Inhomogeneous Atomic Bose-Fermi Mixtures in Cubic Lattices

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We determine the ground state properties of inhomogeneous mixtures of bosons and fermions in cubic lattices and parabolic confining potentials. For finite hopping we determine the domain boundaries between Mott-insulator plateaux and hopping-dominated regions for lattices of arbitrary dimension within mean-field and perturbation theory. The results are compared with a new numerical method that is based on a Gutzwiller variational approach for the bosons and an exact treatment for the fermions. The findings can be applied as a guideline for future experiments with trapped atomic Bose-Fermi mixtures in optical lattices.

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I. Introduction.—Mixtures of ultracold bosonic and fermionic particles have attracted a considerable amount of attention in recent years, to a high extent triggered by the perspective of achieving *prima facie* transitions to superfluidity in systems of neutral fermionic atoms [1]. Spectacular progress has already been achieved in the experimental manipulation of cold atoms in optical lattices with the experimental realization of the superfluid-Mott-insulator phase transition in systems of bosonic atoms [2], and the production of degenerate Fermi gases [1,3]. A perspective of key interest lies in the possibility of discovering and probing new quantum phases of matter in the study of Bose-Fermi mixtures in optical lattices [3–7]. In Ref. [4], the Bose-Fermi Hubbard (BFH) Hamiltonian has been introduced and derived from the microscopic many-body Hamiltonian, linking the experimentally accessible quantities to the model parameters; and a mean-field argument has been presented. In Refs. [5] the phase diagram of homogeneous boson-fermion mixtures in optical lattices has been studied in a mean-field approach, and the existence of a complex structure of phases of composite fermionic particles has been conjectured. In Ref. [6] stable supersolid phases have been predicted for homogeneous Bose-Fermi mixtures. In Ref. [7] the task of assessing the phase diagram of the BFH model using an exact diagonalization approach for systems of small size is addressed, and, finally, in Ref. [8] high-temperature superfluidity of the fermionic atoms induced by the boson-fermion interaction has been predicted.

The investigations in Refs. [5–8] are confined to the homogeneous case, i.e., to the translationally invariant BFH model. While this is a very reasonable approach to discuss the phase diagram in the thermodynamical limit, the actual experimental situations often involve the use of external trapping potentials superimposed on the optical lattice that break the translational symmetry. This fact leads to the appearance of spatial domains of coexisting different phases along the lattice, as recently studied for pure bosonic [9] and pure fermionic systems [10]. Studies of such inhomogeneous systems are thus of immediate relevance for the interpretation of experimental findings.

In this Letter we study the effects of an inhomogeneous confining potential on Mott and superfluid regions emerging in systems of Bose-Fermi mixtures in regular lattices at zero temperature. We show that the BFH model is exactly solvable in the limit of very strong lattices (vanishing bosonic and fermionic hopping), and analyze the related structure of domains of composite particles. We then consider the general case of finite hopping in D-dimensional lattices, study the bulk properties of the system in Landau theory and local density approximation (LDA), and determine the general phase boundaries of the different domains. We introduce a versatile method, applicable to several systems of this kind, that treats the bosons within a Gutzwiller-type ansatz [11,12] and the fermions exactly. This method allows us to present for the first time the domain structure of inhomogeneous lattice mixtures in confining potentials and the respective phase diagrams for the homogeneous case.

The starting point of our analysis is the single-band BFH Hamiltonian [13], which captures the essential properties of dilute mixtures in optical lattices at zero or very low temperatures under fairly general assumptions on the tunable physical parameters [4]. The grand canonical BFH Hamiltonian reads

$$\hat{H} = -\sum_{\langle i,j\rangle}(J_B \hat{b}_i^\dagger \hat{b}_j + J_F \hat{f}_i^\dagger \hat{f}_j + \text{h.c.}) + U_{BF}\sum_i \hat{n}_B^i \hat{n}_F^i + U_{BB}\sum_i \hat{n}_B^i(\hat{n}_B^i - 1) + \sum_i \hat{n}_B^i \tilde{V}_B^i + \sum_i \hat{n}_F^i \tilde{V}_F^i, \quad (1)$$

where $\tilde{V}_B^i = V_B^i - \mu_B$ and $\tilde{V}_F^i = V_F^i - \mu_F$. Here, $\hat{b}_i$ and $\hat{f}_i$ are the on-site bosonic and fermionic annihilation operators, respectively, whereas $\hat{n}_B^i = \hat{b}_i^\dagger \hat{b}_i$ and $\hat{n}_F^i = \hat{f}_i^\dagger \hat{f}_i$. Sites are associated with a cubic D-dimensional lattice with fixed spacing, and $i = (i_1, ..., i_D)$ denotes a

D-tuple labeling the coordinates of a site i. The symbol $\langle i, j\rangle$ denotes summation over pairs of nearest neighbors. The first two terms in Eq. (1) describe independent bosonic and fermionic nearest-neighbor hopping with positive amplitudes J_B and J_F. The subsequent line represents on-site boson-boson and boson-fermion interactions. Finally, the first two terms of the last line incorporate the external confining potential, which, in typical experimental situations, can be taken to be harmonic. The origin of the lattice is chosen to be at the minimum of the trapping potential, assumed to be equal for bosons and fermions, so that $V_B^i = V_F^i = V_i := V_0|i|^2$. This Hamiltonian is a generalization to systems of bosons and fermions of the frequently employed Bose-Hubbard model exhibiting the Mott to superfluid phase transition in bosonic systems [12,14,15]. Expressions linking the model parameters to quantities that can be tuned in an actual experimental situation, such as the depth of the optical lattice and the atomic scattering lengths, are provided in Ref. [4].

II. Exact solution with vanishing hopping.—A surprisingly rich situation is already encountered in the case of vanishing hopping: $J_B = J_F = 0$. In this case the Hamiltonian $\hat{H}_0$ is simply a sum of single-site contributions, and the eigenstates of the BFH model are tensor products of number states with state vectors $|\psi\rangle = |n_0, n_1, \cdots\rangle|m_0, m_1, \cdots\rangle$, where $n_i = 0, 1, 2, \ldots$ and $m_i = 0, 1$ represent the occupation number of bosons and fermions at site i, respectively. For ease of notation, we will fix the energy scale by setting $U_{BB} = 1$. We have $\langle\psi|\hat{H}_0|\psi\rangle = \sum_i[n_i^2 - n_i + U_{BF}n_i m_i + V_i(n_i + m_i) - \mu_B n_i - \mu_F m_i] =: \sum_i E(n_i, m_i)$, where for the ground state with state vector $|\psi_0\rangle$ the occupation numbers take the specific values $\bar{n}_i = \max(0, [(1 + \mu_B - V_i)/2])$ if $E(\bar{n}_i, 0) < E(\bar{n}_i, 1)$ and $\bar{n}_i = \max(0, [(1 + \mu_B - V_i - U_{BF})/2])$ otherwise, whereas $\bar{m}_i = 0$ if $E(\bar{n}_i, 0) < E(\bar{n}_i, 1)$ and $\bar{m}_i = 1$ otherwise, where $[.]$ denotes the closest integer to the value in brackets. According to the above determination, several types of composite particles can be formed. Composites consisting of $\bar{m}_i$ fermions and $\bar{n}_i$ bosons are formed at site i, see Fig. 1. Connected domains with fixed integer particle numbers are formed and, depending on the interaction strength U_{BF} and the relation of the respective chemical potentials μ_B and μ_F, the fermions distribute around the center of the trap or are pushed outwards.

III. Finite hopping: perturbative treatment.—We now turn to the strong coupling limit with small but finite hopping. In a wide range of physical parameters, the strength of the hopping for bosons and fermions are approximately of the same value, $J_F = J_B =: J$, and we treat the small positive parameter J as a perturbation. As in Ref. [16], we introduce a mean-field approximation, which amounts to a replacement $\hat{b}_i^\dagger \hat{b}_j \longmapsto \psi_B^i \hat{b}_j + \hat{b}_i^\dagger \psi_B^j - \psi_B^j \psi_B^i$, the complex numbers ψ_B^i being variational parameters modeling the influence of neighboring

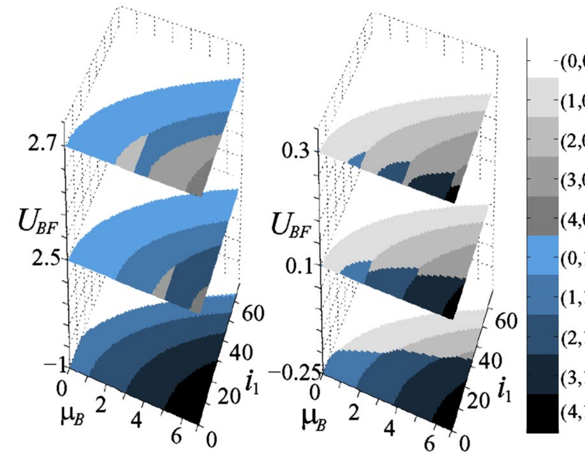

FIG. 1 (color online). Distribution of integer boson and fermion numbers for the case $J_B = J_F = 0$ and $V_0 = 0.002$ for a D-dimensional cubic lattice. This is encoded in the shading as shown in the bar on the right hand side (number of bosons, number of fermions) as a function of the component i_1, the chemical potential μ_B, and U_{BF}. For the left (right) figure, $\mu_F = 6\mu_B/5$ ($\mu_F = \mu_B/5$) is chosen.

atoms with the physical interpretation of a superfluid parameter. We consider the resulting corrections to the ground state energy, $\langle\psi_0|\hat{H}_0|\psi_0\rangle = \sum_i E(\bar{n}_i, \bar{m}_i)$, to second order in J. Moreover, to study bulk properties we will make use of the local density approximation (LDA). This means taking for each lattice site ψ_B^i to be equal to the corresponding values at neighboring sites. This is well justified for a sufficiently shallow trapping potential. In this approximation, the ground state energy reads $E = \langle\psi_0|\hat{H}_0|\psi_0\rangle + \Delta E_B + \Delta E_F + O(J^3)$, where $\Delta E_B = 2Jd\sum_i[|\psi_B^i|^2(1 + Jdr_i)]$, with $r_i = (4\bar{n}_i + 2c_i + 2)/(c_i^2 - 1)$, $c_i = 1 - 2\bar{n}_i - V_i + \mu_B - U_{BF}\bar{m}_i$, and d is the coordination number ($d = 6$ in three dimensions). We are now in the position to apply the Landau argument to determine the phase boundaries within LDA. If $1 + Jdr_B^i > 0$, then the approximate energy functional is minimized by having $|\psi_B^i| = 0$, which corresponds to the incompressible Mott situation for the bosons. In turn, for $1 + Jdr_B^i < 0$ the minimization requires $|\psi_B^i| > 0$, and the bosons are superfluid. Exploiting this property, we can determine the phase boundary between the hopping-dominated and Mott regimes at each site, corresponding to $J = -1/(dr_i)$. To find the boundaries for the fermions, we consider that for small J and within LDA the bosons alter the fermionic chemical potential, introducing an effective site dependent chemical potential $\bar{\mu}_F^i = \mu_F - U_{BF}\bar{n}_i - V_i$. At each site i we then consider the corresponding (infinite) homogeneous problem $\hat{H}_F^i = -J\sum_{\langle l,j\rangle}(\hat{f}_l^\dagger \hat{f}_j + \hat{f}_j^\dagger \hat{f}_l) - \bar{\mu}_F^i \sum_l \hat{n}_F^l$, which is appropriate for sufficiently shallow external potentials. This Hamiltonian is diagonal in Fourier space, so that the exact spectrum is given by $\varepsilon_k = -\bar{\mu}_F^i - 4J\sum_{\delta=1}^{D}\cos(k_\delta)$, where $k = (k_1, ..., k_D)$, the lattice spacing being set to 1 without loss of generality. Therefore, when $-\bar{\mu}_F^i - 2dJ > 0$, the ground state has no fermions present, being obviously a Mott state. Similarly, for $-\bar{\mu}_F^i + 2dJ < 0$ the ground state is a Mott state with exactly one fermion at each site. Figure 2 shows the phase regions for an inhomogeneous Bose-Fermi mixture in a three-dimensional lattice with a weakly confining parabolic potential. The solid lines depict the boundaries between Mott and hopping-dominated regions, as evaluated using the above approach. Not surprisingly, one observes that at the center of the trap, where the potential acquires its minimum, lower values of J are needed for the transition to the hopping-dominated regime. For appropriate fixed J, different spatial domains develop from the center of the trap. Depending on the value of μ_B, one observes an alternating sequence of Mott and hopping-dominated domains. An important new feature that emerges in inhomogeneous BFH systems differing from the situation encountered in pure bosonic or fermionic systems is a modulation of the phase regions due to the boson-fermion interaction. This can be understood by comparing the phase boundaries for the interacting mixture with the noninteracting case $U_{BF} = 0$. The boundaries are represented as dashed lines in Fig. 2. For the chosen parameters, the presence of the fermions in the center of the trap is reflected by a tendency to form Mott domains for bosons. Comparing this functional behavior with the fermion number per site in the case of vanishing hopping as depicted in Fig. 1 we see that the state diagram for the bosons is modified when the fermion number per site is exactly one. In turn, the presence of the bosons

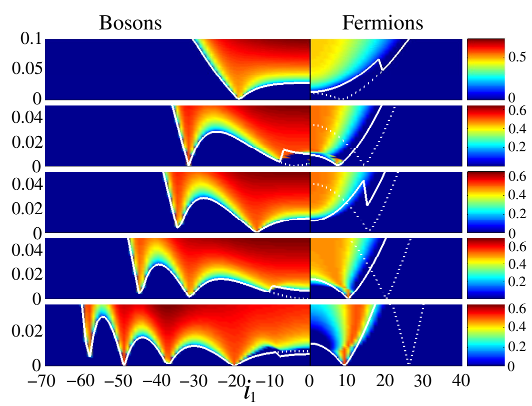

FIG. 2 (color online). The boundaries between Mott and hopping-dominated regions for $D = 3$ ($d = 6$) for bosons (left) and fermions (right), as a function of the site index i_1, and of the hopping $J = J_B = J_F$ at $U_{BF} = 0.3$ and $\mu_F = \mu_B/5$, and, from top to bottom, $\mu_B = (0.7, 2, 2.4, 4, 6.8)$. In each plot, the $J = 0$ axis corresponds to the plots of Fig. 1. The white solid line depicts the phase boundaries as determined in section III. The dashed line reproduces the same plots, but for $U_{BF} = 0$. In the same diagram, the background encodes the variance of the on-site density $\sigma^i_{B/F} = [\langle(\hat{n}^i_{B/F})^2\rangle - \langle\hat{n}^i_{B/F}\rangle^2]^{1/2}$ from the numerical variational analysis discussed in section IV. Dark gray corresponds to the Mott region with $\sigma^i_{B/F} = 0$.

heavily modifies the boundaries between the Mott and the hopping-dominated domains for the fermions: the hopping-dominated regions are pushed outwards, and the value of the integer boson occupation number per site in the Mott phase sets the scale of this phenomenon.

IV. Finite hopping: variational theory.—In Fig. 2 we have also represented the variance of the on-site densities $\sigma^i_{B/F}$. They are determined using the following variational approach. We consider at each bulk site i the corresponding infinite homogeneous lattice Hamiltonian, $\hat{H}_i$. The minimization of $\langle\phi_i|\hat{H}_i|\phi_i\rangle$ over all state vectors will be replaced by a minimization over state vectors respecting the univalence superselection rule, $|\phi_i\rangle = |\phi^i_B\rangle|\phi^i_F\rangle$. For the bosonic sector we introduce a Gutzwiller-type ansatz, $|\phi^i_B\rangle = \prod_l \sum_{n_l} b^i_{n_l}|n_l\rangle$ (see, e.g., Refs. [11,12] and references therein), where the $b^i_{n_l}$ form a probability distribution at each site l, $n_l = 0, 1, \ldots$. After an exact discrete Fourier transformation of the fermionic operators, $\hat{f}_l = \frac{1}{\sqrt{V}}\sum_k \hat{a}_k e^{ikr_l}$, we have for each site i, $\langle\phi_i|\hat{H}_i|\phi_i\rangle = E^i_B + \sum_k \varepsilon^i_k\langle\phi^i_F|\hat{a}^\dagger_k\hat{a}_k|\phi^i_F\rangle$, where

$$E^i_B = -J\sum_{\langle l,j\rangle}\langle\phi^i_B|\hat{b}^\dagger_l\hat{b}_j + \hat{b}^\dagger_j\hat{b}_l|\phi^i_B\rangle + \sum_l\langle\phi^i_B|\hat{n}^l_B(\hat{n}^l_B - 1)|\phi^i_B\rangle + (V_i - \mu_B)\sum_l\langle\phi^i_B|\hat{n}^l_B|\phi^i_B\rangle,$$

with $\varepsilon^i_k = -4J\sum_{\delta=1}^D\cos(k_\delta) - \mu_F - U_{BF}\langle\phi_B|\hat{n}^l_B|\phi_B\rangle - V_i$. Therefore, the state vector $|\phi^0_F\rangle = \prod_{k,\varepsilon^i_k<0}\hat{a}^\dagger_k|0\rangle$ minimizes the energy expectation value at fixed Gutzwiller amplitudes, $E^i_{\min}(b^i_0, b^i_1, \cdots) = E^i_B + \sum_{k,\varepsilon^i_k<0}\varepsilon^i_k$. To determine the ground state, we have to minimize $E^i_{\min}$ at each site i. Because this energy functional is not convex, the energy landscape exhibits local minima and determining the ground state leads to a nonconvex optimization problem. However, the problem can be solved numerically using a simulated annealing method. The regions with exactly vanishing local variance $\sigma^i_{B/F}$ identify the respective Mott regions (dark gray in Fig. 2). Qualitatively, we obtain very similar results in the perturbative and in the variational treatments. The perturbative findings are valid for small hopping only, while the numerical analysis relies on the Gutzwiller ansatz for bosons, which is appropriate in high spatial dimensions ($D = 3$) and in the superfluid regime [17]. For a system of harmonically trapped bosons it has been shown that the appearance of a Mott-insulator domain within a shell of superfluid atoms leads to satellite peaks in the global momentum distribution [18]. This feature is accessible in experiments and can, in particular, be used as an indication for the effect of the fermions on the boson Mott transition.

V. Behavior at the center of the trap: bulk properties.— For the central sites, within LDA, the inhomogeneous case is equivalent to the homogeneous case. To interpret the findings, we first recall the phase diagram of the homogeneous fermionic system in the absence of bosons. In this case the BFH model reduces to a system of spinless

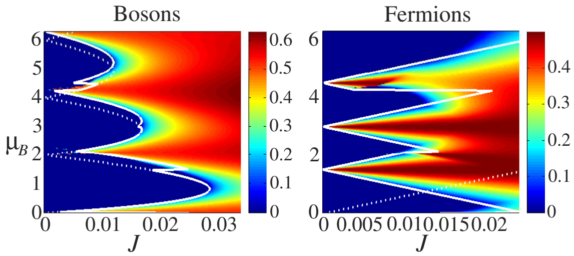

FIG. 3 (color online). State diagram for central sites of bosons (left) and fermions (right) for $U_{BF} = 0.3$ and $\mu_F = \mu_B/5$. Depicted are the phase boundaries as determined using perturbation theory in LDA (solid lines) and Gutzwiller variational theory (shading). The dashed lines correspond to boundaries for $U_{BF} = 0$, determined by the Landau argument for the bosons, and exactly for the fermions.

fermion system with hopping contributions only, and can again be solved exactly by discrete Fourier transformation. The Mott states with exactly one or zero fermions per site can be distinguished from the hopping-dominated states, yielding a linear behavior of the phase boundary as a function of $J = J_F$ (see section III). This is depicted in Fig. 3 with a dashed line. Within the perturbative treatment, the effect of the bosons is to give rise to an effective fermionic chemical potential. This in turn leads to integer discontinuous jumps in the phase boundaries. In turn, the presence of the fermions modulates the phase diagram for the bosons as compared to the standard mean-field phase diagram of the pure Bose-Hubbard model. Notably, the lobes associated to different boson numbers per site in the Mott insulator do not necessarily touch the straight line corresponding to $J = 0$. Again, we have compared these findings with the results obtained from the numerical analysis introduced in section IV. The general behavior of the regions with exactly vanishing density variances is very similar in both approaches. However, the discontinuities are less pronounced within the variational approximation. This is due to the fact that in perturbation theory the zeroth order contribution is manifestly discontinuous. We have compared this behavior with the results obtained from an exact diagonalization of the Hamiltonian for small systems, obtaining qualitatively identical conclusions.

In conclusion, we have studied in detail the phase structure of the ground state of trapped inhomogeneous Bose-Fermi mixtures in cubic lattices. The inhomogeneity leads to domains of Mott plateaux and hopping-dominated regions, where a complex interplay between interacting bosons and fermions is displayed. These results will be compared with density matrix renormalization group methods in forthcoming work. The findings reported in the present work should provide a guideline and should be amenable to direct testing in the upcoming experiments [3] with trapped mixtures of bosonic and fermionic atoms in optical lattices.

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