Fermion-induced decoherence of bosons in optical lattices

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Abstract. Bose-Fermi mixtures with attractive Bose-Fermi interactions in one-dimensional optical lattices are studied by using Quantum Monte Carlo simulations of an extended Bose-Fermi Hubbard model. We first derived the extended Hubbard model with the hopping terms of each species modified to include interaction effects. Bosonic Mott transition induced by introducing fermions into bosons is demonstrated by the simulations.

1. Introduction

Ultracold atoms in optical lattices presented a new way of analyzing particles on periodic potentials [1]. Various phenomena have been realized in the experiments. For example, superfluid-Mott insulator transition [2], shell structure formation in real-space distribution under a confining potential [3], and localizations [4, 5, 6] were observed in bosonic systems. These phenomena can be well described with conventional Hubbard models.

Bose-Fermi mixtures are also an interesting target of ultracold atom experiments and physical properties of the mixtures are well described with a Bose-Fermi-Hubbard model [7]. However, phenomena that this model cannot explain have been observed in experiments of Bose-Fermi mixtures in optical lattices [8, 9, 10]. In these experiments, bosons lost their coherence and underwent a Mott transition as fermions, which attractively interacted with the bosons, were introduced to the system. The analysis of ordinary Bose-Fermi-Hubbard model with a confining potential however showed an opposite result that the bosons maintained the superfluid coherency even in the presence of the fermions [11, 12].

Lühmann et al. [13] discussed a self-trapping effect caused by the attractive boson-fermion interactions to explain the disappearance of the superfluid coherency. When there are some bosons in a well of the lattice potential, the wave function of the fermion in the same well would be squeezed through the boson-fermion interactions. Then the squeezed wave function would produce a narrower and deeper effective potential for the bosons, which makes the bosonic hopping parameter smaller and induces a bosonic Mott transition.

We propose another scenario about the change of the hopping parameters with focus on the terms that are usually ignored in the Hubbard model. In the followings it will be shown that the hopping parameter of the bosons/fermions could locally changes depending on the presence/absence of the fermions/bosons nearby.

For the observation of physical properties of our extended Hubbard model, numerical simulations were conducted and the fermion-induced Mott transition of the bosons was successfully demonstrated. In the simulations the superfluid density and the visibility were calculated as functions of the number of the fermions. It was then confirmed that the superfluid coherency of the bosons vanished with the introduction of the fermions when the attractive boson-fermion interactions were large enough.

The paper is organized as follows. We derive an extended Hubbard model in section 2. Section 3 presents the results of the simulations. A brief summary and discussions are given in section 4.

2. Extended Bose-Fermi Hubbard model

We introduce an effective model of bosons and fermion strongly correlating with each other. One-dimensional bosons and (spin-polarized) fermions in an optical lattice with contact interactions can be generally written as follows.

$$H = \int dx \psi_B^\dagger(x) \left[\frac{p_x^2}{2m_B} + V(x) \right] \psi_B(x) + \int dx \psi_F^\dagger(x) \left[\frac{p_x^2}{2m_F} + V(x) \right] \psi_F(x) \tag{1}$$

$$+ \frac{g_{BB}}{2} \int dx \psi_B^\dagger(x) \psi_B^\dagger(x) \psi_B(x) \psi_B(x) + g_{BF} \int dx \psi_B^\dagger(x) \psi_F^\dagger(x) \psi_F(x) \psi_B(x),$$

where $V(x)$ presents the optical lattice potential and $\psi_B(x)$ and $\psi_F(x)$ are the boson and fermion field operators respectively. The coupling constants are given by $g_{BB} = \frac{4\pi a_{BB}\hbar^2}{m_B}$ and $\frac{2\pi a_{BF}\hbar^2}{M}$ where $M = \frac{2m_B m_F}{m_B + m_F}$ is the reduced mass, and a_{BB} and a_{BF} are boson-boson and boson-fermion s-wave scattering lengths respectively.

In the periodic optical lattice, the field operators can be expanded by Wannier functions as $\psi_B(x) = \sum_i b_i w_B(x - x_i)$ and $\psi_F(x) = \sum_i f_i w_F(x - x_i)$. Here, b_i and f_i are annihilation operators of the bosons and the fermions respectively at the i-th well of the potential and $w(x)$ is the Wannier function. Since we are only interested in low energy behaviors of the system, we only take account of the lowest energy Wannier function $w(x)$. Ordinary Bose-Fermi Hubbard Hamiltonian can be derived from the Hamiltonian H by using the expansion. In the derivation, the terms of relatively small overlap integrals are all discarded. For example, the following gives largest contribution to the boson-fermion interaction term.

$$g_{BF} \sum_i \int dx \, |w_B(x - x_i)|^2 \, |w_F(x - x_i)|^2 \, b_i^\dagger b_i f_i^\dagger f_i. \tag{2}$$

On the other hand, the terms of the following type contain smaller overlap integrals and are usually omitted in Bose-Fermi Hubbard model.

$$g_{BF} \sum_{\langle i,j \rangle} \int dx \, |w_F(x - x_i)|^2 \, w_B^*(x - x_i) w_B(x - x_j) f_i^\dagger f_i b_i^\dagger b_j. \tag{3}$$

However we consider that this kind of terms would be a key for the explanation of the experimentally observed fermion-induced Mott transition. Including (3), the hopping term of the bosons can be expressed as

$$H_B^{hop} = -\sum_{\langle i,j \rangle} \left[t_B^0 - \Delta_B (f_i^\dagger f_i + f_j^\dagger f_j) \right] b_i^\dagger b_j + h.c., \tag{4}$$

where t_B^0 is ordinary hopping parameter in the tight binding approximation and $\Delta_B = -(|g_{BF}|/2) \int dx \, |w_F(x-x_i)|^2 \, w_B^*(x-x_i)w_B(x-x_j)$. Here we assumed attractive boson-fermion interactions, $g_{BF} < 0$. t_F^0 and Δ_F are defined in a similar manner. With this hopping term, our extended Hamiltonian can be written in the form

$$H = -\sum_{\langle i,j \rangle} \left[t_B^0 - \Delta_B(n_{F,i} + n_{F,j}) \right] b_i^\dagger b_j - \sum_{\langle i,j \rangle} \left[t_F^0 - \Delta_F(n_{B,i} + n_{B,j}) \right] f_i^\dagger f_j + h.c. \qquad (5)$$

$$+ \frac{U_{BB}}{2} \sum_i n_{Bi}(n_{Bi} - 1) + U_{BF} \sum_i n_{Bi} n_{Fi},$$

where n_{Bi} (n_{Fi}) is the number operator of the bosons (fermions) at the site i, and U_{BB} and U_{BF} present on-site boson-boson and boson-fermion interactions respectively.

Note that, in this model, the hopping energy of the bosons (fermions) changes depending on the presence of the fermions (bosons) at each site. In a pure boson system with no fermions, the hopping parameter of the bosons is always t_B^0 at any site. With the introduction of fermions to the system, the hopping parameter of the bosons becomes $t_B^0 - \Delta_B$ or $t_B^0 - 2\Delta$ at the sites where the fermions are present. Figure 1 illustrates these three cases.
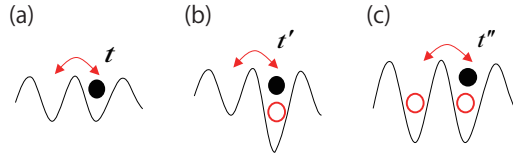

Figure 1. (a), (b) and (c) illustrate effective potential wells of the bosons (filled black circle). In (a) with no fermions, the boson hops to the next site with the transfer energy $t(= t_B^0)$. In (b) with a single fermion (open red circle) the boson hops with $t'(= t_B^0 - \Delta_B)$. In (c) with two fermions, the boson hops with $t''(= t_B^0 - 2\Delta_B)$.

In a mean-field sense, the average hopping energy of the bosons would decrease as the number of the fermions increases. We could therefore expect that the bosons would undergo a Mott transition when a sufficient number of the fermions are introduced to the system and when other conditions of e.g. the number of the bosons and the boson-boson interactions are met.

3. Numerical results

To confirm that the above scenario is correct, we performed Quantum Monte Carlo Simulation(QMC) of the extended Hubbard Hamiltonian (6) that we derived. The QMC is based on a stochastic Green's function method in the canonical ensemble [14, 15]. Since fermions in one dimension can be mapped on hard-core bosons exactly through the Jordan-Wigner transformation, we employ the hard-core bosons in the simulations to avoid a negative sign problem but have to take account of the transformation effect in the calculation of physical quantities of the fermions. We simulated 64 bosons on 64 sites and changed the number of the fermions N_f from 0 to 64. To obtain a qualitative view of the transition we set $t_B^0 = t_F^0 = 1$ for simplicity. The boson-boson interaction was set to $U_{bb} = 4$ with which the bosons are in a superfluid state in the absence of the fermions. The inverse temperature and the boson-fermion interaction were set to $\beta = 64$ and $U_{BF} = -4$ respectively.

Calculation result of the superfluid density ρ_b is shown in figure 2 as a function of N_f with different Δ_B. The superfluid density is calculated by $\rho_b = \frac{\langle W^2 \rangle}{2t_B^0 \beta L^{-1}}$ [16] where W is the winding number and L is the system size. As explained above, in the absence of fermions, the hopping

parameter of the bosons is t_B^0 at any site and the bosons are in the superfluid state as we chose relatively small boson-boson interactions. In the presence of 64 fermions on 64 lattice sites, on the other hand, the hopping energy t_B is given by $t_B^0 - 2\Delta_B$ for any sites. While with $\Delta_B > 0.2$ the ratio U_{BB}/t_B becomes large enough to form a bosonic Mott state. Figure 2 shows that the superfluid density vanishes at around $N_f = 45$ with $\Delta_B = 0.3$ and at around $N_f = 35$ with $\Delta_B = 0.4$. When the attractive interaction U_{BF} is sufficiently large, the superfluid density decreases as the fermions are introduced, forming a bosonic Mott state. We confirmed that this fermion-induced bosonic decoherence could also be observed in a Bose-Fermi mixture with a confinement potential.
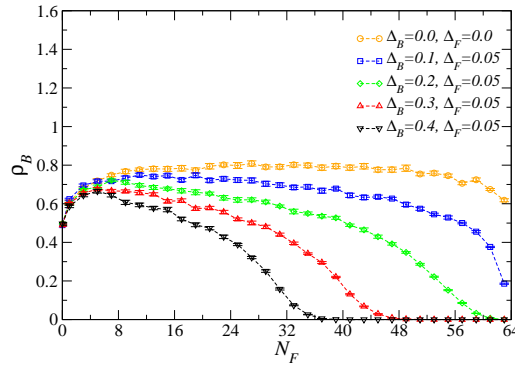

Figure 2. Superfluid density as a function of N_F with different Δ_B and Δ_F.

4. Conclusions
We numerically studied Bose-Fermi mixtures with attractive Bose-Fermi interactions on optical lattices using an extended Bose-Fermi-Hubbard model, which was derived to take account of the effective change of particle hopping energies due to the Bose-Fermi interactions. It was observed in the simulations that the introduction of the fermions induced a bosonic Mott transition as found in the experiments. More detailed calculation results will be given elsewhere.

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