# Mixtures of Strongly Interacting Bosons in Optical Lattices

P. Buonsante,[1] S. M. Giampaolo,[2,3] F. Illuminati,[2,3,4] V. Penna,[1] and A. Vezzani[5]

[1]*C.N.I.S.M. and Dipartimento di Fisica, Politecnico di Torino, C.so Duca degli Abruzzi 24, I-10129 Torino, Italy*
[2]*Dipartimento di Matematica e Informatica, Università degli Studi di Salerno, Via Ponte don Melillo, 84084 Fisciano (SA), Italy*
[3]*CNR-INFM Coherentia, Napoli, Italy,*
*and CNISM Unità di Salerno, and INFN Sezione di Napoli, Gruppo collegato di Salerno, Baronissi (SA), Italy*
[4]*Institute for Scientific Interchange, Viale Settimio Severo 65, 10133 Torino, Italy*
[5]*CNR-INFM and Dipartimento di Fisica, Università degli Studi di Parma, V.le G.P. Usberti n.7/A, I-43100 Parma, Italy*
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We investigate the properties of strongly interacting heteronuclear boson-boson mixtures loaded in realistic optical lattices, with particular emphasis on the physics of interfaces. In particular, we numerically reproduce the recent experimental observation that the addition of a small fraction of $^{41}$K induces a significant loss of coherence in $^{87}$Rb, providing a simple explanation. We then investigate the robustness against the inhomogeneity typical of realistic experimental realizations of the glassy quantum emulsions recently predicted to occur in strongly interacting boson-boson mixtures on ideal homogeneous lattices.

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Ultracold degenerate gases in optical lattices provide an unprecedented toolbox for realizing experimentally what were once just toy models sketching the key features of complicated condensed matter systems. One prominent example is the Bose-Hubbard (BH) model, originally introduced as a variant of the better known Hubbard model [1] and later adopted for the description of superfluid $^4$He trapped in porous media [2]. Several years after the introduction of this simple yet challenging toy model, Jaksch and co-workers suggested that it could be realized in terms of ultracold bosonic gases trapped in optical lattices [3] and were soon proved right by a breakthrough experiment where the hallmark superfluid-insulator quantum phase transition of the BH model was observed [4].

Recently, several experimental groups directed their efforts to the realization of more complex generalizations of the Hubbard model, involving mixtures of particles obeying either the same or different statistics. Beyond their theoretical appeal, these systems are relevant to interesting applications such as implementation of disorder [5], association of dipolar molecules [6], schemes for quantum computation [7], and mapping of spin arrays [8].

Most of the experimental efforts on optical lattice systems have been directed to boson-fermion mixtures [5,9,10], while fermion-fermion and boson-boson (BB) mixtures have been somewhat ignored. Very recently, the Florence group performed an experiment on a harmonically trapped BB mixture of atomic $^{41}$K and $^{87}$Rb with strong interspecies repulsion [11]. Expectedly, the presence of a relevant K fraction modifies the quantum phase transition occurring in Rb. More surprisingly, this effect turns out to be sizable even for a small overlap between the two atomic species [11]. Strongly interacting BB mixtures are also the subject of a recent theoretical investigation, whose main observation is that strong interspecies repulsion can substitute for disorder, driving a mixture loaded in a homogeneous 1D lattice into metastable quantum emulsion (QE) states exhibiting glassy features [12].

In the present work, we introduce a unified framework for the description of lattice BB mixtures with strong interspecies interactions in realistic conditions and different physical regimes encompassing and generalizing the above-described findings [11,12]. In particular, we explain the apparently surprising observation that the coherence properties of a bosonic system can be reduced significantly even in the presence of a single interface with a second bosonic species [11]. Furthermore, we establish the range of parameters for which the intuitively expected opposite behavior of increased coherence is recovered. Concerning QEs, we show that they are, in principle, compatible with the inhomogeneity arising from confining potentials typical of experiments, albeit in a restricted range of parameters. Specifically, while in the homogeneous case a sufficiently strong interspecies repulsion ensures the occurrence of QE states [12], in the experimentally relevant inhomogeneous case, the difference of intraspecies repulsions turns out to be a fundamental critical parameter.

The systems under concern provide a realization of the two-flavor BH Hamiltonian

$$H = U_{12}\sum_j n_{1,j}n_{2,j} + \sum_{f,j}\left[\frac{U_f}{2}n_{f,j}(n_{f,j}-1) + v_{f,j}n_{f,j} - J_f\sum_{\ell\sim j}(a^\dagger_{f,j}a_{f,\ell} + a^\dagger_{f,\ell}a_{f,j})\right], \quad (1)$$

where the lattice boson operators $a^\dagger_{f,j}$, $a_{f,j}$, and $n_{f,j} = a^\dagger_{f,j}a_{f,j}$ create, destroy, and count atoms of type $f$ at site $j$, respectively. The parameters $U_f$ and $U_{12}$ quantify the intra- and interspecies BB (repulsive) interaction, respectively, $J_f$ is the hopping amplitude, and $v_{f,j} = k_f(j - j^0_f)^2$ is the standard harmonic trapping potential felt by bosons of species $f$ at lattice site $j$. By $m_f$, $k_f$, and $j_f^0$, we denote, respectively, the mass, the curvature, and the minimum point of the harmonic potential $v_{f,j}$ of species $f$.

Since our aim is the study of strongly interacting mixtures, it is convenient and effective to adopt a mean-field approach based on the assumption that the ground state of the system is the product of on-site factors $|\Psi\rangle = \prod_j |\psi_j\rangle$, $|\psi_j\rangle = \sum_{n_1,n_2} c^{(j)}_{n_1,n_2} (a^\dagger_{1,j})^{n_1} (a^\dagger_{2,j})^{n_2} |\Omega\rangle$, where $|\Omega\rangle$ is the vacuum state, $a_{f,j}|\Omega\rangle = 0$, and the coefficients $c_{n_1,n_2}$ are determined via energy minimization at fixed atomic populations $N_1$ and $N_2$. Owing to a much lower computational demand, this mean-field approach provides qualitative results on systems that would be beyond the present capabilities of more quantitative numerical methods, such as quantum Monte Carlo (QMC), density matrix renormalization group, or time-evolving block-decimation algorithms.

Hamiltonians similar to Eq. (1) have been considered previously [3,6,8,13–22], possibly referring to different internal states of the same bosonic species [8,15] to spin-1 [18] or dipolar bosons [6,21]. Most of the previous work focuses on the phase diagram of homogeneous lattices, often adopting a mean-field approximation similar to ours [6,13,15–18]. However, our approach is characterized by some features that have not been considered in the literature, at least simultaneously. First, our mean-field is fully site-dependent and does not reduce to an effective single-site theory. This allows us to describe phase-separated systems and to consider realistic harmonic trapping potentials. Furthermore, we fix the bosonic populations $N_1$ and $N_2$ rather than the corresponding chemical potentials $\mu_1$ and $\mu_2$. Again, this allows us to make direct contact with experimentally relevant situations and avoids the ‘‘species depletion’’ problem discussed in Refs. [15,17].

The method is first applied to a situation reproducing the experimental conditions in Ref. [11], where a bosonic mixture of Rb and K was loaded in an optical lattice. The potentials trapping the two atomic species had the same curvature $k_f$, but, since $m_1 \neq m_2$, their minima were displaced in the vertical direction: $j_f^0 = m_f g\lambda/(4k_f)$, where $g$ is the gravitational constant and $\lambda/2$ is the optical lattice spacing (henceforth, the subscripts 1 and 2 will denote Rb and K, respectively). An important consequence of the interplay between the ensuing asymmetry and the strong interspecies repulsion is the tendency towards full phase separation, minimizing the number of interfaces between the two species. In fact, in the Florence experiment, the interspecies overlap is estimated to be limited to one lattice site in the vertical direction. Despite the occurrence of a single phase interface, the effect of K on the coherence properties of Rb turns out to be sizable [11]. More in detail, it has been observed that a modest quantity of K (around 10% of Rb) reduces the coherence of Rb significantly, moving the superfluid-insulator transition point to smaller values of the optical lattice depth $s$. The authors of Ref. [11] also remark that a naive argument based on Ref. [6] results in a prediction opposite to the observed behavior: The presence of K increases the local density of Rb, which would cause an increase in the coherence of the latter.

This argument is indeed valid for most of the phase diagram of the BH model describing an atomic cloud loaded in a homogeneous optical lattice. However, clear exceptions are found in the proximity of the Mott lobes, where an increase of the (local) density—or chemical potential—results in a sharp drop in the condensate fraction. Furthermore, it should be emphasized that such a phase diagram describes a homogeneous system in the thermodynamic limit, whereas here we are dealing with a finite and inhomogeneous system. The site-dependent potential acts like a local chemical potential for a system with fixed total population. As a result, at sufficiently high ratios of interaction to kinetic energy, configurations of the system can be found where superfluid and Mott-insulating domains coexist [23,24]. The density of the system assumes the so-called wedding-cake or ziggurat profile, the plateaus corresponding to (quasi-)Mott-insulator domains. When the configuration is such that the topmost plateau involves a fair number of sites, the density profile responds to an increase in the total population according to a predictable sequence. At first, a domelike essentially superfluid structure appears on top of the highest plateau. Subsequently, the width and height of this structure increase, leading to an increase in the system coherence. When the tip of the dome gets too close to the next level of the ziggurat, the dome flattens, its central part turning gradually into a plateau. Correspondingly, there is a drop in the overall coherence of the system [23].

The above-described single-species scenario is captured quite satisfactorily by the Gutzwiller mean-field approximation [3,25–27]. We will now show that it bears a strict relation with the experimental observations reported in Ref. [11] about the Rb-K BB mixture. Figure 1 shows results obtained from a double-species Gutzwiller mean-field approach where we have adopted physical parameters—$J_f$, $U_f$, $U_{12}$, $k_f$, atomic density at the trap center, population ratios—in the experimentally determined range [11,28]. For the sake of simplicity, we have focused on a 1D lattice as mean-field results are essentially independent of the dimensionality [29]. Figure 1(a) shows the local superfluid parameter $|\alpha_{1,h}|^2 = |\langle\Psi|a_{1,h}|\Psi\rangle|^2$ of Rb alone as a function of the relevant population $N_1$ and lattice site label $h$ (the darker the hue, the larger $|\alpha_{1,h}|^2$). The drop in the superfluid parameter at the trap center signals the formation of new ziggurat levels from the flattening of coherent domes. Figure 1(b) shows the same quantity as in Fig. 1(a) yet in the presence of 30 atoms of K ($|\alpha_{2,j}|^2$ is not shown). The main effect of the addition of K is that the new structures of the (now asymmetric) ziggurat appear at smaller populations $N_1$. Figure 1(c) shows an estimate of the coherence of Rb measured in terms of the relevant condensate fraction $f_C^1$ [30] for the data in Figs. 1(a)

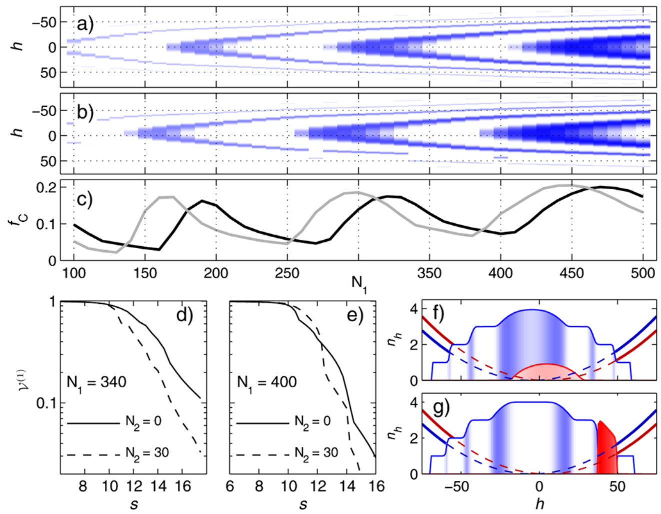


FIG. 1 (color online). (a) $|\alpha_{1,h}|^2$ vs $N_1$ ($s = 11$, $J_1 \approx 0.022U_1$, $k_1 \approx 7.9 \times 10^{-4}U_1$); (b) same as (a) but in the presence of K ($N_2 = 30$, $U_2 \approx 0.65U_1$, $J_2 \approx 0.21U_1$, $U_{12} \approx 2.22U_1$, $k_2 = k_1$); (c) $f_C$ of Rb corresponding to (a) (black curve) and (b) (gray curve); (d),(e) visibility of Rb vs lattice strength. (f),(g) Configurations of 340 Rb (blue) and 30 K (red) atoms for $s = 11$, along with the relevant trapping potentials (arbitrary units). The height of each bar represents the local population $n_h$, whereas the darkness of the shading is proportional to $|\alpha_{j,h}|^2$. In (f) we set $U_{12} = 0$.

(black) and 1(b) (gray). The presence of K is indeed equivalent to an increase in Rb population, but, given the oscillatory behavior of $f_C^1$, this does not necessarily result in an increase of the overall coherence of Rb. A small fraction of $N_2$ can cause either an increase or a decrease of $f_C^1$, depending on the value of $N_1$. The experimental measure of coherence, i.e., the so-called visibility $\mathcal{V}$ [11,31], exhibits similar oscillations as in Fig. 1(c), albeit with a different envelope. Figures 1(d) and 1(e) show the changes in $\mathcal{V}^{(1)}$ produced by $N_2 = 30$ K atoms, for two values of $N_1$. Note that Fig. 1(d) considers the same population ratio as estimated in the experiment [11] and reproduces quite satisfactorily the observed loss of coherence. Guided by Fig. 1(c), in Fig. 1(e) we change $N_1$ from 340 to 400 to probe the opposite phenomenon. It turns out that the presence of K enhances $\mathcal{V}^{(1)}$ only at relatively low lattice depths, while at large $s$ the effect is again a loss of coherence, albeit less pronounced. This result agrees with experiments, where an increase of coherence was never observed [28]. We now turn our attention to another interesting feature of strongly interacting BB mixtures, i.e., the possible occurrence of low-energy metastable states characterized by a large number of interfaces, recently discussed in the ideal case of homogeneous lattices $k_f = 0$ [12]. The authors of Ref. [12] observe that the QMC simulations employed to determine the ground state of the total Hamiltonian $H$ fail to equilibrate as soon as $U_{12} \geq U_f$ and ascribe this behavior to the presence of many low-energy metastable states (where metastable refers to the robustness of these configurations against the QMC minimization algorithm, which is equipped with nonlocal moves). Being characterized by a large number of interfaces separating single-species droplets, these metastable states are dubbed quantum emulsions. The relevant energies are found to be linearly dependent on the number of interspecies interfaces. One interesting feature of these QEs is their spontaneous randomness, i.e., the fact that the droplets exhibit a disordered spatial arrangement despite the absence of any randomness in the Hamiltonian parameters.

By adopting a self-consistent dynamical search algorithm for the ground state of the homogeneous system in its Gutzwiller form [32], we find that the BB mixture gets trapped into a QE state whose energy depends on the number of interfaces, in complete analogy with Ref. [12]. This is evident from Fig. 2 illustrating the situation on a homogeneous lattice for different values of the hopping to interaction ratios [33]. However, the homogeneous lattice of Ref. [12] is a strongly idealized situation, in which the only requirement for the occurrence of QEs is that $U_{12}$ be sufficiently larger than $U_1$ and $U_2$ [12,13]. Moving to the inhomogeneous case typical of actual experimental situations, we find that $\Delta U = |U_1 - U_2|$ becomes a further critical parameter for the existence of QEs. This is clearly illustrated in Fig. 3. Figure 3(a) shows the average number of interfaces as a function of $\Delta U$, while the inset is analogous of the leftmost panel in Fig. 2. Figures 3(b) and 3(c) show typical configurations at small and large values of $\Delta U$, respectively. Note that the former is characterized by a significant number of randomly arranged single-species droplets. In this case $J_1 = J_2 = 0.1U_1$, but we obtain similar results also for $J_1 \neq J_2$, provided that $\Delta U \approx 0$. Clearly, the number of QE states at a given energy will be smaller than in the homogeneous case, owing to the reduced degree of symmetry of the system. Indeed, in this case, the energy of each droplet does depend on its position in the lattice, due to the local potential contribution. Unlike the 1D case, in higher dimensions the interface energy of a droplet depends on its size. This fact, along with the larger lattice connectivity, is expected to hinder the occurrence of QEs.

In summary, we have investigated the properties of a strongly interacting bosonic mixture loaded into an optical

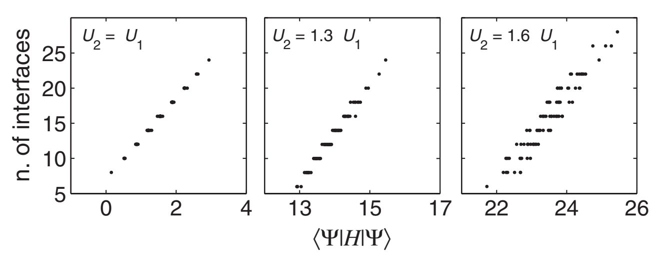


FIG. 2. Number of interfaces vs energy for $N_1 = N_2 = 180$ particles on a 300-site 1D lattice. In all cases $J_1 = J_2 = 0.1U_1$ and $U_{12} = 1.5U_1$.

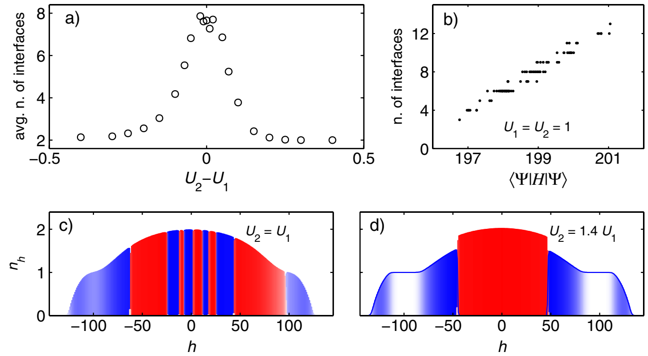


FIG. 3 (color online). QEs in the presence of a harmonic confinement; (a) average number of interfaces (over 100 realizations) vs $U_2 - U_1$; (b) same as Fig. 2(a); (c),(d) local densities of bosons in two limiting situations. The color key is the same as Figs. 1(f) and 1(g). In all cases $N_1 = N_2 = 180$ and $k_1 = k_2 = 10^{-4}U_1$;other parameters are as in Fig. 2.

lattice, going beyond the idealized situation of a homogeneous system. We considered the inhomogeneities arising from the presence of the harmonic trapping potential typical of standard experimental setups as well as from the differential gravitational sag originated by the difference in the masses of the two bosonic species. We reproduced the apparently surprising results of the first experiment involving a BB mixture [11], providing a simple explanation for the observed loss of coherence of $^{87}$Rb in the presence of a small fraction of $^{41}$K. Furthermore, our results predict that the opposite phenomenon, i.e., the increase of coherence predicted by the "naive argument" proposed in Ref. [11], is limited to sufficiently shallow lattice depths. A complete agreement between theory and experiment would require the scaling to higher dimensions, more refined—and very likely, far more demanding—numerical algorithms, and/or more involved analytical studies than the present mean-field approach. However, such a program is not likely to add significant new elements to the scenario inferred by our analysis, which captures the essential physics of the phenomenon under examination.

We then investigated the effect of inhomogeneity on the QE states formerly predicted on homogeneous lattices [12]. In particular, we found that, at variance with the homogeneous case, a large $U_{12}$ is not sufficient for their occurrence, a further critical condition being a small $U_2 - U_1$. This suggests that Feshbach resonances could be a crucial ingredient for the experimental observation of QEs in heteronuclear mixtures. An intriguing alternative possibility for the realization of lattice BB mixtures with directly built-in conditions $J_1 = J_2$ and $U_1 = U_2$ could be provided by a generalization of the models considered in Ref. [21], by considering dipolar bosons placed on two neighboring lattices with angular relations such that the two sets of atoms interact via a strong interspecies repulsion $U_{12}$.

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