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 by studying the Bose-Fermi Hubbard model including parabolic confining potentials. We present the exact solution in the limit of vanishing hopping (ultradeep lattices) and study the resulting domain structure of composite particles. For finite hopping we determine the domain boundaries between Mott-insulator plateaux and hopping-dominated regions for lattices of arbitrary dimensionality within 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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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\textsuperscript{1}. Spectacular progress has already been achieved in the experimental manipulation of cold atoms in optical lattices with an astonishingly high degree of control. Most prominently, the superfluid-Mott insulator phase transition in systems of bosonic atoms in optical lattices has been experimentally observed\textsuperscript{2}, and the production of degenerate Fermi gases in optical lattices has been recently achieved\textsuperscript{3}. A perspective of key interest in this field lies in the possibility of discovering and probing new quantum phases of matter by combining ideas from the study of Bose-Fermi mixtures in solid state systems and of cold quantum gases in optical lattices\textsuperscript{4-8}. In Ref.\textsuperscript{4}, the Bose-Fermi Hubbard (BFH) Hamiltonian has been introduced and derived from the underlying microscopic many-body Hamiltonian, linking the experimentally accessible quantities to the model parameters. A mean field argument has been presented for the onset of a bosonic superfluid transition, and in a numerical analysis the behavior of on-site quantities in several situations has been studied. In Refs.\textsuperscript{5, 6} the phase diagram of inhomogeneous 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 suggested. In Ref.\textsuperscript{7} stable supersolid phases have been predicted for homogeneous Bose-Fermi mixtures in two-dimensional lattices. Finally, Ref.\textsuperscript{8} addresses the task of assessing the phase diagram of the BFH model using an exact diagonalization approach for systems of small size.

The investigations in Refs.\textsuperscript{4, 5, 6, 7, 8} are confined to the homogeneous case, i.e., to a translationally invariance BFH Hamiltonian. While this is a very reasonable approach as far as the discussion of the actual phases in the thermodynamical limit is concerned, it is not quite the one encountered experimentally, e.g. in the case of trapped, ultracold atomic gases. The external confining potential, superimposed to the optical lattice potential, breaks the translational symmetry, and leads to profound modifications of the phase structure by allowing for the appearance of spatial domains of coexisting different phases along the lattice, as recently studied for pure bosonic\textsuperscript{9} and pure fermionic systems\textsuperscript{10}. Studies of such inhomogeneous systems are of immediate relevance for the interpretation of experimental findings, where some confinement in a trap is necessary.

In the present paper 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 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. Notably, we introduce a method to treat the bosons within a Gutzwiller-type ansatz\textsuperscript{11, 12} and the fermions exactly, a versatile method that is applicable to several systems of this kind. This method allows us to present for the first time the domain structure of inhomogeneous atomic mixtures in confining potentials and the respective phase diagrams for the homogeneous case.

Starting point of our analysis is the single-band BFH Hamiltonian\textsuperscript{13}, which captures the essential properties of dilute mixtures in optical lattices under fairly general assumptions on the tunable physical parameters\textsuperscript{4}. The grand canonical BFH Hamiltonian reads

\[
\hat{H} = -J_B \sum_{\langle i,j \rangle} (\hat{b}_i \hat{b}_j + \hat{b}_i^\dagger \hat{b}_j^\dagger) - J_F \sum_{\langle i,j \rangle} (\hat{f}_i \hat{f}_j + \hat{f}_i^\dagger \hat{f}_j^\dagger) + U_{BB} \sum_i \hat{n}_B^i (\hat{n}_B^i - 1) + U_{BF} \sum_i \hat{n}_B^i \hat{n}_F^i + \mu_B \sum_i \hat{n}_B^i - \mu_F \sum_i \hat{n}_F^i \tag{1}
\]

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
\( \hat{n}_F = \hat{f}_F \hat{f} \). Sites are associated with a cubic \( D \)-dimensional lattice with fixed spacing, and \( i = (i_1, \ldots, i_D) \) denotes a \( D \)-tuple labeling the coordinates of a site \( i \) with coordination number \( d \) (i.e., the number of nearest neighbors). 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 to the corresponding values at neighboring sites.

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. [3].

1) 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 \( |\psi\rangle = |n_0, n_1, \ldots, n_D \rangle \), where \( n_i = 0, 1, 2, \ldots \) and \( n_{i_k} = 0 \) represent the occupation number of bosons and fermions at site \( i \), respectively. For simplicity 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

\[
\hat{n}_i = \left\{ \begin{array}{ll}
\text{max}(0, [(1 + \mu_B - V_i)/2]), & \text{if } E(\hat{n}_i, 0) < E(\hat{n}_i, 1), \\
\text{max}(0, [(1 + \mu_B - V_i - U_{BF})/2]), & \text{otherwise},
\end{array} \right.
\]

\[
\hat{m}_i = \left\{ \begin{array}{ll}
0, & \text{if } E(\hat{n}_i, 0) < E(\hat{n}_i, 1), \\
1, & \text{otherwise},
\end{array} \right.
\]

where \([\cdot]\) 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 \( \hat{m}_i \) fermions and \( \hat{n}_i \) bosons are formed at site \( i \), see Fig. 1. Connected domains with fixed integer particle number are formed and, depending on the interaction strength \( U_{BF} \) and the relation of the respective chemical potentials \( \mu_B \) and \( \mu_F \), the fermions distribute around the center of the trap or are pushed outwards.

2) Finite hopping: perturbative treatment. – We now turn to the strong coupling limit where also small but finite hopping is allowed for. In a wide range of physical parameters, the strength of the hopping for bosons and fermions are approximately of the same value, for instance for neutral atoms in optical lattices [4]. We set subsequently \( J_F = J_B = J \), and treat the small positive parameter \( J \) as a perturbation. As in Refs. [10], we introduce a mean field approximation, which amounts to a replacement of the bosonic operator products in Eq. (1) according to \( \hat{b}^\dagger_i \hat{b}_j \rightarrow \psi_B^i \psi_B^j + \psi_B^i \psi_B^j \), the complex numbers \( \psi_B^i \) being variational parameters modeling the influence of neighboring atoms with the physical interpretation of a superfluid parameter. We consider the resulting corrections to the ground state energy, \( \langle \psi_0 | \hat{H}_0 | \psi_0 \rangle = \sum_i E(\hat{n}_i, \hat{m}_i) \), 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 \( \psi_B^i \) 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 \( E = \langle \psi_0 | \hat{H}_0 | \psi_0 \rangle = \Delta E_B + \Delta E_F + O(J^2) \), where \( \Delta E_B = 2J d \sum_i \left( |\psi_B^i|^2 (1 + J d r_i) \right) \), with \( r_i = (4\hat{n}_i + 2c_i + 2)/(c_i^2 - 1) \), \( c_i = 1 - 2\hat{n}_i - \hat{V}_i - \mu_B - U_{BF}\hat{n}_i \), and \( d \) is the coordination number of a \( D \)-dimensional cubic lattice (\( d = 6 \) in three dimensions). We are now in the position to apply the Landau argument to determine the phase boundaries within LDA. If \( J > J_{dr}^B \), then the approximate energy functional is minimized by having \( |\psi_B^i|^2 = 0 \), which corresponds to the incompressible Mott situation for the bosons. In turn, for \( J > J_{dr}^F \) the minimization requires \( |\psi_F^i|^2 > 0 \), and the bosons are superfluid. Exploiting this property, we can determine the phase boundary between the hopping-dominated and the Mott regime at each site, corresponding to \( J = 1 / (d r_i) \). 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 \( \tilde{\mu}_F^i = \mu_F - U_{BF} \hat{n}_i - \hat{V}_i \). At each site \( i \) we then consider the corresponding (infinite) homogeneous problem

\( \hat{H}_F = -J \sum_{\langle i, j \rangle} (\hat{f}_i \hat{f}_j + \hat{f}_i^\dagger \hat{f}_j^\dagger) - \tilde{\mu}_F \sum_i \hat{n}_F^i \), which is appropriate for sufficiently shallow external potentials. This Hamiltonian is diagonal in Fourier space, so that the exact

FIG. 1: 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 color as shown in the bar on the right hand side (number of bosons, number of fermions) as a function of the component \( t_i \), the chemical potential \( \mu_B \), and \( U_{BF} \). For the left (right) figure, \( \mu_F = 0 \) (\( \mu_F = \mu_B / 5 \)) is chosen.
The values of \( p_x = \mu_F/5 \) are chosen (corresponding to the topmost plot on the right of Fig. 1), and, from top to bottom, \( J = (0.7, 2, 2.4, 4, 6.8) \). 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 II. The dashed line reproduces the same plots, but for \( U_{BF} = 0 \). In the same diagram, the background color encodes the variance of the on-site densities \( \sigma_{B/F} = \langle (\hat{n}_{B/F})^2 \rangle - \langle \hat{n}_{B/F} \rangle^2 \) from the numerical variational analysis discussed in section III. Dark blue (gray) corresponds to the Mott region with \( \sigma_{B/F} = 0 \).

The spectrum is given by \( \varepsilon_k = -\mu_F^\prime - 4J \sum_{\delta=1}^{D} \cos(\delta k) \), where \( k = (k_1, \ldots, k_D) \), the lattice spacing being set to 1 without loss of generality. Therefore, when \( -\mu_F^\prime - 2dJ > 0 \), the ground state has no fermions present, being obviously a Mott state. Similarly, for \( -\mu_F^\prime + 2dJ < 0 \) the ground state is a Mott state with exactly one fermion at each site. Fig. 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, respectively, 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 the hopping 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 \( \mu_B \), 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 non-interacting 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 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.

III) Finite hopping: variational theory. – In Fig. 2 we have also represented the variance of the on-site densities \( \sigma_{B/F} \). 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 \( \langle \phi_i \rangle \langle \hat{H}_i \rangle \) over all state vectors will be replaced by a minimization over state vectors respecting the univalence superselection rule, \( \langle \phi_i \rangle = \langle \phi_B^i \rangle \phi_F^i \). For the bosonic sector we introduce a Gutzwiller-type ansatz, \( \langle \phi_B^i \rangle = \prod_l \sum_j b_l \langle n_j \rangle \) (see, e.g., Refs. [11, 12] and references therein), where the \( b_l \) form a probability distribution at each site \( l, n_l = 0, 1, \ldots \). After an exact discrete Fourier transformation of the fermionic operators, \( \tilde{f}_l = \frac{1}{\sqrt{l}} \sum_k \tilde{a}_k e^{ik l} \), we have for each site \( i \),

\[
\langle \phi_i \rangle \langle \hat{H}_i \rangle = E_B^i + \sum_k \varepsilon_k \langle \phi_F^i \rangle \langle \tilde{a}_k \tilde{a}_k \rangle \langle \phi_F^i \rangle,
\]

\[
E_B^i = -J \sum_{\langle i,j \rangle} \langle \phi_B^i \rangle \langle \tilde{b}_j \rangle + \langle \tilde{b}_j \rangle \langle \phi_B^i \rangle + \sum_l \langle \phi_B^i \rangle \langle \tilde{n}_l \rangle (\langle \tilde{n}_l \rangle - 1) \langle \phi_B^i \rangle + \langle V_l - \mu_B \rangle \langle \phi_B^i \rangle \langle \phi_B^i \rangle,
\]

\[
\varepsilon_k = -4J \sum_{k=1}^{D} \cos(k \delta) - \mu_F - U_{BF} \langle \phi_B^i \rangle \langle \tilde{n}_l \rangle \langle \phi_B^i \rangle - V_l.
\]

Therefore, the state vector \( \langle \phi_B^i \rangle = \prod_{k, \varepsilon_k < 0} \langle \tilde{a}_k \rangle \rangle \langle \phi_F^i \rangle \langle \phi_F^i \rangle \) minimizes the energy expectation value at fixed Gutzwiller amplitudes,

\[
E_{\text{min}}^i(\tilde{b}_0, \tilde{b}_1, \ldots) = E_B^i + \sum_{k, \varepsilon_k < 0} \varepsilon_k.
\]

To determine the ground state, we have to minimize \( E_{\text{min}}^i \) 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 non-convex optimization problem. However, the problem can be solved numerically using a simulated annealing method [13]. The regions with exactly vanishing local variance, \( \sigma_{B/F} \), identify the respective Mott regions (dark blue/grey 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 [12]. The behavior shown in Fig. 2 is thus a genuine effect of the boson-fermion interaction in the mixture, as it is predicted by the considered approximation schemes. 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 [20]. 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.
IV) 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 how the phase diagram for the fermions would look like in the homogeneous case in the absence of bosons. In this case the BFH model describes a spinless fermion system with hopping contributions only. It can be solved without approximation as before with the help of a 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 II). 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, reflecting the change of the number of bosons per site in the Mott phase. This in turn leads to integer discontinuous jumps in the phase boundaries. In this way, the presence of the bosons modifies the fermionic phase diagram. 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 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 III. The general behavior of the regions with exactly vanishing density variance within Gutzwiller approximation, and Mott regions according to the perturbative results is very similar. 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 optical lattices. The inhomogeneity leads to domains of Mott plateaux and hopping-dominated regions, where a complex interplay between interacting bosons and fermions is displayed. Introducing a new numerical method that treats fermions without approximation, we were able to visualize for the first time the effects of this complex interplay on the domain structure of both species and present the phase diagrams for the homogeneous case. These results will be compared with DMRG-methods for one-dimensional lattices 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 with trapped mixtures of bosonic and fermionic atoms in optical lattices.

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[1] A.G. Truscott et al., Science 291, 2570 (2001); F. Schreck et al., Phys. Rev. Lett. 87, 080403 (2001); Z. Hadzibabic et al., ibid. 88, 160401 (2002); G. Roati et al., ibid. 89, 150403 (2002); W. Hofstetter et al., ibid. 89, 220407 (2002).
[2] M. Greiner et al., Nature 415, 30 (2002); M. Greiner et al., ibid. 419, 51 (2002).
[3] G. Modugno et al., Phys. Rev. A 68, 011601 (2003).
[4] A. Albus, F. Illuminati, and J. Eisert, Phys. Rev. A 68, 023606 (2003).
[5] M. Lewenstein et al., Phys. Rev. Lett. 85, 45404 (2004).
[6] H. Fehrmann et al., Opt. Express 12, 55 (2004).
[7] A. Albus, F. Illuminati, J. Eisert, and M. Lewenstein, Phys. Rev. Lett. 108, 110401 (2012).
[8] R. Roth and K. Burnett, Phys. Rev. A 69, 021601 (2004).
[9] G.G. Batrouni et al., Phys. Rev. Lett. 89, 117203 (2002).
[10] M. Rigol et al., Phys. Rev. Lett. 91, 130403 (2003).
[11] W. Krauth, M. Caffarel, and J.-P. Bouchaud, Phys. Rev. B 45, 3137 (1991).
[12] D. Jaksch et al., Phys. Rev. Lett. 81, 3108 (1998).
[13] Necessary conditions for the single-band approximation to be valid are a sufficiently low temperature and a fermionic filling factor smaller than one. Furthermore, the lowest band needs to be well separated from the other bands, which in optical lattices can be realized by sufficiently deep lattices, and the interaction energies must be sufficiently small.
[14] M.P.A. Fisher et al., Phys. Rev. B 40, 546 (1989).
[15] S. Sachdev, Quantum phase transitions (Cambridge University Press, Cambridge, 1999).
[16] K. Sheshadri et al., Europhys. Lett. 22, 257 (1993).
[17] S. Kirkpatrick, C.D. Gelatt, and M.P. Vecchi, Science 220, 671 (1983).
[18] J.J. Garcia-Ripoll et al., Opt. Express 12, 42 (2004).
[19] For purely bosonic systems, we were able to reproduce the findings for the local density of Ref. [11] without noticeable difference, providing an indication for the validity of the LDA.
[20] V.A. Kashurnikov, N.V. Prokof’ev, and B.V. Svistunov, Phys. Rev. A 66, 031601(R) (2002).

[21] This diagonalization has been performed for 8 lattice sites, 5 fermions and 3 bosons, employing Arnoldi techniques.