Quantum phase structure of Bose-Bose mixtures in optical lattices

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Abstract. We study the phase structure of mixtures of strongly interacting bosonic atoms in a combined potential of a parabolic trap and an optical lattice. We apply a mean-field approximation and a local density approximation to the Bose-Hubbard model for the Bose-Bose mixture, and calculate the superfluid order parameter and the number of particles per site for both species. We find that the mixture is phase-separated due to the strong onsite inter-species repulsion. Considering a zero-hopping limit, we find that the coexisting phase can appear when onsite inter-species repulsion interaction is weak.

1. Introduction
The ultracold Bose atoms in optical lattices have attracted attention. One of the interesting phenomena exhibited by ultracold Bose atoms in optical lattices is superfluid to Mott insulator phase transition, as experimentally observed [1]. The properties of this system can be well captured by Bose-Hubbard model [2–4].

In 2003, Moore et. al. [5] suggested a loading of a two-species Bose-Einstein condensate into an optical lattice. Recently, Catani et al. [6] produced experimentally a heteronuclear quantum degenerate mixture of $^{87}\text{Rb}$ and $^{41}\text{K}$ in a 3D optical lattice. Superfluid to Mott insulator phase transition of Bose-Bose mixtures was studied by applying the Hubbard model using the perturbation theory [7], the Gutzwiller approach [8], and the quantum Monte Carlo simulation [9]. In particular, Ref.[7] considered the homogeneous case (no trap potential) and concluded that the following phases appear: (1) atomic components are in the SF phase; (2) one component is in SF phase, while the other is in MI phase; (3) both components are in MI phase.

In this paper we focus on Bose-Bose mixtures in a combined potential of a parabolic trap and an optical lattice, using the Bose-Hubbard model. We apply the mean-field approximation and the local density approximation to calculate the spatial profiles of the superfluid order parameters and local number density in a trap potential of this system. In order to gain qualitative insight, we also present the phase diagram in a zero-hopping limit.

2. Bose Hubbard Hamiltonian
We consider the phase structure of mixtures of $^{87}\text{Rb}$ and $^{41}\text{K}$ in a combined potential of a parabolic trap and an optical lattice. We have the following Bose Hubbard hamiltonian for a Bose-Bose mixture;
\[ H = -t_1 \sum_{\langle i,j \rangle} (b_{i1}^\dagger b_{j1} + b_{i1} b_{j1}^\dagger) + \frac{U_1}{2} \sum_i \hat{n}_{i1} (\hat{n}_{i1} - 1) - \mu_1 \sum_i \hat{n}_{i1} \\
- t_2 \sum_{\langle i,j \rangle} (b_{i2}^\dagger b_{j2} + b_{i2} b_{j2}^\dagger) + \frac{U_2}{2} \sum_i \hat{n}_{i2} (\hat{n}_{i2} - 1) - \mu_2 \sum_i \hat{n}_{i2} \\
+ U_{12} \sum_i \hat{n}_{i1} \hat{n}_{i2}, \]

where \( b_{i1}(b_{i2}) \) and \( b_{i2}^\dagger(b_{i2}) \) is the creation (annihilation) operators of \( ^{87}\text{Rb} \) and \( ^{41}\text{K} \) at site \( i \), \( \hat{n}_{i1} \equiv b_{i1}^\dagger b_{i1} \) is the number operator, and \( \langle i,j \rangle \) denotes sum over nearest neighbor sites. \( t_{\alpha}, U_{\alpha} \) and \( \mu_{\alpha} \) (\( \alpha = 1 \) or \( 2 \)) are the hopping amplitude, onsite interaction and the chemical potential for \( ^{87}\text{Rb} \) (\( \alpha = 1 \)) or \( ^{41}\text{K} \) (\( \alpha = 2 \)), respectively. \( U_{12} \) is onsite interaction between \( ^{87}\text{Rb} \) and \( ^{41}\text{K} \). In a mean-field approximation, the hopping term is decoupled as

\[ b_{i1}^\dagger b_{i1} \simeq \langle b_{i1} \rangle b_{i1} + b_{i1}^\dagger \langle b_{i1} \rangle - \langle b_{i1} \rangle^2 \]
\[ = \phi b_{i1} + b_{i1}^\dagger \phi - \phi^2, \]
\[ b_{i2}^\dagger b_{i2} \simeq \langle b_{i2} \rangle b_{i2} + b_{i2}^\dagger \langle b_{i2} \rangle - \langle b_{i2} \rangle^2 \]
\[ = \psi b_{i2} + b_{i2}^\dagger \psi - \psi^2, \]

where \( \phi = \langle b_{i1} \rangle, \psi = \langle b_{i2} \rangle \) are the superfluid order parameters. The Hamiltonian can be written as a sum over single-site terms, \( H = \sum_i H_i \), where

\[ H_i = -zt_1 \phi (b_{i1}^\dagger + b_{i1}) + \frac{U_1}{2} \hat{n}_{i1} (\hat{n}_{i1} - 1) - \mu_1 \hat{n}_{i1} + zt_1 \phi^2 \\
- zt_2 \psi (b_{i2}^\dagger + b_{i2}) + \frac{U_2}{2} \hat{n}_{i2} (\hat{n}_{i2} - 1) - \mu_2 \hat{n}_{i2} + zt_2 \psi^2 \\
+ U_{12} \hat{n}_{i1} \hat{n}_{i2}, \]

with \( z \) being the coordination number. One can obtain the zero-temperature properties of Bose-Bose mixtures by diagonalizing the Hamiltonian \( H_i \) in the occupation number basis \( \{ |n_1, n_2 \rangle \} \) truncated at finite values \( n_{i1} \) and \( n_{i2} \). In order to include the effect of trap potential, we apply a local density approximation (see Ref. [2]). We set local chemical potential for each species as \( \mu_{\ell}^\text{eff} = \mu_{\ell} - \epsilon_{\ell} \) (\( \ell = 1, 2 \)). It should be noted that two species feel different trap potentials because the masses are different.

### 3. Numerical Results

Our main results are shown in Figs. 1-4. From the experiment of Ref.[6], we estimate the parameters as \( U_1: U_2: U_{12} = 1 : 0.34 : 1.85 \) and \( t_1 : t_2 = 1 : 2.39 \) for \( U_1/zt_1 = 40 \). In Fig. 1, we plot the density and superfluid density \( ^{87}\text{Rb} \), when \( ^{41}\text{K} \) is absent. The density of system exhibits the so-called wedding-cake profile, with the plateaus corresponding to Mott-insulator \( (n_1 = 1) \) domains.

Fig. 2 shows the density profile of \( ^{87}\text{Rb} \) and \( ^{41}\text{K} \) mixture. The total number of \( ^{87}\text{Rb} \) is the same as in Fig. 1. This figure exhibits the phase-separation of mixture, since \( U_{12} \) is stronger than \( U_1 \) and \( U_2 \). This result is consistent with the result in Ref.[8]. Comparing Fig. 1 with Fig. 2, the Mott core changes to the superfluid at center of a parabolic trap.

To understand the nature of the phase-separation, we consider a zero-hopping limit \( t_1(t_2) \to 0 \). In Fig. 3, we plot the phase boundaries of occupation number per site.
Figure 1. Density distribution of only $^{87}$Rb in combined potential. Solid line is average number at $i$ site, dash line is superfluid density.

Figure 2. Density distribution of $^{87}$Rb and $^{41}$K mixture in a combined potential. Solid line is the occupation number of $^{87}$Rb, while dotted line is superfluid density of $^{87}$Rb. Chain line is the occupation number of $^{41}$K, while dashed line is superfluid density of $^{41}$K.

Figure 3. The phase boundary of occupation number $(n_1, n_2)$ in the zero-hopping limit, with $U_1 : U_2 : U_{12} = 1 : 0.34 : 1.85$ for $U_1/\varepsilon t_1 = 40$. Solid line shows the boundary between $^{87}$Rb and $^{41}$K. Dotted lines show boundary between the same species with different occupation numbers. In the case of $t_1(t_2) \to 0$, solid line is linear and the slope of solid line changes at the intersections with dotted lines.

Figure 4. The phase boundary of occupation number $(n_1, n_2)$ in the zero-hopping limit, with $U_1 : U_2 : U_{12} = 1 : 0.34 : 0.6$ for $U_1/\varepsilon t_1 = 40$. Solid lines is boundary between $^{87}$Rb and $^{41}$K. Dotted lines are boundaries between the same species with different occupation numbers. Contrary to Fig. 3, the coexisting phase appears in the region enclosed by solid line.

The phase boundary between two phase-separated states $(n_1, 0)$ state and $(0, n_2)$ state is analytically given by

$$\mu_2 = \frac{n_1}{n_2} \mu_1 + \frac{U_2}{2} (n_2 - 1) - \frac{U_1}{2} \frac{n_1}{n_2} (n_1 - 1),$$  \tag{5}$$

where the following relations between the number of $^{87}$Rb ($^{41}$K) and the chemical potential must
be satisfied

\[ U_1(n_1 - 1) + U_{12} n_2 \leq \mu_1 \leq U_1 n_1 + U_{12} n_2 \]
\[ U_2(n_2 - 1) + U_{12} n_1 \leq \mu_2 \leq U_2 n_2 + U_{12} n_1. \]  

(6)

In Fig. 3, we plot the results using the parameters of $^{87}\text{Rb}$ and $^{41}\text{K}$. We see that there is no coexisting phase in the limit $t_1(t_2) \to 0$. This is consistent with Fig. 2.

In Fig. 4, we show the phase diagram obtained by using a smaller value of $U_{12}$. There appears a coexisting phase in a small region. The phase boundary between the coexisting phase and separated phase are now given by a complex formula, so we do not present an explicit form.

4. Conclusions

We studied the quantum phase transition of Bose-Bose mixtures in a combined potential of a parabolic trap and an optical lattice. We found that the spatial phase separation occur for $^{87}\text{Rb}$ and $^{41}\text{K}$ mixtures in a combined potential. This result is understood by considering the Bose-Bose mixtures in a zero-hopping limit $t_1(t_2) \to 0$. When $U_{12}$ is small, the coexisting phase can appear in the system.

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5. References

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