Multicriticality and interaction-induced first-order phase transitions in mixtures of ultracold bosons in an optical lattice

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We study a critical behavior of mixtures of two species of ultracold bosons trapped in an optical lattice. Using mean-field approximation, we determine the ground-state phase diagram of the system for a wide range of parameters. The introduction of interactions between different species of atoms strongly renormalizes the phase diagram. It can alter the critical behavior modifying multicriticality of crossing points and order of phase transitions in their vicinity between mixed and superfluid states. For selected values of model parameters, the behavior of the system falls out of the XY model universality class, which usually is a hallmark of superfluid phase transition. We supplement our analysis with analytical calculations to explain the observed scenario.

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I. INTRODUCTION

Multicritical systems have been extensively studied in recent years [1]. Their uniqueness lies in the possibility of coupling between multiple different order parameters that may give rise to surprising critical properties. The most interesting situation appears when the coupling occurs around the intersection of at least two critical lines on the phase diagram of the system, when the underlying phase transitions coincide for the same or similar parameters of the system. If the coupling happens to be large, the nature of the multicritical points can be altered along with the character of the individual phase transitions. Multicritical phenomena have been investigated in many contexts: anisotropic antiferromagnets [2], He^3-He^4 solutions [3], ferromagnetic superconductors [4], etc. However, they can also be observed in systems of ultracold atomic gases in optical lattices, which provide an ideal, highly controllable model setup, for simulating complicated processes of quantum many-body physics. Properties of these atoms can be tuned in a wide range of parameters such as geometry of trapping potential, nature and strength of interatomic interactions, and accurate control of particle tunneling [5]. Optical lattices provide an opportunity to investigate various systems: purely bosonic [6] or fermionic gases, or mixtures of different types [7,8] or states of atoms [9]. High tunability in connection with multiple order parameters that can be present, renders them very good objects to investigate the multicritical phenomena. This has stimulated interest in the investigation of mixtures of atoms of different species or the same atoms, but in two or more different states, i.e., multicomponent gases. The problem has been studied both experimentally [10,11] and theoretically [12–18]. In the case of bosons, changing the ratio between kinetic energy and interparticle interactions drives the system through the zero-temperature superfluid-Mott insulator phase transition, which belongs to the XY model universality class. Recently, the finite-temperature phase diagram of binary bosonic mixtures has been determined using multiple methods [19]. Various phases have been identified along with critical lines and crossing points. Furthermore, finite-size scaling of quantum Monte Carlo simulations in the hard-core limit determined the universality class of the transition lines that correspond to the Bose-Einstein condensation of one of the two species. This proved that the critical behavior of the system belonged to the three-dimensional XY universality class characterized by the breaking of a global U(1) symmetry and by short-range effective interactions. It has been further confirmed by a renormalization group analysis of the Landau-Ginzburg Φ^4 theory of two complex fields with global $\mathrm{U}(1) \oplus \mathrm{U}(1)$ symmetry.

In the present paper we show that strong interactions between two bosonic condensates can lead to previously unobserved behavior around selected crossing points, where in the presence of a condensate of one type of atom, the other condenses abruptly with the first-order phase transition. We systematically analyze the phase diagram of such mixtures to find out how the competition between order parameters influences the nature of the phase transitions present in the system. We show that, in order to qualitatively describe the observed scenario, it is necessary to go beyond the quartic Landau theory. The remainder of the paper is as follows. In Sec. II we briefly present the model and method of reduced occupation basis that is used for numerical calculations. In the following section, we present phase diagrams in the symmetric (two identical sets of bosons interacting with each other) and asymmetric cases and discuss the nature of phase transition occurring in the system. In Sec. IV we perform analytical calculations based on the free-energy expansion, which allow us to confirm our numerical results and determine the criteria for types of multicritical points. Finally, in Sec. V we conclude with our results.

II. MODEL AND METHOD

Strongly interacting ultracold bosons in optical lattices are well described by the Bose-Hubbard model [20]. In this paper we study a behavior of a mixture of two atomic gases (A and B) that are coupled together with an on-site density-density interaction. The Hamiltonian of the systems is as follows:

$$\begin{aligned}\hat{H} = &-t_A \sum_{\langle i,j\rangle} \hat{a}_i^\dagger \hat{a}_j - \mu_A \sum_i \hat{n}_i + \frac{U_A}{2} \sum_i \hat{n}_i(\hat{n}_i - 1) \\ &- t_B \sum_{\langle i,j\rangle} \hat{b}_i^\dagger \hat{b}_j - \mu_B \sum_i \hat{m}_i + \frac{U_B}{2} \sum_{\mathbf{r}} \hat{m}_i(\hat{m}_i - 1) \\ &+ W \sum_i \hat{n}_i \hat{m}_i, \end{aligned} \tag{1}$$

where $\hat{a}_i^\dagger$ ($\hat{b}_i^\dagger$), $\hat{a}_i$ ($\hat{b}_i$) are the creation and annihilation operators of bosons A and B, respectively. The lattice is characterized by the total number of lattice sites N and the coordination number z, while i and j label the lattice sites. The movement of the particles between the neighboring sites is described by 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, $\hat{n}_i = \hat{a}_i^\dagger \hat{a}_i$ and $\hat{m}_i = \hat{b}_i^\dagger \hat{b}_i$ are the number operators for A and B bosons. The density of particles is controlled by the chemical potentials μ_A and μ_B. The bosonic operators then can be represented as a fluctuation around their average values:

$$\begin{aligned} \hat{a}_i &= \langle \hat{a}_i \rangle + \delta\hat{a}_i \equiv \phi_A + \delta\hat{a}_i, \\ \hat{b}_i &= \langle \hat{b}_i \rangle + \delta\hat{b}_i \equiv \phi_B + \delta\hat{b}_i. \end{aligned} \tag{2}$$

Here, ϕ_A and ϕ_B are the statistical averages of the bosonic operators and play the role of order parameters, whose nonzero values indicate the presence of the superfluid phase (condensate):

$$\begin{aligned} \phi_A &\equiv \langle \hat{a}_i \rangle = \frac{1}{Z} \operatorname{Tr} \hat{a}_i e^{-\beta \hat{H}}, \\ \phi_B &\equiv \langle \hat{b}_i \rangle = \frac{1}{Z} \operatorname{Tr} \hat{b}_i e^{-\beta \hat{H}}. \end{aligned} \tag{3}$$

Introducing substitution (2) into the Hamiltonian (1) and neglecting quadratic fluctuation terms ($\delta\hat{a}_i^\dagger \delta\hat{a}_i = 0$, $\delta\hat{b}_i^\dagger \delta\hat{b}_i = 0$) one obtains the mean-field approximation Hamiltonian:

$$\begin{aligned} \hat{H}_{\mathrm{MF}} &= \phi_A^2 t_A z N + \phi_B^2 t_B z N \\ &\quad - \phi_A t_A z \sum_i (\hat{a}_i^\dagger + \hat{a}_i) - \phi_B t_B z \sum_i (\hat{b}_i^\dagger + \hat{b}_i) \\ &\quad + \frac{U_A}{2} \sum_i \hat{n}_i(\hat{n}_i - 1) + \frac{U_B}{2} \sum_i \hat{m}_i(\hat{m}_i - 1) \\ &\quad + W \sum_i \hat{n}_i \hat{m}_i - \mu_A \sum_i \hat{n}_i - \mu_B \sum_i \hat{m}_i \end{aligned} \tag{4}$$

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

$$\begin{aligned} Z &= \operatorname{Tr} e^{-\beta \hat{H}_{\mathrm{MF}}} \\ &= e^{-\beta N z t_A \phi_A^2 - \beta N z t_B \phi_B^2} \sum_{n,m=0}^{\infty} \langle m,n | e^{-\beta N \hat{H}_{\mathrm{os}}} | m,n \rangle, \end{aligned} \tag{5}$$

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

$$\begin{aligned} &\langle m',n' | \hat{H}_{\mathrm{os}} | m,n \rangle \\ &= \delta_{n',n}\delta_{m',m} \Big[-\mu_A n - \mu_B m \\ &\quad + \frac{U_A}{2} n(n-1) + \frac{U_B}{2} m(m-1) + W n m \Big] \\ &\quad - \delta_{m',m} z t_A \phi_A (\delta_{n',n-1}\sqrt{n} + \delta_{n',n+1}\sqrt{n+1}) \\ &\quad - \delta_{n',n} z t_B \phi_B (\delta_{m',m-1}\sqrt{m} + \delta_{m',m+1}\sqrt{m+1}). \end{aligned} \tag{6}$$

This leads to the following expression for the free energy:

$$\begin{aligned} f &= -\frac{1}{\beta N} \ln Z \\ &= z t_A \phi_A^2 + z t_B \phi_B^2 - \frac{1}{\beta N} \ln \sum_{n,m=0}^{\infty} \langle m,n | e^{-\beta N \hat{H}_{\mathrm{os}}} | m,n \rangle. \end{aligned} \tag{7}$$

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 one to reduce the Hamiltonian basis and truncate the summation in Eq. (7) at some arbitrarily selected value $N_{\max}$ ($n,m = 0, \ldots, N_{\max}$). The validity of this truncation can be checked by observing the effect of a variation of $N_{\max}$ on the obtained results.

III. PHASE DIAGRAM

In order to determine the phase diagram of the system, minimization of the free energy in Eq. (7) in terms of values of order parameters ϕ_A and ϕ_B is required. In the following, we limit ourselves to $N_{\max} = 5$, which allows us to correctly describe systems with up to four bosons of each kind at every lattice site in the ground state (here, in numerical calculations $\beta = 1/k_B T = 500$). Depending on the value of the order parameters ϕ_A or ϕ_B the atoms are in the superfluid (SF, $\phi_{A,B} \neq 0$) or in the Mott insulating (MI, $\phi_{A,B} = 0$) state. As a result, it can lead to one of four possible states of the system as a whole: (a) $A_{\mathrm{SF}}(\phi_A \neq 0) + B_{\mathrm{SF}}(\phi_B \neq 0)$, (b) $A_{\mathrm{SF}}(\phi_A \neq 0) + B_{\mathrm{MI}}(\phi_B = 0)$, (c) $A_{\mathrm{MI}}(\phi_A = 0) + B_{\mathrm{SF}}(\phi_B \neq 0)$, or (d) $A_{\mathrm{MI}}(\phi_A = 0) + B_{\mathrm{MI}}(\phi_B = 0)$. To treat both species of particles (A and B) on an equal footing, we use the following parametrization of the system parameters:

$$t_B = \gamma t_A = \gamma t, \quad \mu_B = \xi \mu_A = \xi \mu, \quad U_B = \zeta U_A = \zeta U, \tag{8}$$

which allows for the introduction of differences between the types of bosons, when γ, ξ, and ζ coefficients depart a value of 1. 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 the behavior of both types of particles is identical. However, each type of boson interacts with other atoms of the same type, while the interaction between two types is controlled by W (for $W = U$ the particles interact identically with others). Such case was studied earlier by means of various methods [13–16]. For $W = 0$, the phase transition lines of both condensates coincide and are the same as for an ultracold bosonic gas with a single type of particles [21] [see Fig. 1(a)]. For hopping lower than the critical value, both species of bosons are in the Mott insulating state ($A_{\mathrm{MI}} + B_{\mathrm{MI}}$), while for higher, in the superfluid phase ($A_{\mathrm{SF}} + B_{\mathrm{SF}}$). When the interaction W is turned on, extra lobes of Mott insulator phase appear between the original lobes of a single condensate and their width in units of μ/U is equal to W/U. Densities of each kind of boson can be calculated from the following expressions:

$$\begin{aligned} n_A &= \langle n \rangle = \frac{1}{Z} \operatorname{Tr} \hat{n}_i e^{-\beta \hat{H}_{\mathrm{MF}}}, \\ n_B &= \langle m \rangle = \frac{1}{Z} \operatorname{Tr} \hat{m}_i e^{-\beta \hat{H}_{\mathrm{MF}}}. \end{aligned} \tag{9}$$

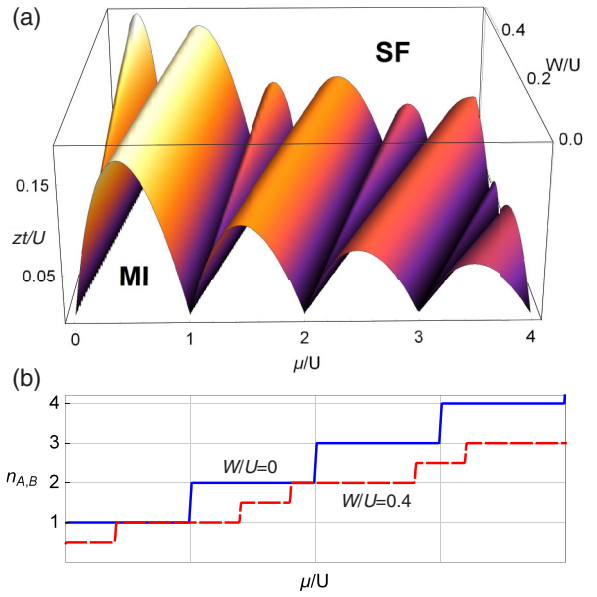

FIG. 1. Phase diagram (a) and density of particles of each type in the Mott insulating state (b) in symmetric case $t_B = t_A$, $\mu_B{=}\mu_A{=}\mu$, $U_B = U_A = U$ for interactions between different species W/U ranging from 0 to 0.5.

Their values in the Mott insulating state ($t/U = 0$) are shown in Fig. 1(b). It appears that the extra lobes are on average half-filled with particles of each type ($\frac{1}{2}, \frac{3}{2}, \frac{5}{2} \ldots$ particle of each type per lattice site), while the original lobes are filled with an integer number of particles of both species. However, the total filling $n_A + n_B$ is still an integer.

In a nonsymmetric case, critical lines of two sorts of particles no longer coincide. As a result, the ground state of each condensate may be dependent on the state of the other:

$$\left.\frac{\partial f(\phi_A,\phi_B)}{\partial \phi_A}\right|_{\phi_A=0} = 0,$$
$$\left.\frac{\partial f(\phi_A,\phi_B)}{\partial \phi_B}\right|_{\phi_B=0} = 0 \qquad (10)$$

as both ϕ_A and ϕ_B can have nonzero values at the same time. Consequently, the order parameters have to be determined using their definitions in Eq. (3) and the resulting phase diagrams have to be calculated from the set of Eqs. (10) and (3). The critical lines for different values of asymmetry parameters (γ, ζ, and ξ) are shown in Fig. 2. The lobes, which separate superfluid and Mott insulating phases of both sorts of bosons, no longer have a regular shape. Depending on the values of γ, ζ, and ξ, they can be significantly modified in the presence of the other order parameter, which is especially visible around the multicritical (crossing) points. The possible ground states of the system are the combination of SF and MI states of each kind of particle and all four of them can be observed on the phase diagram. The profile of densities of two species of bosons in the Mott insulating phases ($t/U \to 0$) is presented in Fig. 3. Except for the small vicinity of the zero value of the chemical potential, the densities are integers and change in consecutive Mott insulator lobes.

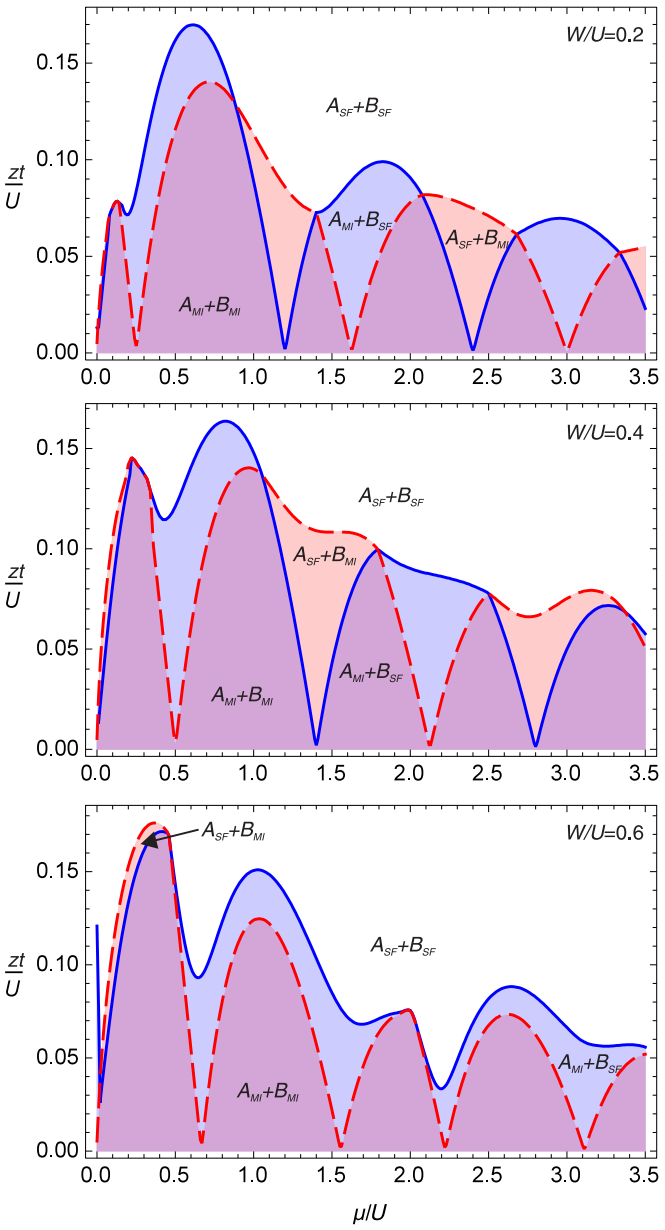

FIG. 2. Phase diagrams of a mixture of two atomic gases in an optical lattice for $\gamma = 1.1$, $\xi = 0.8$, and $\zeta = 0.9$ and selected values of interaction between two species $W/U = 0.2, 0.4, 0.6$ (from top to bottom). Solid (blue) lines denote critical lines of bosons A, while dashed (red) ones are for the bosons B. Areas below each line represent the Mott insulator of the respective type of bosons.

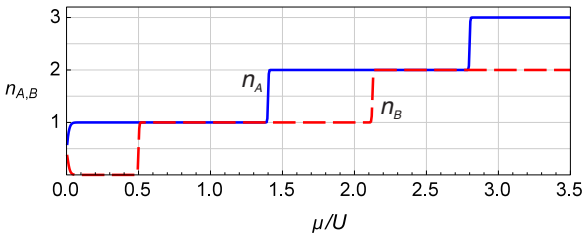

FIG. 3. Density of bosons A (solid line) and B (dashed line) in the Mott insulating phase ($t/U \to 0$) as a function of the chemical potential μ/U for $W/U = 0.4$, $\gamma = 1.1$, $\xi = 0.8$, $\zeta = 0.9$ [corresponding to Fig. 2(b)].

TABLE I. Multicritical points in the region $\mu/U = 0.2, \ldots, 2.5$ of the phase diagram from Fig. 2(b).

Critical point number	μ/U	zt/U
1	1.05291	0.13710
2	1.79352	0.09971
3	2.49943	0.07788

The exact behavior of the critical lines near the crossing points is strongly dependent on their position on the phase diagram. The presence of another order parameter does not influence the critical lines around some crossing points, while next to some others, it strongly modifies their shapes. In order to analyze this behavior, we focus on a chosen asymmetric phase diagram with $W/U = 0.4$, $\gamma = 1.1$, $\xi = 0.8$, and $\zeta = 0.9$ [see Fig. 2(b)] and three multicritical points that lie in the region of the chemical potential $\mu/U = 0.2, \ldots, 3.0$ (see Table I). At point 1, critical lines of both condensates do not show any deflection at the crossing point. However, near points 2 and 3 significant deflection is observed. Therefore, we calculate the values of order parameters as a function of hopping t/U at the multicritical points and for slightly lower and higher chemical potential μ/U. The results are presented in Fig. 4. Close to point 3, the phase transition from $A_{\mathrm{MI}} + B_{\mathrm{MI}}$ phase to $A_{\mathrm{MI}} + B_{\mathrm{SF}}$ or $A_{\mathrm{SF}} + B_{\mathrm{MI}}$ is continuous. However, while hopping is increased, the finite jump of the order parameters ϕ_A or ϕ_B during the transitions to the $A_{\mathrm{SF}} + B_{\mathrm{SF}}$ state is observed, which means that this transition is of the first order.

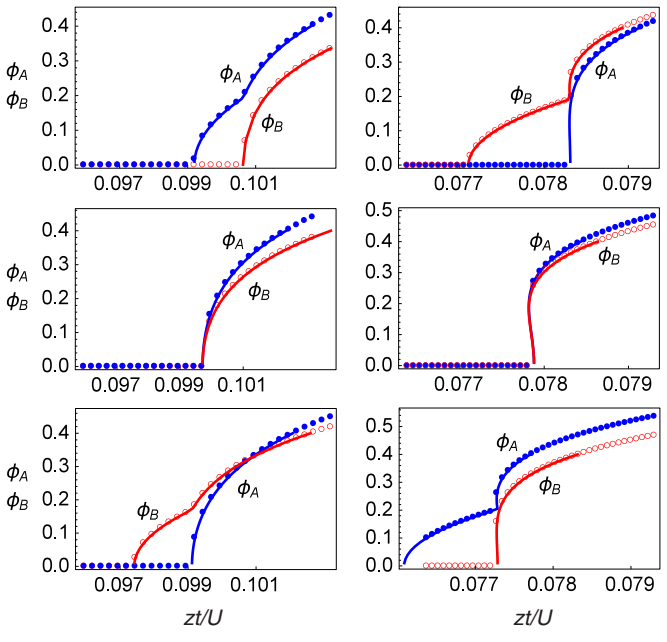

FIG. 4. Dependence of order parameters ϕ_A and ϕ_B on hopping t/U for $W/U = 0.4$, $\gamma = 1.1$, $\xi = 0.8$, $\zeta = 0.9$ and the three values of the chemical potential $\mu = \mu_c - 0.01, \mu_c, \mu_c + 0.01$ (from top to bottom) surrounding two multicritical points $\mu_c = 1.793\,52$ (left), $2.499\,43$ (right) demonstrating the second-order (left) and the first-order (right) phase transitions in the presence of condensed atoms of the other type, respectively. Filled (blue) circles denote ϕ_A, while empty (red) circles correspond to ϕ_B.

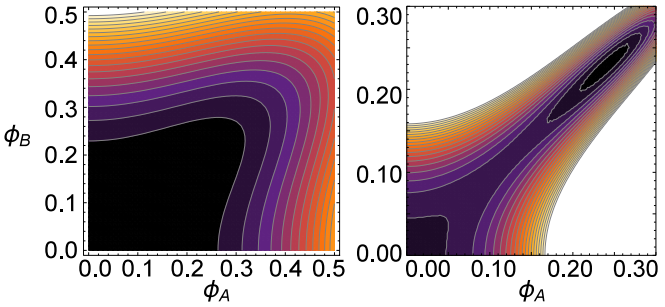

FIG. 5. Free energy of the mixture of atomic gases for W/U=0.4, $\gamma = 1.1$, $\xi = 0.8$, and $\zeta = 0.9$, near points 2 (left) and 3 (right) from Table I and Fig. 2(b). Darker colors denote lower energy.

Investigating the behavior of the order parameters exactly at the critical point, a discontinuous transition from Mott insulator to the superfluid state ($A_{\mathrm{MI}} + B_{\mathrm{MI}}$ to $A_{\mathrm{SF}} + B_{\mathrm{SF}}$) can be observed. On the other hand, point 2 is an intersection of two second-order transition lines. These observations can be verified by calculating the free energy of the system at critical points 2 and 3. The result is shown in Fig. 5. The free energy of the system at point 3 has two minima that are typical for the first-order phase transition and coexisting metastable states of the Mott insulator ($\phi_A = 0$, $\phi_B = 0$) and the superfluid ($\phi_A \neq 0$, $\phi_B \neq 0$). This situation differs significantly from the results of Ref. [4], where such scenario was not present. We provide further investigations of this case in the next section.

The existence of the first-order phase transition lines in the phase diagrams precludes the determination of the positions of the critical lines using minimization of the free energy in Eq. (10) since instead of a single, global minimum, multiple minima can occur. In this case, the thermodynamic phase transition can be determined by comparing and equating the values of the free energy of both phases:

$$f(\phi_A = 0, \phi_B = 0) = f(\phi_A \neq 0, \phi_B \neq 0), \qquad (11)$$

where nonzero values of order parameters are calculated self-consistently from Eq. (3). As can be deduced from Fig. 4, the first-order phase transition is not limited to the multicritical point, but extends to some region of the chemical potential (see Fig. 6). As the distance from the crossing point gets larger, the finite jump of the order parameters becomes smaller until finally continuous phase transitions are restored.

IV. MULTICRITICAL POINTS

In the previous section we have numerically determined the phase diagram of the mixture of two types of bosons for arbitrary values of model parameters. The results suggest that in the vicinity of selected crossing points, where the critical lines for both kinds of particles meet, the type of phase transitions can change from continuous, which is characteristic for regular bosonic condensates (single type of atoms) to discontinuous (of the first order). In the following, we present an analysis based on the free-energy expansion to support the previous results and determine the criteria for the type of multicritical points present in the phase diagram.

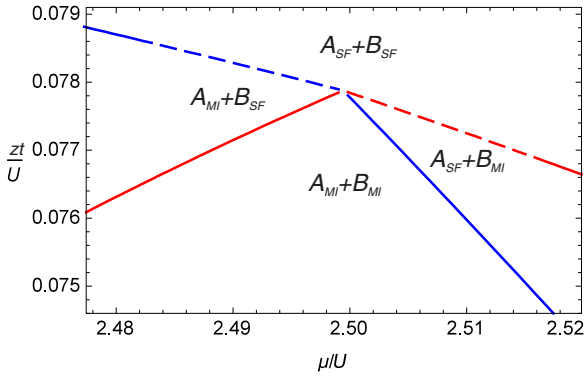

FIG. 6. First-order phase transition lines (dashed) of condensation in the presence of other condensates around the bicritical crossing point no. 3 (see Table I). Solid lines denote continuous phase transitions.

A. Generic free-energy expansion

Expansion of the free energy of a mixture of two kinds of bosons can be written in the standard way up to quartic terms:

$$f = f_0 + \frac{a_A}{2}\phi_A^2 + \frac{a_B}{2}\phi_B^2 + \frac{b_A}{4}\phi_A^4 + \frac{b_B}{4}\phi_B^4 + \frac{d_{AB}}{2}\phi_A^2\phi_B^2, \tag{12}$$

where f_0 is the free energy of the disordered state. This problem has already been analyzed in the case of two general order parameters, which are coupled [22] and in the context of coexistence of superconductivity and magnetism [4]. Since the Landau expansion works in the vicinity of the critical line, in the case of mixtures of particles, it can be used only around crossing points of two critical lines (multicritical points) or to describe condensation of one subsystem, while the other is in the disordered (Mott insulating) state ($\phi_A = 0$ or $\phi_B = 0$). The free energy can be minimized and analytical solutions for order parameters ϕ_A and ϕ_B can be found if the expansion up to quartic terms is taken into account. This leads to two possible scenarios for multicritical points presented in Figs. 7(a) and 7(b) depending on the interplay of the expansion parameters. For $b_A b_B > d_{AB}^2$ four phases are present around the multicritical point (which is tetracritical) with the phase transitions between them being continuous. However, as the difference $b_A b_B - d_{AB}^2$ becomes smaller, the mixed state region ($A_{\mathrm{SF}} + B_{\mathrm{SF}}$, $\phi_A \neq 0$, $\phi_B \neq 0$) becomes narrower and finally closes for $b_A b_B = d_{AB}^2$. When $b_A b_B < d_{AB}^2$ the mixed state is no longer present. Instead, the two states with only one of the atoms groups being superfluid are separated by a

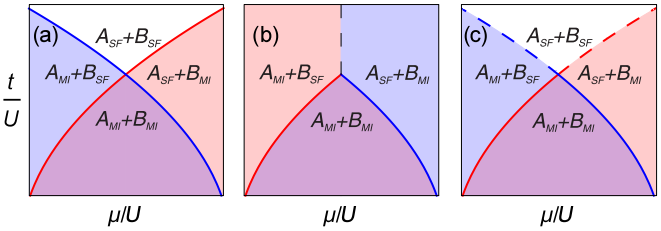

FIG. 7. Possible scenario of the behavior of a system with two interacting orders around the multicritical point.

first-order transition line. Consequently, the multicritical point changes to bicritical. Although the former scenario presented in Fig. 7(a) is observed in the case of a mixture of cold bosons in optical lattice (see Sec. III), the latter is missing. Instead, a different one is observed, which is schematically depicted in Fig. 7(c): around the multicritical point four phases are possible: $A_{\mathrm{SF}} + B_{\mathrm{SF}}$, $A_{\mathrm{SF}} + B_{\mathrm{MI}}$, $A_{\mathrm{MI}} + B_{\mathrm{SF}}$, and $A_{\mathrm{MI}} + B_{\mathrm{MI}}$; however, $A_{\mathrm{MI}} + B_{\mathrm{MI}}$ is separated from $A_{\mathrm{SF}} + B_{\mathrm{MI}}$ with the $A_{\mathrm{MI}} + B_{\mathrm{SF}}$ continuous phase transition, while $A_{\mathrm{SF}} + B_{\mathrm{SF}}$ with the first-order one.

In an analysis of the free-energy expansion, one has to be careful to allow only these values of the expansion parameters, which make the function physically well defined: being divergent to $+\infty$ for $|\phi_A|, |\phi_B| \to \infty$ and as a result having a global minimum. For this reason, in Refs. [4,22] it was assumed that b_A, b_B, and d_{AB} are positive, which limited the possible results to scenarios (a) and (b) in Fig. 7 (although, the analysis in Ref. [4] is valid for $d_{AB} < 0$ as long as $d_{AB}^2 < b_A b_B$). In order to describe the regime from Fig. 7(c), it is required that the free energy has multiple local minima: one for both ϕ_A and ϕ_B being nonzero and the other for only one of them being nonzero. This, in some circumstances, can be achieved if d_{AB} is negative. As it may lead to the free energy being divergent to $-\infty$, the expansion in Eq. (12) has to be taken to higher order. The simplest extension is to include an additional term $\Delta(\phi_A^2 + \phi_B^2)^3$ with positive values of Δ. This leads to the following expansion of the free energy:

$$f = f_0 + \frac{a_A}{2}\phi_A^2 + \frac{a_B}{2}\phi_B^2 + \frac{b_A}{4}\phi_A^4 + \frac{b_B}{4}\phi_B^4 + \frac{d_{AB}}{2}\phi_A^2\phi_B^2 + \Delta\left(\phi_A^2 + \phi_B^2\right)^3. \tag{13}$$

Unfortunately, the expression in Eq. (13) is too complicated to be minimized analytically and to calculate the order parameters dependence on the expansion parameters. However, from a general analysis of the Landau expansion it is known that at the critical line of the continuous phase transitions coefficients of the quadratic terms are equal to zero. As in the scenario in Fig. 7(c), two continuous phase transition lines meet at the critical point; the behavior of the system at this point can be investigated by assuming that $a_A = a_B = 0$. In this case values of the order parameters that minimize the free energy can be calculated. It appears that two solutions exist: one is trivial, $\phi_A = 0, \phi_B = 0$, and it corresponds to the disordered phase $A_{\mathrm{MI}} + B_{\mathrm{MI}}$. The other one is complicated; however, it has the following form:

$$\phi_A \sim i\sqrt{b_B - d_{AB}}\sqrt{b_A b_B - d_{AB}^2},$$
$$\phi_B \sim i\sqrt{b_A - d_{AB}}\sqrt{b_A b_B - d_{AB}^2}, \tag{14}$$

where i is the imaginary unit. For negative values of d_{AB} obeying the condition $d_{AB}^2 > b_A b_B$ this solution is real and nonzero. As a result, at the multicritical point two phases can be present: $A_{\mathrm{MI}} + B_{\mathrm{MI}}$ and $A_{\mathrm{SF}} + B_{\mathrm{SF}}$, each with its own local minimum of the free energy corresponding to point 3 in Fig. 5. Furthermore, the free energy in Eq. (13) can be analyzed numerically to discover that the scenario in Fig. 7(c) can be realized for d_{AB} which is negative and $d_{AB}^2 > b_A b_B$. Obviously, the question is whether the free energy of the

model analyzed in Sec. III falls into this scenario, which will be studied in the following section.

B. Coefficients of the free-energy expansion

In the following, we use a method based on the Laplace transform to calculate the coefficients of the free-energy expansion of the Bose-Hubbard model of a mixture of two types of bosons from Secs. II and III, when both order parameters (ϕ_A and ϕ_B) are zero. This allows one to retrieve the lower (in terms of value of t/U) of the critical lines in Fig. 2 and, as a result, works also at multicritical points. This approach has already been applied to single-component systems [23,24]; here we adapt it to a more complex system. The existence of two heterogenic order parameters makes the calculation more complicated, but the main idea remains the same. The mean-field Hamiltonian in Eq. (4) is decomposed into a diagonal H_0 and a nondiagonal H' part, $\hat{H}_{\rm MF} = \hat{H}_0 + \hat{H}'$:

$$\frac{\hat{H}_0}{N} = \frac{U_A}{2}\hat{n}(\hat{n}-1) + \frac{U_B}{2}\hat{m}(\hat{m}-1) + W\hat{n}\hat{m} - \mu_A\hat{n} - \mu_B\hat{m},$$
$$\frac{H'}{N} = -\phi_A t_A z\sum_i(\hat{a}_i^\dagger + \hat{a}_i) - \phi_B t_B z\sum_i(\hat{b}_i^\dagger + \hat{b}_i). \tag{15}$$

The partition function can be written as

$$Z = e^{-\beta z(t_A\phi_A^2 + t_B\phi_B^2)}Z', \tag{16}$$

where

$$Z' = \mathrm{Tr}\, e^{-\beta(H_0+H')}. \tag{17}$$

The key step of the method is to perform a perturbation expansion of the partition function Z' starting from representation as an integral over a contour Γ, which surrounds all singularities of the resolvent $(s-H)^{-1}$:

$$Z' = \int_\Gamma \frac{ds}{2\pi i}e^{-\beta s}\mathrm{Tr}(s-H)^{-1}$$
$$= \int_\Gamma \frac{ds}{2\pi i}e^{-\beta s}\mathrm{Tr}\left\{(s-H_0)^{-1}\sum_{n=0}^{\infty}[(s-H_0)^{-1}gH']^n\right\}. \tag{18}$$

This can be rewritten in a more compact form:

$$Z' = Z_0 - \beta\sum_{n=1}^{\infty}\int_0^1\frac{dg}{g}\int_\Gamma\frac{ds}{2\pi i}e^{-\beta s}\mathrm{Tr}[(s-H_0)^{-1}gH']^n, \tag{19}$$

where Z_0 is

$$Z_0 = \sum_{n,m=0}^{\infty} e^{-\beta E_{n,m}} \tag{20}$$

and $E_{n,m}$ are eigenvalues of the H_0 Hamiltonian. The partition function can be expanded in the powers of the order parameters:

$$Z = e^{-\beta z(t_A\phi_A^2 + t_B\phi_B^2)}\big(Z_0 + Z_2^A\phi_A^2 + Z_2^B\phi_B^2 + Z_4^A\phi_A^4$$
$$+ Z_4^B\phi_B^4 + Z_4^{AB}\phi_A^2\phi_B^2\big). \tag{21}$$

As a result, the coefficients in the expansion of the free energy in Eq. (12) can be calculated as functions of the model parameters:

$$f_0 = T\ \ln Z_0,$$
$$a_A = 2\left(z\,J - T\frac{Z_2^A}{Z_0}\right),$$
$$a_B = 2\left(z\,J - T\frac{Z_2^B}{Z_0}\right),$$
$$b_A = -\frac{4}{\beta}\left[-\frac{1}{2}\left(\frac{Z_2^A}{Z_0}\right)^2 + \frac{Z_4^A}{Z_0}\right],$$
$$b_B = -\frac{4}{\beta}\left[-\frac{1}{2}\left(\frac{Z_2^B}{Z_0}\right)^2 + \frac{Z_4^B}{Z_0}\right],$$
$$d_{AB} = -\frac{2}{\beta}\left(-\frac{Z_2^A Z_2^B}{Z_0^2} + \frac{Z_4^{AB}}{Z_0}\right). \tag{22}$$

It should be noted that the method allows for analytical calculation of coefficients of higher order expansion of the free energy, although the expressions are becoming more complicated. As a result, one can include the parameters that determine the nature of the phase transitions into the phase diagram of the mixture of bosons. These parameters, according to Sec. IV A, are the values of $b_A b_B - d_{AB}^2$ and d_{AB}. If the former is positive at the intersection of critical lines of two types of bosons, a tetracritical is present. On the other hand, if the value is negative, the lines meet at a bicritical point. If d_{AB} is negative, the mixed phase ($A_{\rm SF} + B_{\rm SF}$) is separated from the single-particle-ordered phases ($A_{\rm SF} + B_{\rm MI}$ and $A_{\rm MI} + B_{\rm SF}$) with the first-order transition line. The interplay of the parameters is presented in Fig. 8, which leads to two tetracritical points at $\mu/U = 1.05$ and $\mu/U = 1.79$ and one bicritical point at $\mu/U = 2.5$ (another one close to

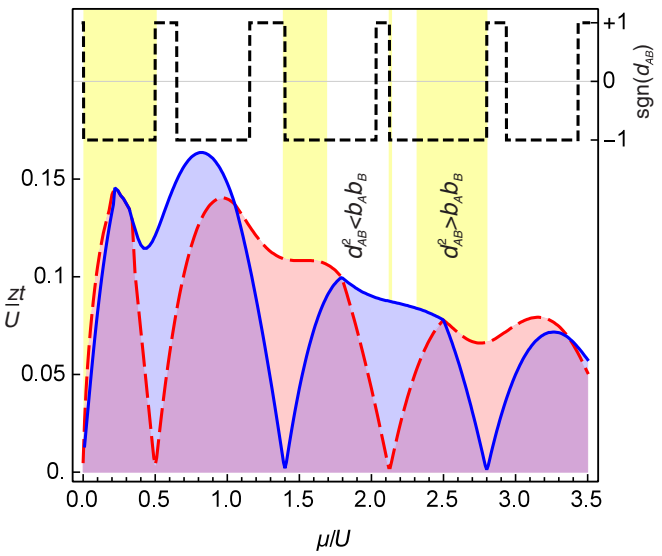

FIG. 8. Phase diagram from Fig. 2(b) with values of coefficients determining the type of multicritical points: the sign of d_{AB} (dashed line on the top) and the negative value of $b_Ab_B - d_{AB}^2$ (vertical shaded regions).

$\mu/U = 0.25$ is not analyzed since critical lines are highly coinciding) since it is the only crossing point at which negative values of $b_A b_B - d_{AB}^2$ and d_{AB} coincide. This confirms the results of the numerical analysis in Sec. III. However, the question on the physical reason for a large negative value of d_{AB} (effective coupling between bosonic order parameters) is still open. From Fig. 3, it seems that it has no connection with the particle densities of the bosonic species. On the other hand, the exact expression for d_{AB} resulting from Eq. (22) is too complicated to be helpful in solving this conundrum.

V. CONCLUSION

We have investigated the phase diagrams of mixtures of atomic gases in an 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 a continuous one. However, we showed that the presence of an additional order parameter in connection with strong interactions between different species of atoms can lead to a change of the nature of the phase transition close to selected multicritical points along with a change of their multicriticality: they change from tetracritical to bicritical, while the critical lines between MI-SF and SF-SF phases become of the first order. As a result, the condensation of bosons in the presence of other bosonic condensates may fall out of the XY model universality class. The reason for this behavior is an effective strong and negative coupling between bosonic parameters resulting from the complicated nature of the many-body quantum problem. In solid-state physics, finding a multicritical system with strongly coupled order parameters is not easy. From our results, it seems that due to high tunability of atoms in an optical lattice this task should be much more fruitful for systems of ultracold bosons.

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