Mixture of Tonks-Girardeau gas and Fermi gas in one-dimensional optical lattices

Shu Chen,1 Junpeng Cao,1 and Shi-Jian Gu2

1Institute of Physics, Chinese Academy of Sciences, Beijing 100190, China
2Department of Physics and ITP, Chinese University of Hong Kong, Hong Kong, China

We study the Bose-Fermi mixture with infinitely boson-boson repulsion and finite boson-Fermion repulsion. By using a generalized Jordan-Wigner transformation, we show that the system can be mapped to a repulsive Hubbard model and thus can be solved exactly for the case with equal boson and fermion masses. By using the Bethe-ansatz solutions, we investigate the ground state properties of the mixture system. Our results indicate that the system with commensurate filling \( n = 1 \) is a charge insulator but still a superfluid with non-vanishing superfluid density. We also briefly discuss the case with unequal masses for bosons and fermions.

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Mixtures of quantum degenerate atoms recently became a subject of intense studies of both experiment and theory. One of particularly interesting systems is mixture of ultracold bosonic and fermionic atoms \[1–3\], which have become accessible through the development of sympathetic cooling \[1, 2\]. The experimental progress in manipulating cold atoms in effective one-dimensional (1D) waveguides and the ability of tuning the effective 1D interactions by Feshbach resonance leads experiment accessible to the strong correlation regime of 1D quantum gas \[4, 5\]. Meanwhile, by loading the atomic system into the optical lattice \[6, 7\], one can simulate not only the solid state systems in a highly tunable way but also new systems which may not be realized in condensed matter, such as mixtures of Bose-Fermi atoms. These advances open a new channel to investigate numerous phenomena of low-dimensional correlated lattice models which play important roles in condensed matter physics.

To gain a deep insight of properties of the low-dimensional quantum mixtures, some refined methods capable of dealing with strong correlations are especially important. For example, the method of Bose-Fermi mapping has been extensively exploited to study the Tonks-Girardeau (TG) gas \[8, 9\]. This method has been also generalized to study the multi-component quantum gas in the infinitely repulsive limit \[10, 11\]. The extended Bose-Fermi mapping method is only limited to a special case with no tunable parameter of interaction, where all the intra- and inter-component interactions go to infinite. In addition, the Bose-Fermi mixture with equal boson-boson and boson-fermion interactions can be exactly solved by Bethe-ansatz \[12–14\]. Unfortunately, its corresponding lattice model is no longer integrable. So far, the ground state phase diagram of the 1D Bose-Fermi Hubbard model in optical lattice has been studied by mean-field theory \[15, 16\], Bosonization method \[17, 18\], exact diagonalization method \[19\], and quantum Monte Carlo method \[20–22\]. Despite the intensive studies of the lattice model \[15, 20, 22, 24\], no analytically exact result has been given except the TG limit \[10\], in which however the model suffers the problem of a huge degeneracy of ground states (GSs). In this work, we shall study the boson-fermion mixtures with the aim to give some exact conclusions apart from the TG limit and focus on the case with an infinite boson-boson repulsion but a tunable boson-fermion interaction, which is found to be exactly solvable when the hopping amplitude \( t_b \) for boson equals to \( t_f \) for fermion.

We consider a mixture system of bosonic and spin-polarized fermionic atoms confined in a deep 1D optical lattice. For sufficiently strong periodic potential and low temperatures, the atoms will be confined to the lowest Bloch band and the low energy Hamiltonian is described by the Hamiltonian

\[
H = -\sum_{i,\sigma=b,f} \left( t_\sigma a_\sigma^\dagger a_{i+1\sigma} + H.c. \right) + \frac{1}{2} \sum_{i} U_b n_{i,b} (n_{i,b} - 1) + U_{bf} \sum_{i} n_{i,b} n_{i,f},
\]

where \( a_{i\sigma} \) are bosonic or fermionic annihilation operators localized on site \( i \), and \( n_{i\sigma} = a_{i\sigma}^\dagger a_{i\sigma} \). In principle, the interaction parameters \( U_{bf} \) and \( U_b \) can be tuned experimentally by the Feshbach resonance. In this work, we shall focus on the case with infinitely strong boson-boson repulsion, i.e., \( U_b = \infty \), and a tunable inter-species repulsion \( U_{bf} = U \). In this case, the boson is a hard-core one or a TG gas, for which the states occupied by more than one boson are prohibited. Similarly, the states occupied by more than one fermion are not permitted due to the Pauli principle. However, a boson and a fermion can occupy the same site which contributes an on-site energy \( U \). In the hard-core limit, the Bose-Fermi mixture model can be simplified to

\[
H_{BF} = -\sum_{i,\sigma=b,f} \left( t_\sigma a_{i\sigma}^\dagger a_{i+1\sigma} + H.c. \right) + U \sum_{i} n_{i,b} n_{i,f},
\]

with additional on-site constraints \( a_{i\dagger}^\dagger a_{i\dagger} = a_{i\dagger} a_{i\dagger} = 0 \) and \( \{ a_{ib}, a_{ib}^\dagger \} = 1 \) assigned to avoid double or higher occupancy.

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\*Electronic address: schen@aphy.iphy.ac.cn
\*Electronic address: sjgu@sun1.phy.cuhk.edu.hk
Mixture with equal masses. — Firstly, we focus on the case that the bosonic and fermion atoms have the same masses, which is approximately satisfied for the Bose-Fermi mixture of heavy isotopic atoms, for example, the $^{174}$Yb-$^{173}$Yb mixture [3]. The Bose-Fermi mixture with equal masses provides a solvable limit, which may serve as a touchstone for various numerical simulations. For the model system with the fermion and the boson having the same mass, we have $t_b = t_f$. It is convenient to use the following extended Jordan-Wigner (JW) transformations

$$a_{ib} = \prod_{j<i} e^{i \pi c_{i,j}^\dag c_{i,j}^\tau}, \quad a_{if} = \prod_{j=1}^N e^{i \pi c_{i,j}^\dag c_{i,j}^\tau},$$

which maps the Hamiltonian of hard-core Bose and Fermi mixture model into a Hubbard model

$$H_F = -\sum_{i,\sigma} \left( t_\sigma c_{i,\sigma}^\dag c_{i+1,\sigma} + H.c. \right) + U \sum_i n_{i\uparrow} n_{i\downarrow}.$$  

The second mapping in eq. (3) is introduced to enforce the Fermion operators $c_{i,\uparrow}$ and $c_{i,\downarrow}$ fulfill the anti-commutation relation $\{c_{i,\uparrow}, c_{i,\downarrow}\} = 0$. The Hamiltonians of $H_{BF}$ and $H_F$ have the same spectrum of energy. Therefore, we can get the eigen-energy of $H_{BF}$ with $t_b = t_f = t$ from the well-known Lieb-Wu solution of the Hubbard model [25], i.e., the eigenenergy is given by $E = -2t \sum_j^N \cos k_j$ with $k_j$ determined by the Bethe-ansatz equations

$$2\pi I_j = k_j L - \sum_{\beta=1}^M \theta_1(\Lambda_\beta - \sin k_j),$$

$$2\pi J_\alpha = \sum_{j=1}^N \theta_1(\Lambda_\alpha - \sin k_j) - \sum_{\beta=1}^M \theta_2(\Lambda_\alpha - \Lambda_\beta) + \phi_f - \phi_b,$$

where $\theta_n(k) = 2 \tan^{-1}(4k/nU)$, $j = 1, \cdots, N$, $\beta = 1, \cdots, M$, $N = N_b + N_f$, $M = N_f$, $N_b$ ($N_f$) is the number of bosons (fermions), and $L$ is the size of the system. Here the set $\{I_j, J_\alpha\}$ play the role of quantum number. We also solve the ground state energy of $H_{BF}$ by using the numerical exact diagonalization method and compare with the result obtained by solving the Bethe-ansatz equations. It is found that the numerical result agrees with the Bethe-ansatz solution exactly.

The unitary mapping builds a bridge between the hard-core Bose-Fermi mixture and the extensively studied Hubbard model. Since these two models sharing the same energy spectrum, we can conclude that they have the same thermodynamic properties. The GS properties of hard-core Bose-Fermi model also share some similarities with the Hubbard model, i.e., there exists no Mott transition from superfluid to Mott insulator for any finite $U$. For the incommensurate filling case, the system is in a superfluid phase, whereas the system with the commensurate filling $n = 1$ is in a Mott phase for any finite $U$, which is characterized by the presence of a charge gap and simultaneously a gapless mode of mixture composition fluctuations.

The superfluid density of the bosonic component can also be characterized by the bosonic phase stiffness, which reflects the response of a superfluid component to the imposed phase gradient and is defined as [26]

$$D_b = \left. \frac{L \partial^2 E_0(\phi_b) }{2 \partial \phi_b^2} \right|_{\phi_b=0},$$

which is proportional to the Drude weight. Similarly, the fermionic stiffness can be represented as

$$D_f = \left. \frac{L \partial^2 E_0(\phi_f) }{2 \partial \phi_f^2} \right|_{\phi_f=0}.$$ 

Here, $E_0$ is the ground-state energy, $\phi_b$ and $\phi_f$ are the component-dependent flux in units of $\hbar c/e$ for the boson and fermion respectively, which can be incorporated in the wavefunction by making the usual gauge transformation $a_{i,\sigma} \to e^{i \phi_{\sigma} r_i/L} a_{i,\sigma}$. A finite bosonic or fermionic stiffness is characteristic of a superfluid or conductor, whereas the stiffness vanishes for an insulator. In the presence of component-dependent flux, the eigenenergy of the system is also given by $E = -2t \sum_j \cos k_j$ with $k_j$ determined by the revised Bethe-ansatz equations [26]

$$2\pi I_j = k_j L - \phi_b - \sum_{\beta=1}^M \theta_1(\Lambda_\beta - \sin k_j),$$

$$2\pi J_\alpha = \sum_{j=1}^N \theta_1(\Lambda_\alpha - \sin k_j) - \sum_{\beta=1}^M \theta_2(\Lambda_\alpha - \Lambda_\beta) + \phi_f - \phi_b.$$ 

By solving the revised BAEs, we can directly calculate the stiffness of system. In order to calculate the charge stiffness $D_c$, we set the magnetic flux of hard-core bosons $\phi_b$ and that of spinless fermions $\phi_f$ to be the same, i.e., $\phi_b = \phi_f = \phi$, whereas the spin stiffness $D_s$ is calculated by taking $\phi_b = -\phi_f = \phi$. Explicitly, we have

$$D_c = \left. \frac{L \partial^2 E_0(\phi) }{2 \partial \phi^2} \right|_{\phi=\phi_b=\phi_f=0}$$

and

$$D_s = \left. \frac{L \partial^2 E_0(\phi) }{2 \partial \phi^2} \right|_{\phi=\phi_b=\phi_f=0}.$$ 

For the case with commensurate filling, we display the charge, spin and boson stiffness in (a), (b) and (c) of Fig. 1, respectively. It is obvious that the charge stiffness goes to zero quickly when the interaction $U$ exceeds a critical value. To extrapolate the critical $U_c$ in the thermodynamic limit, we make finite size analysis of the transition point where the charge stiffness tends to vanish, which is characterized by the minimum of the derivative of the charge stiffness as shown in the Fig. 1(d).
The non-vanishing $D$ order process. For the incommensurate case with $n_b = 1$ and $n_f < 1$, the bosons are in an insulator state which provides a homogeneous background for the fermions which form a conductor with $D_f = t \sin(\pi n_f)/\pi$.

Despite $H_{BF}$ and $H_F$ sharing the same energy level structure, they have different ground state wavefunction due to the intrinsically different exchange symmetry of the wave functions for Bose and Fermi systems. Suppose the wavefunction of the Fermi Hubbard model is given by $\Psi_F(x_1, \cdots, x_n; x_{n+1}, \cdots, x_N)$, the wavefunction of $H_{HB}$ can be constructed as

$$\Psi_{BF}(x_1, \cdots, x_n; y_{n+1}, \cdots, y_N) = \prod_{i<j} sgn(x_i - x_j) \Psi_F(x_1, \cdots, x_n; y_{n+1}, \cdots, y_N),$$

where $sgn(x_i - x_j) = (x_i - x_j)/|x_i - x_j|$ is the sign function. Consequently, the observable associated with the wave functions rather than the energy level structures should display different behaviors, which can be displayed in the off-diagonal density matrix and the momentum distributions of the hard-core boson. Explicitly, the density matrices of boson and fermion are defined as $\rho_{ij}^B = \langle a_{i,b}^\dagger a_{j,b} \rangle$ and $\rho_{ij}^F = \langle a_{i,f}^\dagger a_{j,f} \rangle$ respectively, which exhibit quite different behaviors for boson and fermion. The momentum distribution can be obtained by the Fourier transformation of the corresponding density matrix. For example, we have

$$n^{B,F}(k) = \frac{1}{2\pi L} \sum_{i,j} \rho_{ij}^{B,F} e^{-ik(i-j)}. \quad (9)$$

In Fig. (2), we display the momentum distribution of the Bose and Fermi systems respectively for the case with commensurate filling $n_b = n_f = 1/2$. It is shown that the momentum distribution of the hard-core bosons has a sharp peak, which reflects the bosonic nature of the particles. With the increase in inter-component interactions, the momentum distribution spreads wider and wider but the pronounced peak around the zero momentum is kept. While the momentum distribution of the fermion exhibits the free Fermi distribution for $U = 0$, it becomes more wider and develops a wide tail with the increase in $U$.

**Mixture with unequal masses.**— Finally, we give a brief discussion on the case with $t_b \neq t_f$ which corresponds to the system where the bosonic and fermionic atoms have different masses, such as mixture of $^7\text{Li}$ and $^{40}\text{K}$. In general, the single particle hopping amplitude is inversely proportional to the mass of atoms, i.e., $t_f/t_b = m_b/m_f.$
The Hubbard model still holds true via the generalized mixture of hard-core bosons and fermions is no longer true with the following structure factor of density wave (DW) of fermionic atoms

\[ S_{\text{FDW}}(q) = \frac{1}{L} \sum_{j} e^{iq(j-1)} (\langle n_{j,f} n_{L-f,j} \rangle - \langle n_{j,f} \rangle^2), \]

where \( q = 2n\pi/L \) and \( n = 0, 1, \ldots, L \). We calculate the structure factor as a function of \( t_\beta \) for different modes for systems with different sizes \( L \) and strengths of interactions \( U \). The results show an obvious competition between the modes of \( S_{\text{FDW}}(q = 2\pi/L) \) and \( S_{\text{FDW}}(q = N\pi/L) \). In the heavy fermionic atom limit with small \( t_\beta \), \( S_{\text{FDW}}(q = 2\pi/L) \) dominates, which indicates phase separation in this region \( 24 \) where configurations of fermionic atoms like \( \{f, f, f, f, o, o, o, o, o\} \) are found to be dominant. On the other hand, as \( t_\beta \to 1 \), \( S_{\text{FDW}}(q = N\pi/L) \) exceeds \( S_{\text{FDW}}(q = 2\pi/L) \), which implies that fermionic atoms distribute uniformly on the optical lattice. Then together with bosonic atoms, the ground state becomes the so-called DW state similar to the state of symmetric model, which is the limiting case with \( t_\beta = 1 \) studied in the above section. Consequently, we can determine the transition point on the \( U-t_\beta \) plane for a finite system from the intersection of the structure factor of two modes. In Fig. 3 we plot the phase diagram on the \( U-t_\beta \) plane for systems with a filling factor \( n = 4/5 \) for different system-sizes \( L = 15, 20, 25 \). The infinite size limit is obtained by extrapolation from the finite-size analysis. Below the phase boundary line, the phase-separation phase dominates, while the DW phase is dominated above the boundary line.

In summary, we study the mixture of TG gas and fermions in a 1D optical lattice. We show that this system can be mapped to the Fermi Hubbard model by a generalized Jordan-Wigner transformation and thus is exactly solvable when the bosons and fermions have the same masses. Based on the Bethe-ansatz solution, we calculate the charge stiffness and the superfluid density for the systems with either commensurate or incommensurate filling. Our results show that the system with commensurate filling factor \( n = 1 \) is a charge insulator but remains to be a superfluid characterized by a non-vanishing superfluid density. We also give a brief discussion to the case with unequal boson and fermion masses. In the heavy Fermi mass limit, our result indicates that a phase-separation phase arise. The phase transition from the density wave phase to the phase-separation phase is discussed.

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### Appendix A

In this appendix, we provide a derivation of the relation

\[ D_b = \frac{1}{4}(D_c + D_s). \]

In the presence of flux, the
Hamiltonian (2) becomes
\[ H_{BF} = -t \sum_i (a_{iB} a_{i+1B} e^{i\phi_L/L} + H.c.) \]
\[ -t \sum_i (a_{iF} a_{i+1F} e^{i\phi_L/L} + H.c.) + U \sum_i n_{i,B} n_{i,F}. \]

Expanding the Hamiltonian in terms of \( \phi_L / L \) and \( \phi_L / L \), we have
\[ H_{BF} = \left( T_b - \frac{\phi_L j_b}{L} - \frac{T_b \phi_L^2}{2 L^2} \right) + \left( T_f - \frac{\phi_L j_f}{L} - \frac{T_f \phi_L^2}{2 L^2} \right) \]
\[ + U \sum_i n_{i,B} n_{i,F} + O(\phi_L^3, \phi_L^4), \]

where \( T_\sigma = -t \sum_i (a_{i\sigma} a_{i+1\sigma} + H.c.) \) and \( j_\sigma = it \sum_i (a_{i\sigma} a_{i+1\sigma} - H.c.) \) with \( \sigma = b, f \). So according to the perturbation theory,
\[ D_c = \frac{1}{L} \left[ \frac{1}{2}(-T_c) - \sum_{n \neq 0} \frac{\langle 0| j_n | n \rangle^2}{E_n - E_0} \right], \]
\[ D_s = \frac{1}{L} \left[ \frac{1}{2}(-T_s) - \sum_{n \neq 0} \frac{\langle 0| j_n | n \rangle^2}{E_n - E_0} \right], \]
\[ D_b = \frac{1}{L} \left[ \frac{1}{2}(-T_b) - \sum_{n \neq 0} \frac{\langle 0| j_b | n \rangle^2}{E_n - E_0} \right], \]
\[ D_f = \frac{1}{L} \left[ \frac{1}{2}(-T_f) - \sum_{n \neq 0} \frac{\langle 0| j_f | n \rangle^2}{E_n - E_0} \right], \]

where the current operators: \( j_c = j_b + j_f, \ j_s = j_b - j_f, \) and \( T_c = T_s = T_f + T_b = 2T_b \). Then
\[ D_c + D_s = \frac{1}{L} \left[ \frac{1}{2}(-4T_b) - 2 \sum_{n \neq 0} \frac{\langle 0| j_c | n \rangle^2}{E_n - E_0} - 2 \sum_{n \neq 0} \frac{\langle 0| j_s | n \rangle^2}{E_n - E_0} \right] = 4D_b. \]

Finally, we have
\[ D_b = \frac{1}{4}(D_c + D_s). \]

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