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Phase Diagram of Mixtures of Ultracold Bosons in Optical Lattice

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We study a behaviour of mixture of two species of ultracold bosons trapped in optical lattice. Using mean-field approximation, we determine the phase diagram of the system for wide range of parameters. We observe that each of the groups of atoms can condense into superfluid state or localize and form the Mott insulator, which yields that the whole system is either superfluid, the Mott insulator, or a mixed state. It appears that introduction of interaction between different kinds of atoms can strongly renormalise the phase diagram. It can alter the critical behaviour modifying multi-criticality of crossing points and order of phase transitions between mixed and superfluid states.

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1. Introduction

Ultracold atomic gas in optical lattice provides a perfect, highly controllable model system for simulating complicated phenomena of quantum many-body physics. Properties of atoms can be tuned in wide range starting from geometry of trapping potential, through precise control of particle tunnelling to nature and strength of interatomic interactions [1]. As a result, in bosonic system a phase transition between superfluid and the Mott insulating states can be observed, which is a hallmark of strongly correlated systems [2]. Optical lattices allow for investigation of various systems: purely bosonic or fermionic gases or mixtures of different types or states of atoms. Since particles are trapped in a clean, almost ideal environment, understanding of the underlying phenomena is much easier than in solids, which are perturbed by crystal structure imperfections, or mixing and blending of various effects. However, experimental setups usually require that atoms are in well defined hyperfine states, thus limiting some degrees of freedom by enforcing polarization (e.g. spin). This has stimulated interest in investigation of mixtures of atoms of different kinds [3] or the same atoms, but in two or more different states, i.e. multicomponent gases [4], since it introduces additional degrees of freedom. The problem has also been investigated theoretically within mean-field approach in context of magnetic ordering [5], or superfluid–Mott insulator transition [6]. Two-component bosons have been studied using the Monte Carlo technique, which showed existence of the first-order phase transitions resulting from pairing interactions [7]. Quantum Monte Carlo calculations of properties of binary mixtures of identical bosons allowed for observation of tricritical points on the phase diagram [8]. The problem of competing orders have been also analysed in other contexts, e.g. of ferromagnetic superconductors, where some general scenarios for multicritical systems have been predicted [9]. Here, we systematically analyse phase diagram of mixtures of two kinds of bosons to investigate how competition between order parameters influences the phase diagram and nature of the phase transitions present in the system.

The remainder of the paper is as follows. In Sect. 2 we briefly present the model and method of reduced occupation basis that we use. In the following section, we calculate phase diagrams in the symmetric (two identical sets of bosons interacting with each other) and fully asymmetric case and discuss the nature of phase transition occurring in the system. Finally, in Sect. 4 we conclude our results.

2. Model and method

Strongly interacting atomic gases in optical lattices are well described by the Bose–Hubbard model [10]. Here, we investigate a behaviour of a mixture of two types of bosons (A and B) that are coupled together with density–density on-site interaction. The Hamiltonian is as follows:

$$\begin{aligned}\hat{H} = &-t_A \sum_{\langle i,j\rangle} a_i^{+} a_j - \mu_A \sum_i n_i \\ &+\frac{U_A}{2}\sum_i n_i\,(n_i-1) - t_B \sum_{\langle i,j\rangle} b_i^{+} b_j - \mu_B \sum_i m_i \\ &+\frac{U_B}{2}\sum_r m_i\,(m_i-1) + W\sum_i n_i\, m_i,\end{aligned} \quad (1)$$

where $a_i^\dagger$ ($b_i^\dagger$), a_i (b_i) are creation and annihilation operators of bosons A and B, respectively. Furthermore, i and j label sites of a lattice with coordination number z and total number of lattice sites being N. The particles are moving between the neighbouring sites with hopping elements t_A and t_B. On-site interactions between atoms of the same type occur with energies U_A and U_B, while different types interact with energy W. Finally, $n_i = a_i^\dagger a_i$ and $m_i = b_i^\dagger b_i$ are the densities of A and B bosons, which are controlled by the chemical potentials μ_A and μ_B. The bosonic operators then can be presented as a fluctuation around their average values:

$$a_i = \langle a_i\rangle + \delta a_i = \phi_A + \delta a_i$$

$$b_i = \langle b_i \rangle + \delta b_i = \phi_B + \delta b_i. \quad (2)$$

Here, ϕ_A and ϕ_B are the statistical averages of the bosonic operator and serve as order parameters, whose non-zero values signal presence of the superfluid phase (condensate). Introducing substitution (2) into Hamiltonian (1) and neglecting quadratic fluctuation terms ($\delta a_i^\dagger \delta a_i = 0$, $\delta b_i^\dagger \delta b_i = 0$) one arrives at the mean-field approximation Hamiltonian

$$\begin{aligned}\hat{H}_{\mathrm{MFA}} &= \phi_A^2 t_A z N + \phi_B^2 t_B z N \\ &-\phi_A t_A z \sum_i \left(a_i^+ + a_i\right) - \phi_B t_B z \sum_i \left(b_i^+ + b_i\right) \\ &+\frac{U_A}{2} \sum_i n_i \left(n_i - 1\right) + \frac{U_B}{2} \sum_{\boldsymbol{r}} m_i \left(m_i - 1\right) \\ &+W \sum_i n_i m_i - \mu_A \sum_i n_i - \mu_B \sum_i m_i, \end{aligned} \quad (3)$$

that is only single-site dependent. As a result, site index i can be omitted and summations over lattice sites can be easily performed. The partition function of the system can be written in the occupation number basis

$$\begin{aligned} Z &= \mathrm{Tr}\, \mathrm{e}^{-\beta \hat{H}_{\mathrm{MFA}}} = \mathrm{e}^{-\beta N z t_A \phi_A^2 - \beta N z t_B \phi_B^2} \\ &\times \sum_{n,m=0}^{\infty} \left\langle m, n \left| \mathrm{e}^{-\beta N \hat{H}_{\mathrm{local}}} \right| m, n \right\rangle, \end{aligned} \quad (4)$$

with $\beta = 1/k_B T$ and T being the temperature. The matrix element of the local Hamiltonian reads

$$\begin{aligned} \left\langle m', n' \left| \hat{H}_{\mathrm{local}} \right| m, n \right\rangle &= \delta_{n',n} \delta_{m',m} \Big[-\mu_A n - \mu_B m \\ &+\frac{U_A}{2} n \left(n-1\right) + \frac{U_B}{2} m \left(m-1\right) + W n m \Big] \\ &-\delta_{m',m} z t_A \phi_A \left(\delta_{n',n-1} \sqrt{n} + \delta_{n',n+1} \sqrt{n+1}\right) \\ &-\delta_{n',n} z t_B \phi_B \left(\delta_{m',m-1} \sqrt{m} + \delta_{m',m+1} \sqrt{m+1}\right). \end{aligned} \quad (5)$$

This leads to the expression for the free energy

$$\begin{aligned} f &= -\frac{1}{\beta N} \ln Z = z t_A \phi_A^2 + z t_B \phi_B^2 \\ &-\frac{1}{\beta N} \ln \sum_{n,m=0}^{\infty} \left\langle m, n \left| \mathrm{e}^{-\beta N \hat{H}_{\mathrm{local}}} \right| m, n \right\rangle. \end{aligned} \quad (6)$$

In the strong coupling limit, the separation between energy levels grows quadratically with the number of particles. As a result, in the ground state only finite number of states m, n has significant contribution to the free energy. This allows to reduce the Hamiltonian basis and truncate the summation in Eq. (6) (n, $m = 0, \ldots, N_{\max}$).

3. Phase diagram

In order to determine the phase diagram, it is necessary to minimize the free energy of the system in Eq. (6) in terms of values of order parameters ϕ_A and ϕ_B. Here, we limit $N_{\max} = 5$, which leads to correct description of systems with no more than 4 bosons of each kind at every lattice site in the ground state. Critical line at which ϕ_A or ϕ_B zeros delimits superfluid (SF) and the Mott insulating (MI) states of A or B bosons, respectively. Regions under the critical line (lower values of t/U) correspond to the Mott insulator state of atoms, while in the region over the critical line (larger values of t/U) the bosons are in superfluid state. As a result, the system can occupy one of four possible states: (a) A-SF ($\phi_A \neq 0$), B-SF ($\phi_B \neq 0$), (b) A-SF ($\phi_A \neq 0$), B-MI ($\phi_B = 0$), (c) A-MI ($\phi_A = 0$), B-SF ($\phi_B \neq 0$), or (d) A-MI ($\phi_A = 0$), B-MI ($\phi_B = 0$). Since usually phase diagram of bosons in optical lattices are calculated as a dependence of critical hopping (t/U) on the chemical potential (μ/U), we further parametrize the system to accommodate the differences between sorts of bosons:

$$\begin{aligned} t_B &= \gamma t_A = \gamma t, \\ \mu_B &= \xi \mu_A = \xi \mu, \\ U_B &= \zeta U_A = \zeta U. \end{aligned} \quad (7)$$

First we consider a symmetric case $\gamma = \zeta = \xi = 1$ ($t_B = t_A = t$, $\mu_B = \mu_A = \mu$, $U_B = U_A = U$), in which both groups of particles behave identically. However, coupling W between them can be modified. Such case was studied earlier by the means of different methods [5–8]. For $W = 0$, the phase transition lines of both condensates coincide and are identical as for a ultracold bosonic gas with single kind of particles [11] (see Fig. 1). For hopping lower than the critical value, both species of bosons are in the Mott insulating phase (A-MI, B-MI), while for higher — in the superfluid (A-SF, B-SF). When the interaction W is switched on, extra lobes of the Mott insulator phase appear between the original lobes and their width is equal to W/U.

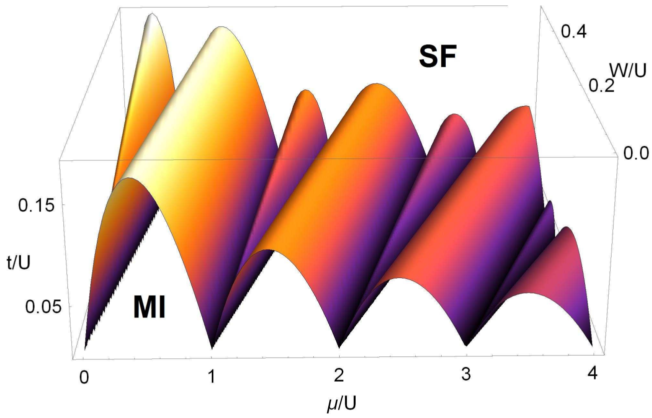

Fig. 1. Phase diagram of a mixture of atomic gases in optical lattice in symmetric case $t_B = t_A$, $\mu_B = \mu_A = \mu$, $U_B = U_A = U$ for interactions between different species $W = 0, \ldots, 0.5$.

In non-symmetric case, critical lines of two kinds of particles no longer coincide. As a result, ground state of each condensate may be dependent on the state of the other

$$\left.\frac{\partial f\left(\phi_A, \phi_B\right)}{\partial \phi_A}\right|_{\phi_A=0} = 0, \qquad \left.\frac{\partial f\left(\phi_A, \phi_B\right)}{\partial \phi_B}\right|_{\phi_B=0} = 0, \quad (8)$$

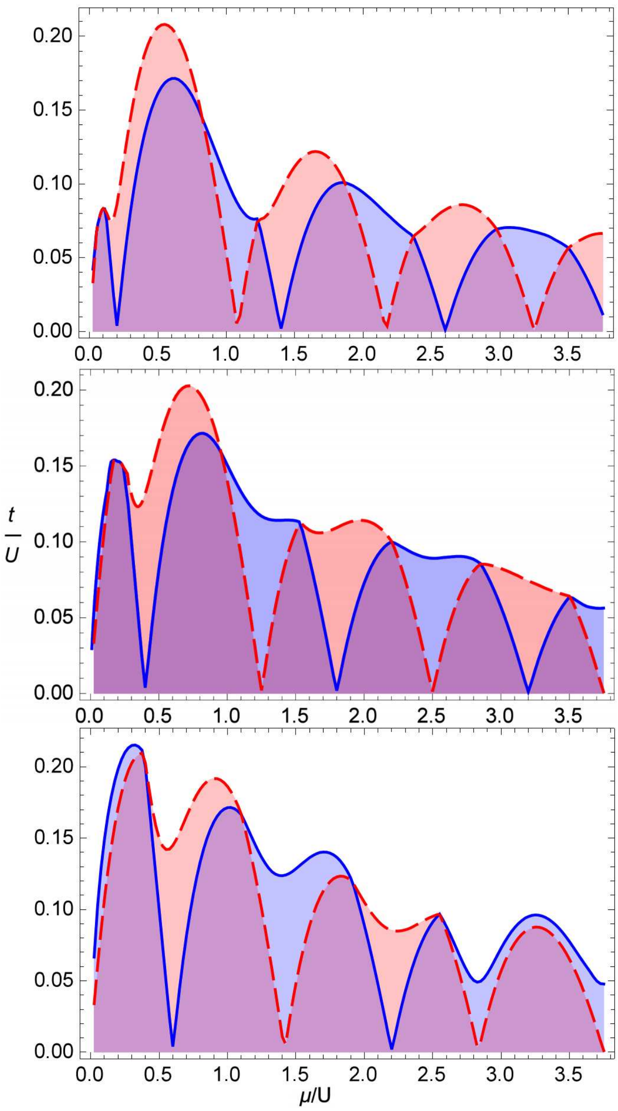

Fig. 2. Phase diagrams of a mixture of two atomic gases in optical lattice for $\gamma = 0.9$, $\xi = 1.2$ and $\zeta = 1.1$ and selected values of interaction between species $W = 0.2, 0.4, 0.6$ (from top to bottom). Solid (blue) line corresponds to bosons A critical line, while dashed (red) line denotes bosons B critical line. Areas below each line represent the Mott insulator of the respective type of bosons.

while ϕ_A and ϕ_B are not simultaneously zero. The order parameters have to be calculated using their definitions:

$$\phi_A = \langle a_i \rangle = \frac{1}{Z} \operatorname{Tr} a_i \, \mathrm{e}^{-\beta \hat{H}_{\mathrm{MFA}}},$$

$$\phi_B = \langle b_i \rangle = \frac{1}{Z} \operatorname{Tr} b_i \, \mathrm{e}^{-\beta \hat{H}_{\mathrm{MFA}}}, \tag{9}$$

and the resulting phase diagrams have to be determined from the set of Eqs. (8) and (9). The critical lines for various values of asymmetry parameters are presented in Fig. 2. The lobes delimiting superfluid and the Mott insulating states of both kinds of bosons no longer have regular shape. Depending on values of γ, ζ and ξ, they can be strongly influenced by the presence of the other order parameter, which is pronounced especially around the multicritical (crossing) points. All four possible ground states of the mixture being the combination of SF and MI states of each kind of particles can be observed.

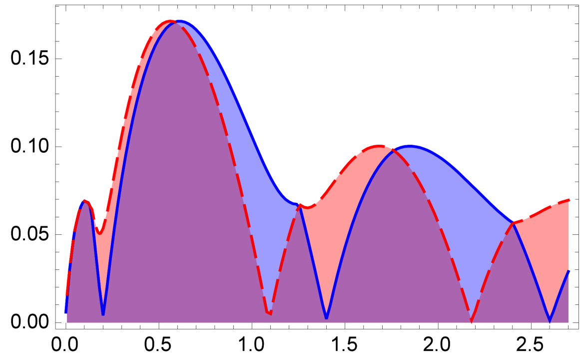

Fig. 3. Phase diagram of a mixture of two atomic gases in optical lattice in case $W = 0.2$, $\gamma = 1$, $\xi = 1.1$ and $\zeta = 1$. Solid (blue) line corresponds to bosons A critical line, while dashed (red) line denotes bosons B critical line. Areas below each line represent Mott insulator of the respective type of bosons.

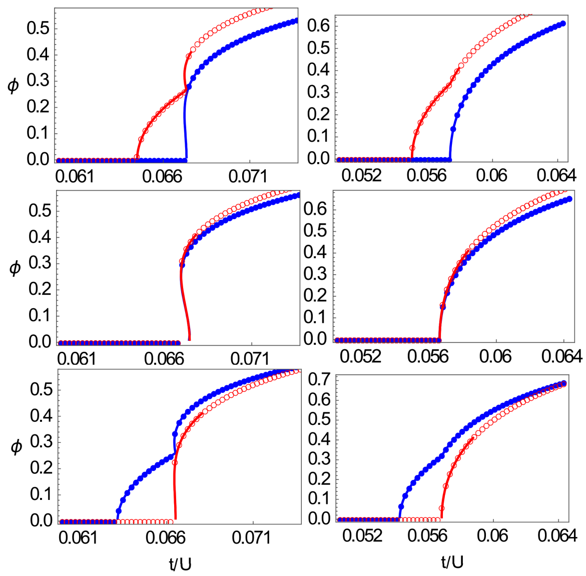

Fig. 4. Dependence of order parameters ϕ_A and ϕ_B on hopping t/U for $W = 0.2$, $\gamma = 1, \xi = 1.1$, $\zeta = 1$ and chemical potential $\mu = \mu_c - 0.01, \mu_c, \mu_c + 0.01$ (from top to bottom), $\mu_c = 1.238$ (left), 2.402 (right). Filled (blue) circles denote ϕ_A, while empty (red) circles correspond to ϕ_B.

The exact behaviour of the critical lines around the crossing points depends on the location on the phase diagram. At some points, the presence of the other order parameter does not influence the critical line, while in others — strongly modifies its shape. In order to investigate this behaviour, we concentrate on a selected asymmetric phase diagram with $W = 0.2$, $\gamma = 1$, $\xi = 1.1$ and

TABLE I

Multicritical points in the region $\mu/U = 0.2, \ldots, 2.5$ in the phase diagram from Fig. 3.

Critical point number	μ/U	t/U
1	0.5852	0.1709
2	1.2537	0.0670
3	1.7629	0.0978
4	2.4022	0.0576

$\zeta = 1$ (see Fig. 3) and four multicritical points that occur in the region of the chemical potential $\mu/U = 0.2, \ldots, 2.5$ (see Table I). At points 1 and 3, critical lines of both condensates do not exhibit any deflection at crossings. However, around points 2 and 4 significant deflection is visible. Therefore, we calculate the values of order parameters along constant chemical potential lines as a function of hopping t/U at the multicritical points and for slightly lower and higher μ/U. The results are presented in Fig. 4. Close to the point 2, the phase transition from A-MI, B-MI phase to A-MI, B-SF or A-SF, B-MI is continuous. However, while hopping is increased, the transitions to A-SF, B-SF state are of the first order, which manifests in the finite jump of the order parameters ϕ_A or ϕ_B. Investigating the behaviour of the order parameters exactly at the critical point, a discontinuous transition from the Mott insulator to the superfluid state (A-MI, B-MI to A-SF, B-SF) can be observed. On the other hand, point 4 is an intersection of two second order transition lines. This observation can be confirmed by calculating the free energy of the system at critical points 2 and 4. The result is depicted in Fig. 5. The free energy of the system at point 2 shows two minima that are characteristic for first-order phase transition and coexisting metastable states of the Mott insulator ($\phi_A = 0$, $\phi_B = 0$) and superfluid ($\phi_A \neq 0$, $\phi_B \neq 0$). This situation is clearly different from scenarios investigated in [9], where such scenario was not present and requires further investigations.

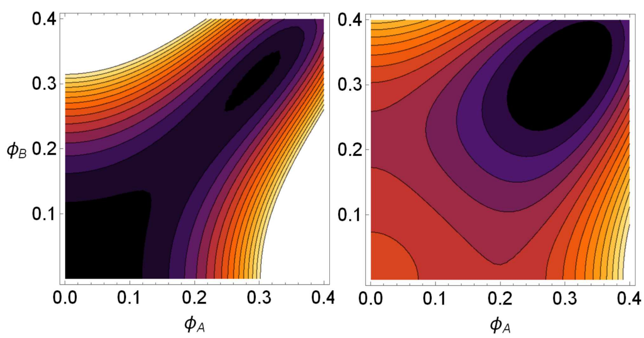

Fig. 5. Free energy of a mixture of atomic gases in optical lattice in case $W = 0.2$, $\gamma = 1$, $\xi = 1.1$ and $\zeta = 1$ near points 2 (left) and 4 (right) from Table I and Fig. 3. Darker colours denote lower energy.

Presence of the first-order phase transition lines in the phase diagrams requires more careful analysis of the condition for the position of the critical lines (minimalisation of the free energy) in Eq. (8) since instead of a single, global minimum, multiple minima can occur. In such case, position of thermodynamic phase transition can be determined by comparing and equating values of the free energy of both phases

$$f(\phi_A = 0, \phi_B = 0) = f(\phi_A \neq 0, \phi_B \neq 0), \tag{10}$$

where non-zero values of order parameters are calculated self-consistently from Eq. (9).

4. Conclusion

We have investigated the phase diagrams of mixtures of atomic gases in optical lattice interacting via density–density coupling for various parameters of the model. In the Bose–Hubbard model of a single condensate the phase transition from the Mott insulator to the superfluid is always continuous. However, we showed that the presence of an additional order parameter in connection with strong interactions between different species of atoms can lead to change of the nature of the phase transition close to some multicritical points. As a result, they change from tetracritical to bicritical, while the critical lines between MI–SF and SF–SF phases become of the first order.

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