states \( |\Phi_0(\sigma)\rangle \) are eigenstates of \( H_V \) and they are degenerate with different \( \sigma \).

By applying the hopping operator \( T_{i\sigma} \) we can generate a subspace \( M(\sigma) \) from the parent state \( |\Phi_0(\sigma)\rangle \), and we denote

\[ |\Phi_1(\sigma)\rangle = T_{N,\sigma} |\Phi_0(\sigma)\rangle \]

or, in general

\[ |\Phi_\nu(\sigma)\rangle = T_{i\sigma} |\Phi_j(\sigma)\rangle. \]

Obviously the dimension of the subspace \( M(\sigma) \) is \( C_{N_i}^N \), and there are \( C_{N_i}^{N_j} \) subspaces. Moreover these different subspaces for different \( \sigma \) are orthogonal.

Next we construct the ground state in the subspace \( M(\sigma) \). For a specific \( \sigma \), we can make the following mapping:

\[ \{\sigma_1 \sigma_2 \sigma_3 \cdots \sigma_N \bigcirc \bigcirc \bigcirc \cdots \bigcirc \} \rightarrow \{\bullet \bullet \bullet \bullet \bullet \bullet \cdots \} \]

(13)

which maps the two component fermions \( c_{i\sigma} \) into a single spinless fermion \( c_i \). It is straightforward to show that in the corresponding new basis the system Hamiltonian can be written as

\[ H_{spinless} = -t \sum_{i=1}^{L-1} (c_i^\dagger c_{i+1} + H.c.) + V a^2 \sum_{i=1}^{L} i^2 n_i \]

(14)

The ground state properties of the fermionic system \( H_{spinless} \) with \( N \) particles have been analyzed in Ref.\textsuperscript{18}. Following the approach therein, we let \( P \) denote the lowest \( N \) eigenfunctions of the Hamiltonian \( H_{spinless} \) which can be obtained by diagonalizing \( H_{spinless} \):

\[ P = \begin{pmatrix}
P_{11} & P_{12} & \cdots & P_{1N} \\
P_{21} & P_{22} & \cdots & P_{2N} \\
\vdots & \vdots & \ddots & \vdots \\
P_{L1} & P_{L2} & \cdots & P_{LN}
\end{pmatrix} \]

(15)

where \( P_{jn} \) are the coefficients of \( n \)-th single particle state \( |\psi_n\rangle = \sum_{i=1}^{L} P_{in} c_i^\dagger |0\rangle \). Then the ground state of the spinless fermion gas is the state with the lowest \( N \) eigenstates of \( H_{spinless} \) fully filled, and the form is:

\[ |\Psi_G^{spinless}\rangle = \prod_{n=1}^{N} \sum_{i=1}^{L} P_{in} c_i^\dagger |0\rangle = \sum_{s=1}^{C_{N_i}^N} \det(P_s) c_s^N |0\rangle \]

(16)

where \( s \) index the combination formed by taking \( N \) numbers from the set \( L = \{1, \cdots, L\} \), \( P_s \) is a square matrix with \( N \) ranks that the \( N \) rows are taken from \( P \) according to the combination \( s \). \( c_s^N \) represents \( c_{i_1}^\dagger c_{i_2}^\dagger \cdots c_{i_N}^\dagger \), and \( s_i \) is the \( i \)-th number in the combination \( s \). We had assumed
that the numbers in combination are all sorted ascending. Now, we can use the reverse mapping of Eq.(13) to get the ground state of the Hamiltonian $H_1$ in the subspace $M(\vec{q})$

$$\Psi^{G}_{H_1}(\vec{q}) = \sum_{q=1}^{C_N^q} \det(P_s)(-1)^{T_q} c_{s,q}^\dagger c_{1,s}^\dagger |0\rangle. \quad (17)$$

where $q$ index the combination formed by taking $N_b$ numbers from the set $\Upsilon = \{1, \cdots, N\}$ which means that the $q_i(i = 1, \cdots, N_b)$-th site in $\vec{q}$ is occupied by $\uparrow$-kind fermion and $q_i$ is the $i$-th number in the combination $q$. $q$ is just another way to index $\vec{q}$. $c_{s,q}^\dagger$ represents $c_{1,s}^\dagger \cdots c_{N_b,s}^\dagger$, $\vec{q}$ represents the combination $\Upsilon - q$, and $T_q$ notes the times of the permutation to put the set $\{s_1, \cdots, s_{N_b}, q_1, \cdots, q_{N_b}\}$ into $s$. Reminding that the forms of Hamiltonian for $\uparrow$ and $\downarrow$-kind fermion are the same, the ground states $|\Psi^{G}_{H_1}(\vec{q})\rangle$ are $C_N^{N_b}$ degree degenerate because of $C_N^{N_b}$ different $\vec{q}$.

Supposing the ground state of $H_1$ given by $|\Phi^{GF}_G\rangle$, the one-particle density matrix function of boson of the system can be written in the form:

$$\rho^{B}_{ij} = \langle \Phi^{GF}_G \rangle_{ij} \langle \Phi^{GF}_G \rangle_{ji}$$

$$= \langle \Phi^{GF}_G \rangle \prod_{\beta=1}^{j-1} \frac{e^{-i\pi(c_{i,1\beta}^\dagger c_{j,1\beta}^\dagger + c_{j,1\beta}^\dagger c_{i,1\beta})}}{c_{i,1\beta}^\dagger c_{j,1\beta}^\dagger \prod_{\gamma=1}^{i-1} e^{i\pi(c_{\gamma,1\beta}^\dagger c_{\gamma,1\beta}^\dagger + c_{\gamma,1\beta}^\dagger c_{\gamma,1\beta})} |\Phi^{GF}_G\rangle$$

$$= \langle \Phi^A |\Phi^B \rangle, \quad (18)$$

where $|\Phi^{GF}_G\rangle$ is the ground state wave function of Bose-Fermi mixture and

$$|\Phi^A\rangle = \left( c_{i,1\beta}^\dagger \prod_{\beta=1}^{j-1} e^{i\pi(c_{\gamma,1\beta}^\dagger c_{\gamma,1\beta}^\dagger + c_{\gamma,1\beta}^\dagger c_{\gamma,1\beta})} |\Phi^{GF}_G\rangle \right)^\dagger,$$

$$|\Phi^B\rangle = c_{i,1\beta} \prod_{\beta=1}^{j-1} e^{i\pi(c_{\gamma,1\beta}^\dagger c_{\gamma,1\beta}^\dagger + c_{\gamma,1\beta}^\dagger c_{\gamma,1\beta})} |\Phi^{GF}_G\rangle. \quad (19)$$

In order to calculate $|\Phi^A\rangle$ (and $|\Phi^B\rangle$), it is convenient to use the following identities: \text{[19]}

$$\prod_{\beta=1}^{i-1} e^{i\pi(c_{j,1\beta}^\dagger c_{\beta,1\beta})} = \prod_{\beta=1}^{i-1} \prod_{\beta=1}^{j-1} e^{i\pi(c_{\gamma,1\beta}^\dagger c_{\gamma,1\beta}^\dagger + c_{\gamma,1\beta}^\dagger c_{\gamma,1\beta})}, \quad (20)$$

and

$$\prod_{\beta=1}^{i-1} e^{i\pi(c_{j,1\beta}^\dagger c_{\beta,1\beta})} c_{j,1\beta} = (-1)^{i(j)} \prod_{\beta=1}^{i-1} e^{i\pi(c_{j,1\beta}^\dagger c_{\beta,1\beta})}, \quad (21)$$

where $z = 1$ if $j < i$, otherwise $z = 0$. Following the same way shown above, we can get the one particle density matrix function of fermion ($\rho^F_{ij} = \langle \Phi^{GF}_G \rangle_{ij}^\dagger \langle \Phi^{GF}_G \rangle_{ji}$) and other quantities such as correlation functions.

FIG. 1: (Color online) Top panels: contour plots of the one particle density matrices. $\rho^{B}_{mix}(Left\ panel), \rho^{B}_{mix}(middle\ panel)$ are the one particle density matrices for the Bose Fermi mixture with $N_b = 3$ and $N_f = 2$. Right panel, the one particle density matrix($\rho^{T,G}_{mix}$) for the pure Fermi gas with $N_f = 5$. Bottom panels: corresponding off-diagonal sections along the anti-diagonal. All the systems are with 13 sites and $V a^2 = 0.02t$, where $V$ is the strength of the harmonic trap and $a$ is the lattice spacing.

III. HARD-CORE BOSON-FERMION MIXTURE IN THE HARMONIC CONFINE POTENTIAL

Since the ground state in the hard-core limit has a degeneracy of $C_N^{N_f}$, for convenience we first consider the case that $|\Phi^{GF}_G\rangle$ is formed by the summation of $|\Psi^{G}_{H_1}(q)\rangle$ with all the degenerate states having the same weight, i.e.,

$$|\Phi^{GF}_G\rangle = \frac{1}{\sqrt{C_N^{N_f}}} \sum_{q=1}^{C_N^{N_f}} |\Psi^{G}_{H_1}(q)\rangle$$

$$= \frac{1}{\sqrt{C_N^{N_f}}} \sum_{q=1}^{C_N^{N_f}} \sum_{s=1}^{C_N^{N_f}} \det(P_s)(-1)^{T_q} c_{1,s}^{\dagger} c_{q,s}^{\dagger} |0\rangle. \quad (22)$$

The ground state $|\Phi^{GF}_G\rangle$ is related to $|\Phi^{GF}_G\rangle$ by the generalized JWT. We note that the above construction is essentially equivalent to the construction of generalized Bose-Fermi mapping by Girardeau et al. at [21]. Then following the method proposed in the above section we can work out the density matrix function and show them in Fig(1) which are found to fulfill the relation

$$\rho_{mix}(i,j) = \sum_{q=1}^{N_b} \rho_{G}(i,j)$$

according to the data, where $\rho_{mix}$ is the one particle density matrix of boson for the Bose Fermi mixture and $\rho^{T,G}_{mix}(i,j)$ is the one particle density matrix of pure TG gas of $N$ bosons obtained by the method proposed by Rigol and Muramatsu [19]. It is easy to see that the one
The bosonic and fermionic one particle density distributions \( n^{B}_{\text{mix}}(i) = \rho^{B}_{\text{mix}}(i, i) \) and \( n^{F}_{\text{mix}}(i) = \rho^{F}_{\text{mix}}(i, i) \) are both proportional to the density \( n^{T G}(i) = \rho^{T G}(i, i) \) of a TG gas of \( N \) bosons \([4]\), i.e.,

\[
\frac{n^{F}_{\text{mix}}(i)}{N_f} = \frac{n^{B}_{\text{mix}}(i)}{N_b} = \frac{n^{T G}(i)}{N} = \frac{n^{F}(i)}{N},
\]

where \( n^{F}(i) \) is the density of the noninteracting gas of \( N \) fermions in trap which is same to \( n^{T G}(i) \) \([13]\). Actually under the state \( |\Psi^{E,F}_{G}\rangle \), the rate of the probabilities that the site \( i \) occupied by the \( \uparrow \)-kind and \( \downarrow \)-kind fermions is \( N_b/N_f \). This result means that there is no phase separation between bosons and fermions. We show the numerical results of the density profiles in Fig.2 which agree with theoretic results obtained by Girardeau et. al \([21]\) and Fang et. al \([24]\). Comparing distributions of the TG gas of 3 bosons and the free fermion gas of 2 fermions with the ones for the mixture \( n^{B(F)}_{\text{mix}} \), we can see that as the other kind particles adding in, the origin particles have to hold the higher energy states and the density distributions become boarder with lower weight.

The momentum distributions are defined by the Fourier transforms with respect to \( i-j \) of the one particle density matrices with the form of

\[
n^{B(F)}(k) = |\Psi(k)|^2 \sum_{n,m=-\infty}^{\infty} e^{-ik(n-m)} \rho^{B(F)}(n,m),
\]

where \( \Psi(k) \) is the Fourier transform of the Wannier function, and \( k \) denotes momentum. Since the bosonic one particle density matrix for the mixture is proportional to the TG one, the bosonic momentum distribution for the mixture is also proportional to the TG one. The numerical results of the momentum distributions are shown in Fig.3. The peak structure in the momentum distribution of boson reflects the bosonic nature of the particle, and is in contrast with the structure of the momentum

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**FIG. 2:** (Color online) The density profiles for several systems. \( n^{B(F)}_{\text{mix}}(i) \) is bosonic(fermionic) density profile for a Bose Fermi mixture with \( N_b = 3 \) and \( N_f = 2 \). PxB stand for the pure TG Bose gas with \( N_b = x \), and PxF stand for the pure free Fermi gas with \( N_f = x \). Again all the systems are with 13 sites and \( V a^2 = 0.02t \).

**FIG. 3:** (Color online) The momentum distributions for several systems. The systems are defined by the same way described in Fig.2. Notice that the momentum \( k \) is in units of \( k_L \) which is the wave vector of the optical lattice.

**FIG. 4:** (Color online) The occupation of the natural orbitals for several systems defined by the same way described in Fig.2.
distribution for the equivalent noninteracting fermions. Again the distributions for the mixture are boarder and lower than the pure ones because of holding higher energy states.

The natural orbitals \( (\phi^B_F(i)) \) are defined as the eigenfunctions of the one particle density matrix \( \rho \):

\[
\sum_{j=1}^{M} \rho_B(i,j) \phi_B^j(i) = \lambda_B^j(i) \phi_B^j(i)
\]

and it can be understood as being effective one particle eigenfunctions of the one particle density matrix \( \rho \):

\[
\lambda_B^j(i) = N_i^B \lambda_T^j(i)
\]

where \( \lambda_T^j(i) \) denotes the occupation of \( j \)-th natural orbital for a pure TG gas composed of \( N \) hard-core bosons. The peak on the lowest orbital of boson is the feature of the boson. As for the fermion, the occupation is no longer the step function with lowest \( N \) orbitals fully filled as the distribution of the pure noninteracting \( N \) fermions. And there is no peak at the lowest orbital.

IV. THE PROPERTY OF THE SYSTEM WITH LARGE BUT FINITE BB AND BF REPULSION

As we have discussed in section II, the ground state in the hard-core limit has a huge degeneracy. However, we expect that the degenerate ground state would be lifted when the on-site interactions deviate the infinite limit. Next we consider the case with \( U_{BB} \) and \( U_{BF} \) being large but finite, for which the second quantized Hamiltonian of \( H \) is the standard Hubbard model of Bose-Fermi mixture with the form of Eq. (3). In the situation that \( U_{bb} \) and \( U_{bf} \) are still large, the state with double occupancy on the same site is a high-energy state and we can use the standard projection method to derive the low-energy effective Hamiltonian of the system which is given by

\[
H_s = -t \sum_{i=1}^{L-1} (b_i^\dagger f_{i+1} + f_i^\dagger b_{i+1} + H.c.) + V a^2 \sum_{i=1}^{L} i^2 n_i^b + V a^2 \sum_{i=1}^{L} i^2 n_i^f - 4t^2 \sum_{i=1}^{L-1} [(S_i^b S_{i+1}^b + S_i^f S_{i+1}^f) - S_i^b S_{i+1}^b] - \frac{2t^2}{U_{bb}} \sum_{i=1}^{L-1} n_i^b n_{i+1}^b
\]

with \( S_i^b = b_i^\dagger f_i, S_z = (n_i^b - n_i^f)/2 \). In the limit \( U_{bb}, U_{bf} \to \infty \), the last two summation terms in the Hamiltonian vanish and the system reduces back to Eq. (21) which we studied in the last section. As \( U_{bb} \) and \( U_{bf} \) become finite but large, the last two summation terms can be viewed as perturbations to the system, so one can expect that they wouldn’t cause significant changes to some properties of the total system such as ground state energy and total density profile (see Fig. 4), because of terms of \( t^2/U_{bf} \) and \( t^2/U_{bb} \) being very small for large \( U_{bb} \) and \( U_{bf} \). Nevertheless, a significant effect induced by these small terms is the lift of the degeneracy of the ground states and the true ground state would be a recombination of \( C_{N_b}^{N_f} \) degenerate states with the weights of states to be determined by minimization of the energy due to perturbation terms.

One observes that terms of \( t^2/U_{bf} \) lead to an effective isotropic antiferromagnetic exchange interactions between “spins” (bosons or fermions) on neighboring sites to lower the ground state energy. On the other hand, terms of \( t^2/U_{bb} \) produce an effective attractive interactions between neighboring bosons and thus states with all the bosons concentrated together have lower energy. Consequently, the relative distribution for the bosons or fermions will be changed and determined by terms of \( t^2/U_{bb} \) and \( t^2/U_{bf} \) to further lower the ground state energy. However, one can expect that the total distribution shall not be changed too much because the terms of \( t^2/U_{bf} \) and \( t^2/U_{bb} \) are very small in comparison with hopping terms. As the system Eq. (25) has no analytical results any more when the interaction parameters \( U_{bb}, U_{bf} \) being finite, as an approximation, we can treat the charge part and spin part separately. Then the charge part, which does not distinguish bosons or fermions, is determined by the matrix \( P \) according to Eq. (15) with the state given by Eq. (16), whereas the spin part, which decides the weight of states with different spin configurations, is determined by Hamiltonian with only \( U_{bf} \) and \( U_{bb} \) terms in Eq. (25). Considering that, with the presence of the harmonic trap, the particles mainly concentrate at the center of the trap with holes around, the spin part is defined on the system with \( N_b \) bosons and \( N_f \) fermions on \( N_b + N_f \) sites. This approximation is similar to the spin charge separation approximation.

First, we consider the situation \( U_{bb} \gg U_{bf} \gg 1 \). In this limit, the terms of \( U_{bf} \) dominate and we can set \( U_{bb} = \infty \). Because of the spin fluctuation terms of \( S_i^z S_j^z + S_i^z S_j^f \), the off-diagonal terms appear between different subspace \( M(q) \), and the ground state of the system becomes complicated. Actually in the limit \( U_{bb} = \infty \), the Hamiltonian \( H_{BB} \) can be mapped to the Fermi Hubbard model by a JW similar to Eq. (3), and they have the same thermodynamic properties \( 48 \). As for the ground state properties, it can be worked out by the mapping from the fermi Hubbard model. When \( U_{bb} \) is away from the infinite limit, there are no analytical results. In Fig. 5 we show the density profiles in the situation \( U_{bb} \gg U_{bf} \gg 1 \) with spin charge separation approximation. From the
data, the total distribution is the same with that of the pure TG boson gas. Because of the effective antiferromagnetic exchanges between bosons and fermions, the specie-dependent distributions for bosons and fermions exhibit quite different behavior with alternating peaks. To check the validity of this approximation method, in Fig. 5, we also show some results of small system of Bose-Fermi Hubbard model gained by exact diagonalization method [38]. We can see that the results gained by the Fermi Hubbard model gained by exact diagonalization. 'EDS' stands for exact diagonalization. 'EDS' stands of the results gained by spin charge separation approximation with the spin part (weights of subspace ground states) is determined by exact diagonalization.

Next we consider the situation $U_{bf} \gg U_{bb} \gg 1$. Then the $U_{bb}$ terms dominate and for simplicity we can first set $U_{bf} = \infty$. Although the $U_{bb}$ term is diagonal in the Hilbert space $\cup_q M(q)$, the states $|\Psi_{H_1}^G(q')\rangle$ (Eq. (17)) with different spin configurations are not degenerate any more for different $q$ because of the $U_{bb}$ term. Since the $U_{bb}$ terms tend to make the boson concentrated together, the ground states of the configuration $q$ with all the boson staying together have the lowest energy. Then the ground states have the degeneracy of $C_1^{N_f+1} = N_f + 1$. We suppose that the ground state $|\Phi_{GF}^F\rangle$ is formed by these degenerate states in subspace $M(q)$ with all the degenerate states having the same weight, say:

$$|\Phi_{GF}^F\rangle = \frac{1}{\sqrt{N_f + 1}} \sum_{q' = 1}^{N_f + 1} |\Psi_{H_1}^G(q')\rangle$$

$$= \frac{1}{\sqrt{N_f + 1}} \sum_{q' = 1}^{N_f + 1} \sum_{s = 1}^{C_1^{N_f}} \text{det}(P_s) (-1)^{T_s} c_{1q'}^\dagger c_{1s}^\dagger |0\rangle.$$ 

Then we can get the density matrices and other quantities. In Fig. 6, we show the density of the system form the state $|\Phi_{GF}^F\rangle$. We can see that there is a phase separation in the system with bosons are in the middle of the trap and fermions surround them. As $U_{bf}$ is away from the limit $\infty$, the $N_f + 1$ fold degeneracy of the ground state is split. For comparison, the density profiles in the limit $U_{bf} \gg U_{bb} \gg 1$ with spin charge separation approximation and exact diagonalization are also shown in Fig. 6a. It is clear that the results obtained by spin charge separation approximation in the density profiles of the Bose Fermi mixture with 3 boson and 2 fermion on 11 sites, the trap strength $Va^2 = 0.2t$, $U_{bb} = 2000t$ and $U_{bf} = 200t$. The curve with symbol circle is the total density profile calculated from the ground state $|\Phi_{GF}^F\rangle$ in Eq. (22) (b): The total density profiles of different $U_{bb}, U_{bf}$ for the Bose Fermi mixture with 3 boson and 2 fermion on 11 sites, the trap strength $Va^2 = 0.2t$. The curve with symbol square is the total density profile calculated from the ground state $|\Phi_{GF}^F\rangle$ in Eq. (22).
separation approximation agree well with the ED ones, however the results gained by the state \(\langle \Phi_{FF}^U \rangle \) (Eq. (29)) do not agree very well with the others because the \( U_{bf} \) terms are neglected. But the results gained by the state \(\Phi_{GG}^F \) (Eq. (29)) and spin charge separation approximation both indicate that there is a phase separation in the system with bosons located in the middle of the trap and fermions surrounded. Again the density distributions of the total particle are almost the same from the data for the three methods (the difference < 10^{-2}).

V. SUMMARY

In conclusions, we have studied in detail the ground state properties of the mixture of the hard-core bosons and noninteracting fermions with point hard-core boson-boson and boson-fermion interactions in the 1D optical lattice with harmonic confine potential. Using extended Jordan-Wigner transformations, we calculate the density matrix, then we yield the density profiles, momentum distribution, the natural orbitals and its occupations. We also discuss the property of the system with large but finite interactions. We find that, despite the total density distribution not sensitive to relative strengths of \( U_{bf} \) and \( U_{bb} \), the boson and fermion distributions rely on \( U_{bb} \gg U_{bf} \gg 1 \) or \( U_{bf} \gg U_{bb} \gg 1 \). We hope that our study could be helpful for the experimental achievement of the ultracold boson-fermion mixtures with hard-core BB, BF interactions in optical lattices.

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