Trapped Bose-Fermi Mixture in an optical lattice

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Abstract. We study distinctive features of local Mott insulator of trapped Bose-Fermi mixture systems on an optical lattice by using Monte-Carlo simulations of one-dimensional Bose-Fermi-Hubbard model. It was found that each species of the bosons and the fermions in a Mott insulator state had a finite stiffness but the density correlation function exhibited a quasi-long-range-order. This strongly suggested that in actual experiments the bosons and fermions of a commensurate filling with the lattice sites would form a Mott insulator state under strong interatomic interactions and have an order in their positional configuration.

1. Introduction
Technologies of confining ultra-cold atoms on optical lattices have opened up new possibilities of quantum phases. Bosonic atoms on a lattice, for example, could become Mott insulator when interatomic repulsive interactions and atomic density per site meet a certain condition[1, 2, 3]. Confinement potential creates a non-uniform density profile, resulting in the coexistence of superfluid and Mott insulator. The boson density has a peak at the deepest position of the confinement potential and decreases as going away from the peak position. It may reach an integer value at some points, where the commensurability with lattice sites is locally satisfied and a local Mott insulator appears under sufficiently large repulsive interactions. The density profile could thus have several plateau areas, called Mott plateaus, at which local Mott insulator is formed.

Situation is more complicated with trapped Bose-Fermi mixture systems on an optical lattice[4]. The density profile of trapped bosons and fermions on an optical lattice could also have Mott plateaus as one sees in the boson systems. However in trapped Bose-Fermi mixture systems in a confinement potential, only the total number of the bosons and the fermions at each site is fixed to an integer value in the Mott plateau and the number of the atoms of each species is not fixed. In other words, in the local Mott state of mixture systems, the total number of the atoms does not fluctuate at each site, but the number of the fermions or that of the bosons at each site could fluctuate compensating each other’s fluctuation to fix the total local density. From this viewpoint, the bosons and fermions seem to be able to move in the local Mott state, unlike bosonic or fermionic Mott insulators. This picture leads to a fundamentally new issue of Mott states.

In this study we conducted quantum Monte-Carlo simulations of one-dimensional Bose-Fermi-Hubbard model to address this issue and find distinctive features of local Mott state of Bose-Fermi mixture systems. Since the Mott plateau in the density profile of the mixture systems,
realized in numerical simulations, is too small to examine its detail, we removed the confinement potential and tuned the number of the atoms instead to realize commensurability.

The paper is organized as follows. Section 2 shows the model that we used in the simulations and Sec. 3 presents the result. Conclusions are given in Sec. 4.

2. Model
We performed world-line quantum Monte Carlo (QMC) simulations of bosons and fermions on a one-dimensional periodic lattice[5, 6, 7]. We employed one-dimensional Bose-Fermi Hubbard Hamiltonian, given by

\[ H = -t_b \sum_i b_i^\dagger b_{i+1} + h.c. - t_f \sum_i f_i^\dagger f_{i+1} + h.c. + \frac{U_{bb}}{2} \sum_i n_{bi}(n_{bi} - 1) + U_{bf} \sum_i n_{bi}n_{fi}, \]  

where \( b_i \) (\( b_i^\dagger \)) is the boson annihilation (creation) operator at site \( i \), \( n_{bi} = b_i^\dagger b_i \), \( f_i \) (\( f_i^\dagger \)) is the fermion annihilation (creation) operator at site \( i \), and \( n_{fi} = f_i^\dagger f_i \). \( U_{bb} \) denotes boson-boson interaction and \( U_{bf} \) boson-fermion interaction. We set \( t_b = t_f = 1 \) as energy unit. Assuming that all the interatomic interactions were repulsive, we measured charge stiffness and B-F correlation function, which we will define below, to clarify the Mott state property of the mixture with significantly strong interactions.

To observe stiffness of the system, we measured the following current-current correlation functions in the zero-frequency limit, which correspond to the averages of squared winding number[6, 7]:

\[ J_b = \lim_{\omega \to 0} \langle j_b(\omega) j_b(-\omega) \rangle, \]
\[ J_f = \lim_{\omega \to 0} \langle j_f(\omega) j_f(-\omega) \rangle, \]
\[ J_{tot} = \lim_{\omega \to 0} \langle (j_b(\omega) + j_f(\omega)) (j_b(-\omega) + j_f(-\omega)) \rangle. \]

Here \( j_b(\omega) \) presents the Fourier transform of current operator \( j_b(\tau) \) of the bosons with \( \tau \) being imaginary time in the path integral formalism, and \( j_f(\omega) \) that of the fermions.

For the observation of particle configuration in the local Mott state, we measured B-F correlation function, defined by

\[ C(l) = (-1)^l \langle S_{i+l} S_i \rangle, \]

where \( S_i = n_{bi} - n_{fi} \). Since in the limit of \( U_{bb}, U_{fb} \to \infty \) our Hamiltonian is equivalent to an antiferromagnetic Heisenberg chain with a constraint that the number of up-spins (say, bosons in our model) and that of down-spins (fermions) are fixed, we can expect staggered spin-density-wave like correlation for \( C \).

It was already shown that the two component systems undergo a mixing-demixing transition[8, 9, 10] at a certain value of \( U_{bf} \) and the transition point shifts as \( U_{bb} \) increases[11]. So we need to choose the interaction parameters appropriately to prevent demixing of the bosons and fermions.

3. Result
3.1. Stiffness
We first present the result of stiffness measurement in the QMC simulations of 30 bosons and 30 fermions on 60 sites at a temperature \( T = 0.04 \) with the Trotter decomposition number \( N_t = 200 \). Figure 1 shows boson stiffness \( J_b \), fermion stiffness \( J_f \) and total stiffness \( J_{tot} \) as functions of the boson-fermion interaction \( U_{bf} \) with the boson-boson interaction \( U_{bb} \) being fixed to 10. We see from the figure that, at around \( U_{bf} = 2 \), \( J_{tot} \) becomes zero and the mixture
forms a Mott insulator. (We also checked the state by measuring compressibility of the mixture system and verified that the system was incompressible in the Mott insulator state.) On the other hand, $J_b$ and $J_f$ remain finite in the Mott insulator state. Therefore the fermions and bosons apparently move around, keeping the total local density fixed to an integer value. $J_b$ and $J_f$ have the same value in the Mott state because, when the total number of the atoms on each site is fixed to 1, the bosons and the fermions move only by exchanging their neighboring positions. Namely, when we have a boson current, we always have a fermion current in the opposite direction.

We show in Fig. 2 the current-current correlation function of the bosons for different system sizes with the total density of the bosons and fermions being kept unchanged. We see almost no recognizable size-dependence of the correlation function, which indicates that the finite stiffness of $J_b$ is not induced by a finite size effect. So, apparently, we have a strange Mott insulator of the boson-fermion mixture, inside which each species of the atoms are moving by switching their positions. As shown below, however, this could be a special case realized in one dimension and would not be expected in three dimensional systems.

![Figure 1. Various stiffnesses as functions of the boson-fermion interaction. The boson-boson interaction is fixed to $U_{bb} = 10$.](image1.png)

![Figure 2. Size dependence of $J_b$ in the Mott state.](image2.png)

3.2. B-F correlation function

Next we present the result of the B-F correlation function $C(l)$ in Figs. 3 and 4. As mentioned above, our Hamiltonian is equivalent to one-dimensional antiferromagnetic Heisenberg model when $U_{bb}$ and $U_{bf}$ are both infinite. We know that the B-F correlation (SDW correlation in the language of spins) of antiferromagnetic Heisenberg model exhibits a power-law decay $l^{-1}$ since we could only have a quasi long-range order in one dimension.

In Fig. 3, $C(l)$ demonstrates a power-law decay $l^{-\alpha}$ for 30 bosons and 30 fermions on 60 sites with $U_{bf}$ fixed to 3.0. The power $\alpha$ depends on the interaction strength and becomes closer to 1 as the interactions get stronger. Figure 4 shows $C(l)$ for 40 bosons and 20 fermions. In this case, the factor $(-1)^l$ in Eq. (3) was modified appropriately according to the number ratio of the bosons and the fermions. (To be more specific, the factor was changed to $(-1)^{l'}$ where $l' = 1$ when $l$ is a multiplier of 3 and $l' = 0$ otherwise.) We could see the power law behavior of the correlation function also in Fig. 4.
4. Conclusions
We performed QMC simulations of one-dimensional bose-fermi mixture systems on a periodic optical lattice with strong repulsive interactions and found that the strong interactions could drive the systems into a Mott insulator state. The calculation of the B-F correlation function indicated the presence of an antiferromagnetic quasi long-range order where the bosons and the fermions align alternately. We could therefore expect a clear long-range order in a three-dimensional mixture.

The stiffness calculation showed that the bosons and fermions moved inside the Mott insulator, unlike pure-boson or pure-fermion Mott insulator. However, we believe that this is characteristic to one-dimensional systems and would not be observed in three-dimensional ones. In one dimension, we have only quasi long-range order in the atom configuration inside the Mott insulator and so the bosons and fermions are located alternately only approximately, which would not contradict the finite stiffness of each species of the atoms. However in three dimensions, this quasi order would become a real long-range order and the bosons and fermions align exactly alternately (if the number of the bosons and that of the fermions are the same), which prohibits the motion of the bosons and fermions. In actual experimental situations, therefore, the bosons and fermions of the mixture systems would have a rigid order in their positional configuration in the Mott insulator state.

5. References
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