Mixtures of bosonic and fermionic atoms in optical lattices

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We discuss the theory of mixtures of bosonic and fermionic atoms in periodic potentials at zero temperature. We derive a general Bose-Fermi Hubbard Hamiltonian in a one-dimensional optical lattice with a superimposed harmonic trapping potential. We study the conditions for linear stability of the mixture and derive a mean-field criterion for the onset of a bosonic superfluid transition. We investigate the ground-state properties of the mixture in the Gutzwiller formulation of mean-field theory, and present numerical studies of finite systems. The bosonic and fermionic density distributions and the onset of quantum phase transitions to demixing and to a bosonic Mott-insulator are studied as a function of the lattice potential strength. The existence is predicted of a disordered phase for mixtures loaded in very deep lattices. Such a disordered phase possessing many degenerate or quasidegenerate ground states is related to a breaking of the mirror symmetry in the lattice.

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I. INTRODUCTION

Recent spectacular progress in the manipulation of neutral atoms in optical lattices [1–3] has opened the way to the simulation of complex quantum systems of condensed-matter physics, such as high-T_c superconductors, Hall systems, and superfluid ^{4}He, by means of atomic systems with perfectly controllable physical parameters [4]. Optical lattices are stable periodic arrays of microscopic potentials created by the interference patterns of intersecting laser beams [5]. Atoms can be confined to different lattice sites, and by varying the strength of the periodic potential it is possible to tune the interatomic interactions with great precision. They can be enhanced well into regimes of strong correlation, even in the dilute limit. The transition to a strong coupling regime can be realized by increasing the depth of the lattice potential wells, a quantity that is directly proportional to the intensity of the laser light. This is an experimental parameter that can be controlled with great accuracy. For this reason, besides the fundamental interest for the investigation of quantum phase transitions [6] and other basic quantum phenomena [7–13], optical lattices have become an important practical tool for applications ranging from laser cooling [14] to quantum control and information processing [15,16], and quantum computation [17–21].

The theory of neutral bosonic atoms in optical lattices has been developed [7] by assuming that the atoms are confined to the lowest Bloch band of the periodic potential. It can then be shown that the system is effectively described by a single-band Bose-Hubbard model Hamiltonian [22]. In such a model the superfluid-insulator transition is predicted to occur when the on-site boson-boson interaction energy becomes comparable to the hopping energy between adjacent lattice sites. This situation can be experimentally achieved by increasing the strength of the lattice potential, which results in a strong suppression of the kinetic-(hopping) energy term. In this way, the superfluid–Mott-insulator quantum phase transition has been realized by loading an ultracold atomic Bose-Einstein condensate in an optical lattice [1].

The present paper is concerned with the study of dilute mixtures of interacting bosonic and fermionic neutral atoms subject to an optical lattice and a superimposed trapping harmonic potential at zero temperature. We assume the fermions to be identical (for instance, spin-polarized in a magnetic trap), so that there are only *s*-wave boson-boson and fermion-boson contact interactions present. We construct an effective single-band Bose-Fermi Hubbard Hamiltonian, and we determine the ground-state energy and on-site density distributions in different mean-field approximations of increasing complexity. Our main aim at this level of description is to determine the basic ground-state properties of the mixture and to study how the bosonic superfluid-insulator transition is influenced by the presence of the fermions. Besides the study of the latter issue, and the assessment of the properties of linear stability of the system against boson-fermion demixing, a remarkable finding of our analysis is that a quantum binary mixture loaded in a very deep optical lattice allows for a disordered phase of very many degenerate or quasidegenerate ground states separated by very high potential energy barriers. In the limit of very large lattice potential strengths, the basic mirror symmetry of the optical lattice is broken.

The plan of the paper is as follows: In Sec. II we set the notation and derive the Bose-Fermi Hubbard model Hamiltonian. We then discuss the range of validity of the approximations and the assumptions used in the derivation. In Sec. III we introduce some basic mean-field descriptions to study the properties of stability of the mixture against phase separation, and we provide a simple analytical criterion for the onset of a superfluid phase for the bosons starting from a Mott-insulating ground state.

In Sec. IV we present numerical simulations for a small number of particles in the framework of the Gutzwiller variational ansatz. Two important cases have to be distinguished: boson-fermion repulsive or attractive interaction (the boson-boson interaction is taken to be always repulsive). In the first

instance, one can observe a continuous transition to a complete demixing of the fermions from the bosons, and to a Mott-insulating phase of the bosons, as the strength of the lattice potential is increased. In the case of attractive boson-fermion interactions there is no transition to demixing or to collapse of the mixture, while one still observes a Mott-insulating transition for the bosons. By studying the behavior of the superfluid order parameter we show that in both cases the transition takes place at the same critical value of the lattice potential strength. Moreover, due to the strong attraction, the fermions and the bosons tend to form together ordered block-crystalline structures at the center of the trap.

In Sec. V we present a numerical analysis that, although constrained to a small number of particles (five bosons and five fermions), seems to indicate the existence of a rich structure of degenerate energy minima for large enough values of the lattice potential strength. Such an energy landscape suggests the possible existence of disordered phases of the mixture due to the delicate interplay between the different physical parameters (boson hopping, fermion hopping, boson on-site energy, boson-fermion on-site energy), the lattice depth, and the symmetries of the problem. Finally, a summary and an outlook to future research are shortly discussed in Sec. VI.

II. MODEL HAMILTONIAN

We start by introducing the Hamiltonian for a Bose-Fermi mixture loaded into optical lattice potentials and confined by additional, slowly varying, external (harmonic) trapping potentials. It is given by

$$\hat{H}=\hat{T}_B+\hat{T}_F+\hat{V}_B+\hat{V}_F+\hat{W}_{BB}+\hat{W}_{BF}, \tag{1}$$

where

$$\hat{T}_B=-\int d^3\mathbf{r}\,\hat{\Phi}^\dagger(\mathbf{r})\frac{\hbar^2\boldsymbol{\nabla}^2}{2m_B}\hat{\Phi}(\mathbf{r}), \tag{2}$$

$$\hat{T}_F=-\int d^3\mathbf{r}\,\hat{\Psi}^\dagger(\mathbf{r})\frac{\hbar^2\boldsymbol{\nabla}^2}{2m_F}\hat{\Psi}(\mathbf{r}) \tag{3}$$

represent the boson and fermion kinetic energies, respectively, while

$$\hat{W}_{BB}=\frac{1}{2}\frac{4\pi\hbar^2 a_{BB}}{m_B}\int d^3\mathbf{r}\,\hat{\Phi}^\dagger(\mathbf{r})\hat{\Phi}^\dagger(\mathbf{r})\hat{\Phi}(\mathbf{r})\hat{\Phi}(\mathbf{r}), \tag{4}$$

$$\hat{W}_{BF}=\frac{2\pi\hbar^2 a_{BF}}{m_R}\int d^3\mathbf{r}\,\hat{\Phi}^\dagger(\mathbf{r})\hat{\Psi}^\dagger(\mathbf{r})\hat{\Psi}(\mathbf{r})\hat{\Phi}(\mathbf{r}) \tag{5}$$

denote the boson-boson and the fermion-boson contact-interaction energies. They are parametrized by the boson-boson and the fermion-boson s-wave scattering lengths a_{BB} and a_{BF}, respectively, and by boson mass m_B and reduced mass $m_R=m_Bm_F/(m_B+m_F)$, where m_F denotes the fermion mass. Potential energies

$$\hat{V}_B=\int d^3\mathbf{r}\,\hat{\Phi}^\dagger(\mathbf{r})[V_B(\mathbf{r})+P_B(\mathbf{r})]\hat{\Phi}(\mathbf{r}), \tag{6}$$

$$\hat{V}_F=\int d^3\mathbf{r}\,\hat{\Psi}^\dagger(\mathbf{r})[V_F(\mathbf{r})+P_F(\mathbf{r})]\hat{\Psi}(\mathbf{r}) \tag{7}$$

are due to the trapping and lattice potentials. We consider pure magnetic trapping for bosons and fermions so that fermions are spin-polarized and their s-wave interaction energy $\hat{W}_{FF}$ can be neglected: $\hat{W}_{FF}=0$. In the subsequent analysis we will consider the harmonic approximation of a typical quadrupolar magnetic field with strong anisotropy in transverse directions y and z, i.e.,

$$V_B(\mathbf{r})\simeq m_B\omega_B^2(x^2+\lambda^2y^2+\lambda^2z^2)/2 \tag{8}$$

and

$$V_F(\mathbf{r})\simeq m_F\omega_F^2(x^2+\lambda^2y^2+\lambda^2z^2)/2, \tag{9}$$

where $\lambda\gg1$ is the anisotropy parameter. Moreover, if we assume trapping in the same magnetic state for the bosons and the fermions, then the trapping frequencies are related according to $\omega_F/\omega_B=(m_B/m_F)^{1/2}$ so that the two potentials coincide: $V_B(\mathbf{r})=V_F(\mathbf{r})$. The ground-state harmonic-oscillator lengths, however, are different due to the different masses, and also differ for the x direction on the one hand and the y and z directions on the other hand:

$$\ell_{B/F}^{\parallel}=\sqrt{\hbar/(m_{B/F}\omega_{B/F})} \tag{10}$$

in the x direction and $\ell_{B/F}^{\perp}=\ell_{B/F}^{\parallel}/\sqrt{\lambda}$ in the y and z directions. We next consider a lattice structure for the bosons and the fermions in the x direction, associated with the corresponding bosonic and fermionic one-dimensional (1D) optical lattice potentials $P_B(x)$ and $P_F(x)$:

$$\begin{aligned}P_B(x)&=V_B^0\sin^2(\pi x/a),\\ P_F(x)&=V_F^0\sin^2(\pi x/a),\end{aligned} \tag{11}$$

where a is the lattice spacing associated with wave vector $k=\pi/a$ of the standing laser light. If the lattice potentials are produced by a far off-resonant laser for both species, the lattice potential strengths are equal for both fermions and bosons: $V_F^0=V_B^0=V_0$, and the two optical lattices coincide exactly. This is the situation we will always consider in the following.

In the presence of a strong optical lattice and a sufficiently shallow external confinement in the x direction, the field operators can be expanded in terms of the single-particle Wannier functions localized at each lattice site x_i. Further, the typical interaction energies involved are normally not strong enough to excite higher vibrational states, and we can retain only the lowest vibrational state in each lattice potential well both for bosons and fermions (single-band approximation). In case of stronger external confinements, or interactions, one should include higher Bloch bands as well in the expansion of the field operators, a case we do not consider in the present context. In the harmonic approximation, Wannier functions $w(\mathbf{r})$ factorize in the product of harmonic-oscillator states in each direction, with the trapping potential almost constant between adjacent lattice sites. We then have

$$\hat{\Phi}(\mathbf{r})=\sum_i \hat{a}_i w_x^B(x-x_i)w_y^B(y)w_z^B(z), \tag{12}$$

$$\hat{\Psi}(\mathbf{r})=\sum_i \hat{b}_i w_x^F(x-x_i)w_y^F(y)w_z^F(z), \tag{13}$$

where $\hat{a}_i$ and $\hat{b}_i$ are, respectively, the bosonic and fermionic annihilation operators at the ith lattice site, $x_i=ia$, and index i runs on positive and negative integers, the origin of the lattice being fixed at $i=0$ so that it coincides with the center (the minimum) of the external trapping potential. In each lattice potential well, the Wannier local ground states for bosons and fermions are Gaussians in the harmonic approximation:

$$w_y^{B/F}(y)=\frac{\exp[-y^2/2(\ell^{\perp}_{B/F})^2]}{\pi^{1/4}(\ell^{\perp}_{B/F})^{1/2}}, \tag{14}$$

$$w_z^{B/F}(z)=\frac{\exp[-z^2/2(\ell^{\perp}_{B/F})^2]}{\pi^{1/4}(\ell^{\perp}_{B/F})^{1/2}}, \tag{15}$$

and

$$w_x^{B/F}(x-x_i)=\frac{\exp[-(x-x_i)^2/2(\ell^{0}_{B/F})^2]}{\pi^{1/4}(\ell^{0}_{B/F})^{1/2}}, \tag{16}$$

where

$$\ell^0_{B/F}=a/[\pi(V_0/E^R_{B/F})^{1/4}] \tag{17}$$

is the width of the harmonic-oscillator potential wells at each lattice site, with $E_B^R=(\pi\hbar)^2/2a^2m_B$ and $E_F^R=(\pi\hbar)^2/2a^2m_F$ being the boson and fermion recoil energies, respectively.

In this paper we will consider the physical situation of very shallow trapping potentials, such that $\ell^{\parallel}_{B/F}\gg aN_{B/F}$ and consequently local-density approximation (LDA) can be applied in the study of the ground-state properties of the system. Therefore, when exploiting the Wannier function expansions (12) and (13) to map the full Hamiltonian (1) into its lattice version, we discard all terms that are of order $(aN_{B/F}/\ell^{\parallel}_{B/F})^2$ or of higher powers of it. Otherwise, nonlocal effects caused by the trapping potential, such as site-dependent hopping terms, have to be considered [23]. Finally, this approximation scheme leads to the following Hubbard-type Hamiltonian:

$$\begin{aligned}\hat{H}=&-\frac{1}{2}\sum_i (J_B\hat{a}^\dagger_{i+1}\hat{a}_i+J_F\hat{b}^\dagger_{i+1}\hat{b}_i+\text{H.c.})\\&+\frac{U_{BB}}{2}\sum_i \hat{n}_B^{(i)}(\hat{n}_B^{(i)}-1)+U_{BF}\sum_i \hat{n}_B^{(i)}\hat{n}_F^{(i)}+\sum_i V_B^{(i)}\hat{n}_B^{(i)}\\&+\sum_i V_F^{(i)}\hat{n}_F^{(i)}+\hbar(\lambda\omega_B+\omega_B^0/2)\hat{N}_B+\hbar(\lambda\omega_F+\omega_F^0/2)\hat{N}_F.\end{aligned} \tag{18}$$

The first line in the above Bose-Fermi Hubbard Hamiltonian describes independent nearest-neighbor hopping of bosons and fermions, with amplitudes J_B and J_F, respectively. The terms in the second line describe boson-boson on site repulsion (with $U_{BB}>0$) and boson-fermion on-site interaction. This interaction can be repulsive or attractive, depending on the sign of U_{BF}. The third line describes the energy offset at each lattice site due to the x component of external trapping potentials $V_{B/F}(\mathbf{r})$, and the last line contains the overall constant zero-point energy terms due to the y and z components of $V_{B/F}(\mathbf{r})$ and to the lattice potential $P(x)$. The on-site interaction and offset energy terms are simple functions of the on-site boson and fermion occupation number operators $\hat{n}_B^{(i)}=\hat{a}_i^\dagger\hat{a}_i$ and $\hat{n}_F^{(i)}=\hat{b}_i^\dagger\hat{b}_i$, while the zero-point energy terms are proportional to the total particle number operators $\hat{N}_B=\Sigma_i\hat{a}_i^\dagger\hat{a}_i$ and $\hat{N}_F=\Sigma_i\hat{b}_i^\dagger\hat{b}_i$. Frequency

$$\omega^0_{B/F}=\hbar/[(\ell^0_{B/F})^2m_{B/F}] \tag{19}$$

fixes the bosonic and fermionic harmonic oscillations in each lattice well. The relevant parameters entering in the Hamiltonian are the on-site values of trapping harmonic potential

$$V^{(i)}_{B/F}=\frac{m_{B/F}}{2}\omega^2_{B/F}x_i^2, \tag{20}$$

the nearest-neighbor hopping amplitudes between adjacent sites x_i and x_{i+1} for bosons and fermions

$$\begin{aligned}J_{B/F}=\int dx\, w_x^{B/F}(x-x_i)\Bigg[&-\frac{\hbar^2}{2m_{B/F}}\frac{d^2}{dx^2}\\&+V_0\sin^2\left(\pi\frac{x}{a}\right)\Bigg]w_x^{B/F}(x-x_{i+1}),\end{aligned} \tag{21}$$

the strength of the on-site repulsion energy between two bosonic atoms at the same lattice site

$$\begin{aligned}U_{BB}=&\frac{4\pi\hbar^2a_{BB}}{m_B}\int dx[w_x^B(x-x_i)]^4\\&\times\int dy[w_y^B(y)]^4\int dz[w_z^B(z)]^4,\end{aligned} \tag{22}$$

and the strength of the on-site interaction energy (either repulsive or attractive) between a bosonic and a fermionic atom at the same lattice site

$$\begin{aligned}U_{BF}=&\frac{2\pi\hbar^2a_{BF}}{m_R}\int dx[w_x^B(x-x_i)w_x^F(x-x_i)]^2\\&\times\int dy[w_y^B(y)w_y^F(y)]^2\int dz[w_z^B(z)w_z^F(z)]^2.\end{aligned} \tag{23}$$

In typical situations we may neglect next-to-nearest neighbor hopping amplitudes and nearest-neighbor interaction couplings that are usually some orders of magnitude smaller, so that Hamiltonian (18) provides a rather accurate model for

the dynamics of a Bose-Fermi mixture with three-dimensional scattering in a one-dimensional periodic potential. Terms involving nearest-neighbor interaction strengths or next-to-nearest neighbor hopping amplitudes can become relevant and need to be included, e.g., when considering phonon exchange between fermions, and this would lead to a Bose-Fermi analog of the so-called extended Hubbard models. To evaluate estimates for the parameters entering the Bose-Fermi Hubbard Hamiltonian (18) using Eqs. (14), (15), and (16), we will set boson recoil energy $E_B^R = \hbar^2\pi^2/(2m_B a^2)$ as the unit of energy. We then introduce a dimensionless quantity $\tilde{V}_0 = V_0/E_B^R$ and, analogously, dimensionless quantities $\tilde{U}_{BB}$, $\tilde{U}_{BF}$, $\tilde{V}_B^{(i)}$, $\tilde{V}_F^{(i)}$, $\tilde{J}_B$, and $\tilde{J}_F$. We then have

$$\tilde{U}_{BB} = \sqrt{\frac{8}{\pi^3}}\frac{a_{BB}a}{(\ell_B^\perp)^2}\tilde{V}_0^{1/4}, \tag{24}$$

$$\tilde{U}_{BF} = \sqrt{\frac{8}{\pi^3}}\left(1+\frac{m_B}{m_F}\right)\frac{a_{BF}a}{(\ell_B^\perp)^2+(\ell_F^\perp)^2}\tilde{V}_0^{1/4}, \tag{25}$$

$$\tilde{V}_B^{(i)} = \frac{i^2}{\pi^2(\ell_B^\parallel/a)^4}, \quad \tilde{V}_F^{(i)} = \frac{m_B}{m_F}\frac{i^2}{\pi^2(\ell_F^\parallel/a)^4}, \tag{26}$$

$$\tilde{J}_B = \left(\frac{\pi^2}{4}-1\right)\tilde{V}_0 \exp\left[-\frac{\pi^2}{4}\sqrt{\tilde{V}_0}\right], \tag{27}$$

$$\tilde{J}_F = \left(\frac{\pi^2}{4}-1\right)\tilde{V}_0 \exp\left[-\frac{\pi^2}{4}\sqrt{\frac{m_F}{m_B}\tilde{V}_0}\right]. \tag{28}$$

In Fig. 1 we show the dependencies of these parameters on the potential strength $\tilde{V}_0$ (compare also Ref. [16]). For reference we have also included the overlap integral $\langle w(x-x_i)|w(x-x_{i+1})\rangle$ of adjacent Wannier functions. The overlap is negligible, but for very small values of the potential strength, confirming that terms of the order of the overlap integral can be neglected in the Hamiltonian. The Gaussian approximation holds rather well, as can be seen by comparing the associated bosonic hopping amplitude J_B with the one obtained by using the exact 1D Mathieu equation [13].

Besides the conditions mentioned earlier, all the expressions derived in the present section are justified under the following circumstances. First of all, we must require that the two-body scattering processes are not influenced by the confinements, a condition that is guaranteed if the lengths of the confining and lattice potentials in all directions are much larger than the boson-boson and fermion-boson scattering lengths. Next, the single-band structure of the lattice Hamiltonian is assured if lattice spacing a is much greater than the harmonic confinements in each direction at all lattice sites. On the other hand, in this limit the harmonic approximation for the Wannier functions at each lattice well is automatically satisfied. Finally, as mentioned earlier, the assumption of a slowly varying confining potential such that LDA is applicable leads to condition $\ell_{B/F}^\parallel \gg a N_{B/F}$. We can summarize all the above conditions with the following chain of inequalities:

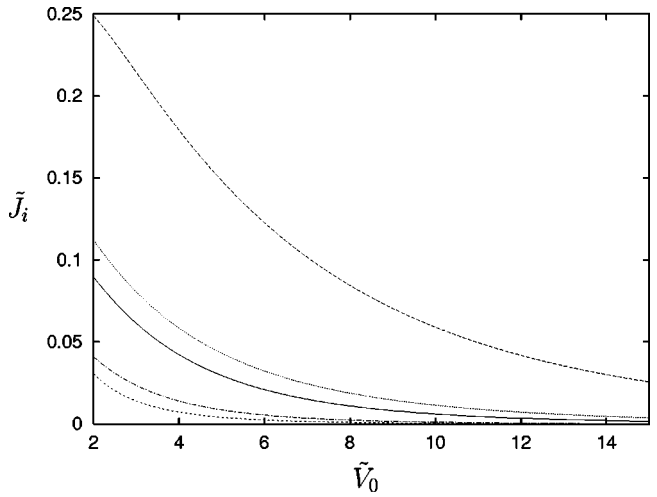

FIG. 1. Top to bottom: fermion hopping amplitude $\tilde{J}_F$ for $m_F/m_B = 0.5$ in the Gaussian approximation; boson hopping amplitude $\tilde{J}_B$ from the exact 1D Mathieu equation; boson hopping amplitude $\tilde{J}_B$ in the Gaussian approximation; the fermion hopping amplitude for $m_F/m_B = 1.5$ in the Gaussian approximation; and, for comparison, overlap integral $\langle w(x-x_i)|w(x-x_{i+1})\rangle$ of adjacent Wannier functions in the Gaussian approximation. All quantities are dimensionless.

$$\{|a_{BF}|, a_{BB}\} \ll \{\ell_{B/F}^0, \ell_{B/F}^\perp\} \ll a \ll \ell_{B/F}^\parallel/N_{B/F}. \tag{29}$$

Our model is for some aspects unrealistic, since in present experimental situations the transverse confinements cannot be made very strong. Therefore a multiband structure can appear with several radial states being occupied, as reported in a recent experiment by the Florence group on Bose-Fermi mixtures in a 1D optical lattice [24].

III. PHASE STABILITY AND THE SUPERFLUID TRANSITION

In this section we investigate the zero-temperature ground-state properties of the system in a mean-field approximation. In the following, we will adopt a grand-canonical description through Hamiltonian

$$\hat{K} = \hat{H} - \mu_B \hat{N}_B - \mu_F \hat{N}_F, \tag{30}$$

where μ_B and μ_F are the bosonic and fermionic chemical potentials. According to the Hohenberg-Kohn theorem, ground-state energy

$$E = \langle \Psi_0 | \hat{K} | \Psi_0 \rangle \tag{31}$$

is a functional of the on-site bosonic and fermionic densities $n_B^{(i)} = \langle \hat{a}_i^\dagger \hat{a}_i \rangle$ and $n_F^{(i)} = \langle \hat{b}_i^\dagger \hat{b}_i \rangle$, where the expectation values are taken with respect to the ground state with state vector $|\Psi_0\rangle$. We decompose functional E according to

$$E = E_B + E_F + E_{BF} - \mu_B \sum_i n_B^{(i)} - \mu_F \sum_i n_F^{(i)}, \tag{32}$$

where E_B is the energy contribution depending only on boson parameters J_B, U_{BB}, and $V_B^{(i)}$; E_F is the energy depending only on the fermion parameters; and E_{BF} is the term due to boson-fermion interactions. We treat this latter term in mean-field approximation; neglecting exchange-correlation effects;

$$E_{BF}=U_{BF}\sum_i n_B^{(i)}n_F^{(i)}. \tag{33}$$

Exchange-correlation effects have been recently studied for the case of homogeneous mixtures in the continuum [25,26]. For fermion energy E_F, we take the energy of the noninteracting homogeneous system and exploit local-density approximation (LDA) on it:

$$E_F=-\frac{2J_F}{\pi}\sum_i \sin(\pi n_F^{(i)})+\sum_i V_F^{(i)}n_F^{(i)}. \tag{34}$$

This approximate description of the fermions is well justified in the presence of a slowly varying trapping potential (so that LDA can be applied), when there are no direct interactions among the fermions (as in our case) and moreover, when one can neglect induced phonon-mediated self-interactions due to the presence of the bosons. Therefore, in this situation, the nontrivial features of different quantum phases will regard only the bosonic sector and not the fermionic one. However, the presence of the fermions will indirectly contribute to the properties of the different bosonic phases, and this is the subject that we will study in the following.

In order to find an expression for boson energy E_B, we will proceed in steps of increasing accuracy. First, we perform a very simple mean-field analysis in two extreme limits: a completely superfluid boson ground state and a totally Mott-insulating boson ground state. In the latter case we will provide a simple criterion for stability of the mixture against demixing. Next, we will perform a perturbation expansion around the Mott-insulating boson ground state to recover perturbatively the phase boundary against transition to superfluidity. Finally, in the following section, we will study the ground-state properties of the mixture using a Gutzwiller ansatz for the bosons capable of describing the intermediate regimes between the insulating and superfluid bosonic phases.

We first consider the bosons to be superfluid. In this regime the chemical potential and the number of particles in a homogeneous system are related, to lowest order in U_{BB}, via [8]

$$\mu_B=U_{BB}n_0-2J_B, \tag{35}$$

where n_0 is the density of condensed bosons. Additionally, for very weak interaction, $n_0\approx n_B$. Exploiting this result in LDA and using the mean-field expression for the Bose-Fermi interaction energy, we can then write for the inhomogeneous Bose-Fermi mixture at a given lattice site:

$$U_{BB}n_B^{(i)}=\mu_B+2J_B-V_B^{(i)}-U_{BF}n_F^{(i)}. \tag{36}$$

Next, we consider the case of a Mott-insulating bosonic phase. To lowest order in J_B we neglect the kinetic term altogether. Then it is easily shown that the relation between the bosonic chemical potential and the bosonic density for a homogeneous system is given by

$$\mu_B=U_{BB}n_B-U_{BB}/2. \tag{37}$$

Exploiting LDA as before, we have in the inhomogeneous case at a given lattice site,

$$U_{BB}n_B^{(i)}=\mu_B+U_{BB}/2-V_B^{(i)}-U_{BF}n_F^{(i)}. \tag{38}$$

Comparing Eqs. (36) and (38), we observe the same behavior of the on-site density profiles but for a constant correction to the boson chemical potential, depending on whether the bosons are in a superfluid or in a Mott-insulating state. Finally, differentiating the energy functional with respect to the on-site populations of the fermions, we determine the associated density field and the set of coupled equations describing the ground state of the mixture at any lattice site:

$$U_{BB}n_B^{(i)}=\mu_B'-V_B^{(i)}-U_{BF}n_F^{(i)}, \tag{39}$$

$$-2J_F\cos(\pi n_F^{(i)})=\mu_F-V_F^{(i)}-U_{BF}n_B^{(i)}, \tag{40}$$

where μ_B' is the proper expression of the boson chemical potential according to whether the bosons are in the Mott-insulating or superfluid regime. These equations are valid at a given lattice site i if $\mu_B'-V_B^{(i)}-U_{BF}n_F^{(i)}>0$, otherwise one must set $n_B^{(i)}=0$. On the other hand, if

$$(\mu_F-V_F^{(i)}-U_{BF}n_B^{(i)})/2J_F<0 \tag{41}$$

we must impose $n_F^{(i)}=0$ at the given lattice site, while $n_F^{(i)}=1$ must be imposed when $(\mu_F-V_F^{(i)}-U_{BF}n_B^{(i)})/2J_F>1$. These expressions are the lattice analogs of the Thomas-Fermi description of boson-fermion mixtures in the continuum. We remark that in the Mott-insulating regime the boson on site populations $n_B^{(i)}$ must be rounded off to the integer closest to the solutions of Eqs. (39) and (40).

In the Mott-insulating regime we can determine a criterion of linear stability against phase separation of the two species if we expand energy functional E to second order in the small density variations $\delta n_{B/F}^{(i)}$ around the minimum provided by the solution of Eqs. (39) and (40):

$$\delta^2E=\tfrac{1}{2}\sum_i (\delta_{nB}^{(i)}\ \ \delta_{nF}^{(i)})\begin{pmatrix} U_{BB} & U_{BF} \\ U_{BF} & 2\pi J_F\sin(\pi n_F^{(i)})\end{pmatrix}\begin{pmatrix}\delta n_B^{(i)}\\ \delta n_F^{(i)}\end{pmatrix}. \tag{42}$$

This quadratic form is positive at a given site i if and only if

$$2\pi J_F\sin(\pi n_F^{(i)})U_{BB}>U_{BF}^2 \tag{43}$$

and $2\pi J_F\sin(\pi n_F^{(i)})+U_{BB}\geqslant 0$. This last condition is always satisfied for $U_{BB}>0$ and identical fermions. If this is not the case for every site i, then the ground state is not stable against demixing. This result is similar to that recently obtained for a mixture of two different boson species on a

lattice [27], which states that the mixture is stable if $U_1U_2 > U_{12}^2$, where U_1 and U_2 are the boson-boson interaction strengths of species 1 and 2, respectively, and U_{12} is the interspecies coupling. The form of expression (43) then suggests that the Pauli on-site energy $2\pi J_F \sin(\pi n_F^{(i)})$ has the meaning of a density-dependent interaction strength. A similar correspondence was previously pointed out for homogeneous Bose-Fermi mixtures in the continuum [28].

Introducing a perturbation expansion with respect to J_B around the Mott-insulating ground state, we can recover the zero-temperature phase transition to the superfluid phase. The reverse, i.e., to build a perturbative expansion in powers of U_{BB} around the superfluid ground state fails to describe the transition to a Mott insulator, as pointed out in Ref. [8] for the pure Bose case. We follow the procedure adopted in Ref. [27] for the two-component boson mixture, with the due modifications for the present case of a boson-fermion mixture, by treating the bosonic kinetic (hopping) term as the perturbation with respect to the bosonic Mott-insulating ground state. This scheme was first introduced for one-component Bose systems in Refs. [8,29,30]. We proceed by expanding the ground-state energy with respect to the (local) bosonic superfluid parameter $\psi^{(i)} = \mathrm{Re}\langle a_i \rangle$. At the phase boundary between a Mott insulator (MI) and a superfluid (SF) the expansion coefficients must vanish, yielding the following criterion for the onset of the transition to the (local) SF state:

$$\begin{aligned} U_{BB}(2n_B^{(i)}-1) - 2J_B - (U_{BB}^2 - 4U_{BB}^2(2n_B^{(i)}+1) + 4J_B^2)^{1/2} \\ < \mu_B - V_B^{(i)} - U_{BF} n_F^{(i)} < U_{BB}(2n_B^{(i)}-1) - 2J_B \\ + (U_{BB}^2 - 4U_{BB}^2(2n_B^{(i)}+1) + 4J_B^2)^{1/2}. \end{aligned} \tag{44}$$

The minimum value of U_{BB}/J_B, where a MI phase can exist, is given by condition

$$U_{BB}/J_B = 4n_B^{(i)} + 2 + 2\sqrt{(2n_B^{(i)}+1)^2 - 1}, \tag{45}$$

and it involves the fermionic sector indirectly through the dependence of $n_B^{(i)}$ on the fermionic parameters and density distributions provided by Eqs. (39) and (40). Apart from this important modification, the phase diagram, at this level of approximation, is analogous to that of a one-component Bose system.

IV. GUTZWILLER ANSATZ AND NUMERICAL ANALYSIS

The simplest ansatz for the boson ground state, which is capable of describing both the SF and the MI phases, is the Gutzwiller ansatz, which contains the mean-field approximations previously discussed as special cases. It consists of factorizing the amplitudes of superpositions of all possible Fock states consistent in the following way:[1]

$$|\Psi\rangle_B \mapsto \prod_i \sum_{n_i} f_{n_i}^{(i)} \frac{(\hat{a}_i^\dagger)^{n_i}}{\sqrt{n_i!}} |0\rangle, \tag{46}$$

where the $f_{n_i}^{(i)}$ are taken to be real and positive. Using the Gutzwiller ansatz in the determination of the energy functional, while keeping the same approximations previously introduced for the boson-fermion interaction and the fermion energy, the total ground-state energy reads

$$E = E_B + E_F + U_{BF} \sum_i n_B^{(i)} n_F^{(i)}, \tag{47}$$

where the subsidiary conditions ensuring particle number conservation are

$$\sum_i n_B^{(i)} = \sum_i \langle \hat{a}_i^\dagger \hat{a}_i \rangle = N_B, \tag{48}$$

$$\sum_i n_F^{(i)} = \sum_i \langle \hat{b}_i^\dagger \hat{b}_i \rangle = N_F. \tag{49}$$

The boson energy contribution is now

$$\begin{aligned} E_B = -\frac{1}{2} J_B \left(\sum_i \psi^{(i+1)*} \psi^{(i)} + \mathrm{c.c.} \right) + \sum_i \frac{U_{BB}}{2} (\sigma_B^{(i)} - n_B^{(i)}) \\ + \sum_i V_B^{(i)} n_B^{(i)}, \end{aligned} \tag{50}$$

and the bosonic observables are related to the Gutzwiller amplitudes by

$$n_B^{(i)} = \sum_{n=0}^{\infty} n (f_n^{(i)})^2, \tag{51}$$

$$\sigma_B^{(i)} = \langle \hat{a}_i^\dagger \hat{a}_i \hat{a}_i^\dagger \hat{a}_i \rangle = \sum_{n=0}^{\infty} n^2 (f_n^{(i)})^2, \tag{52}$$

$$\psi^{(i)} = \mathrm{Re}\langle \hat{a}_i \rangle = \sum_{n=0}^{\infty} \sqrt{n+1} f_n^{(i)} f_{n+1}^{(i)}. \tag{53}$$

Moreover, we must impose the natural constraints that

[1]Recently we have performed as an alternative approach an exact numerical diagonalization of the Bose-Fermi Hubbard Hamiltonian without approximation, which is feasible for a small number of particles. This analysis shows that the behavior of the on-site quantities as considered here is qualitatively very much in agreement with the Gutzwiller ansatz, even for this small number of particles. In turn, the Gutzwiller ansatz does not grasp all relevant properties of the ground state in an appropriate manner, in particular in this 1D situation. For example, one should expect the transition to a MI state at larger values of the lattice strength in an exact treatment, as Ref. [31] suggests.

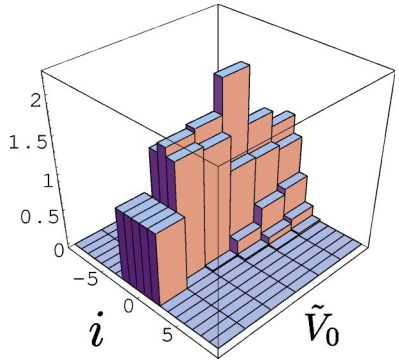

FIG. 2. On-site bosonic densities for a Bose-Fermi repulsion $a_{BF}=0.04$, as a function of the lattice potential strength. In this figure, as well as in the following figures, $\tilde{V}_0$ runs from 1 to 8.

$$\sum_{n=0}^{\infty} (f_n^{(i)})^2 = 1, \tag{54}$$

$$0 \leqslant n_F^{(i)} \leqslant 1, \tag{55}$$

for each lattice site i, reflecting the fact that the Gutzwiller amplitudes form a probability distribution for each lattice site, and that the on-site fermion occupation number cannot exceed one.

Identifying the ground state amounts to solving a constrained optimization problem: one has to minimize energy functional (50) subject to the constraints given by Eqs. (48) and (49), together with Eqs. (54) and (55). We have solved the problem numerically for a small system of ten particles (five bosons and five fermions). The first observation is that the optimization problem is not a convex optimization problem. Hence, one has to expect several local, ''poorer'' extrema in addition to the (not necessarily unique) global one. The numerical solution of this optimization problem has been performed first using a simulated annealing method [32] with an appropriate logarithmic annealing schedule. Quadratic constraints (54) and (55) have been incorporated in a dynamical penalty formulation (see, e.g., Ref. [33]). Finally, for the local refinement the Nelder-Mead downhill simplex method [34] has been applied.

In Fig. 2 we show the change of the on-site bosonic densities with increasing lattice potential strength $\tilde{V}_0$ for a system of five bosons and five fermions with moderate repulsive boson-fermion interaction. We note from Fig. 2 that as the strength of the lattice potential increases, the bosons go in a complete Mott-insulating phase, forming a block crystalline configuration around the center of the trap (which coincides with the origin of the optical lattice) with exactly one boson per lattice site. The corresponding on-site fermionic densities are plotted in Fig. 3. From both figures we can see that if $U_{BF}>0$, by increasing the lattice potential strength the system eventually undergoes simultaneously a boson MI transition and complete phase separation, in accordance with Eq. (43) along with Eqs. (24)–(28).

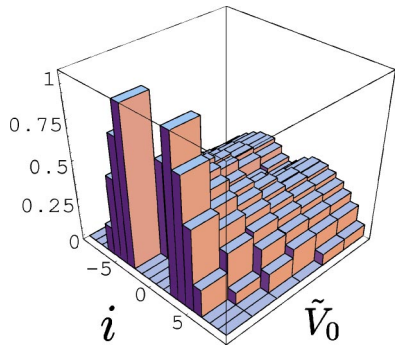

FIG. 3. On-site fermionic densities for a Bose-Fermi repulsion $a_{BF}=0.04$, as a function of the lattice potential strength.

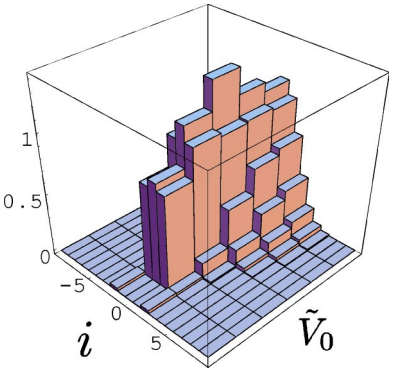

FIG. 4. The bosonic superfluid on-site order parameter for a Bose-Fermi repulsion $a_{BF}=0.04$, as a function of the lattice potential strength.

The local bosonic superfluid parameter $\psi^{(i)}$ for the same physical situation is shown in Fig. 4. Although we are dealing with a finite system, we can already see a rather clear signature of the onset of a phase transition to a Mott-insulator regime when the superfluid parameter suddenly drops to very low values at an approximate critical lattice potential strength $\tilde{V}_0^c \simeq 7$.

We next consider the ground-state properties in the case of an attractive boson-fermion interaction. Because of the strong attraction with growing lattice depth, the fermions follow the bosons in building a sharp crystalline block around the center of the trap, as can be seen from Figs. 5 and 6. We cannot expect in this case to observe a simultaneous mean-field collapse like the one predicted for a trapped Bose-Fermi

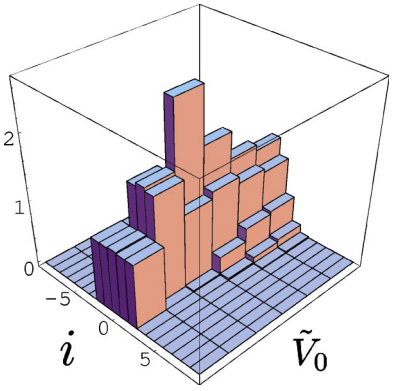

FIG. 5. On-site bosonic densities for a Bose-Fermi attraction $a_{BF}=-0.04$, as a function of the lattice potential strength.

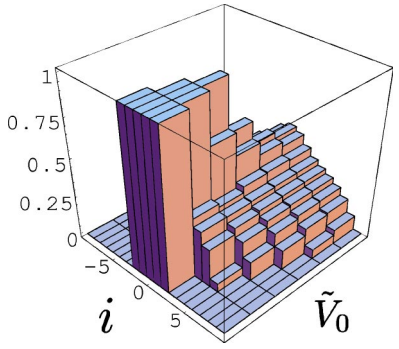

FIG. 6. On-site fermionic densities for a Bose-Fermi attraction $a_{BF}=-0.04$, as a function of the lattice potential strength.

mixture in the continuum [35,36] (for the effects beyond mean field, see Ref. [37]), as this possibility is forbidden in a single-band approximation. Finally, we consider the behavior of the bosonic superfluid on-site parameter in the case of a boson-fermion attractive interaction.

Comparing Fig. 7 with Fig. 4, we see that the transition to a Mott-insulating phase for the bosons takes place at the same lattice potential strength, irrespective of the repulsive or attractive nature of the boson-fermion interaction. This finding confirms the results of the mean-field analysis presented in the preceding section.

V. MIRROR SYMMETRY BREAKING AND TRANSITION TO DEGENERACY

The above optimization problem associated with the constrained minimization of the energy is not convex, hence there can be many local minima in addition to the global one. However, even the ground state may be approximately or exactly degenerate. In fact, this is what happens in the case of boson-boson and boson-fermion repulsion for large values of lattice potential strength $\tilde{V}_0$. As $\tilde{V}_0$ grows, it becomes eventually energetically more favorable for the bosons to be arranged in single-particle occupancy of the available sites around the center of the external trap. The bosonic and fermionic on-site occupation numbers can only assume values 0 or 1, and a definite boson-fermion symmetry is established

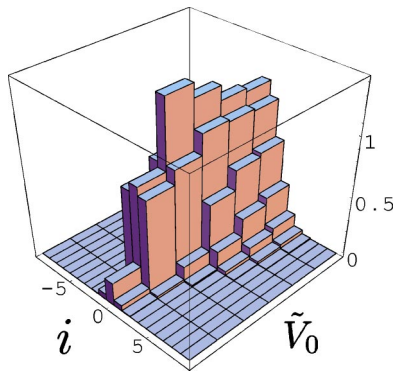

FIG. 7. The bosonic superfluid on-site order parameter for a Bose-Fermi attraction $a_{BF}=-0.04$, as a function of the lattice potential strength.

in the Bose-Fermi Hubbard Hamiltonian assuming that the on-site fermionic and bosonic trapping potentials coincide.

A similar transmutation of bosons into fermions in strong optical lattices has been pointed out by Paredes and Cirac in a recent paper [11]. They consider a model of pure bosons in an optical lattice and show that in the limit of very strong boson-boson on-site interaction, the bosonic operators can be mapped into fermionic operators by means of the well-known Jordan-Wigner transformation. Let us consider what happens in the case of a boson-fermion mixture. As the lattice strength grows, configurations of lowest energy, which are mirror-symmetric with respect to the center of the lattice, like, e.g., those of Figs. 2 and 3, become approximately energetically equivalent to other symmetric configurations (e.g., a checkerboard of alternating bosons and fermions with one particle per lattice site) as well as to nonsymmetric configurations (like a succession of four fermions followed by five bosons and then a last fermion, again with one particle per lattice site), and mirror symmetry breaking takes place. We may thus consider sequences of energy functionals with increasing lattice potential strengths $\tilde{V}_0$. For each value of $\tilde{V}_0$, one may identify a ground state. Then, the difference in energy of this ground state to those states that can be obtained by interchanging the role of fermions and bosons will converge to zero as $\tilde{V}_0$ grows. The boson hopping contribution will become negligible, whereas the behavior of $\tilde{U}_{BB}$ will enforce the mean bosonic on-site occupation number to be at most one. Hence, for each lattice site, the constraints on the boson and fermion occupation numbers become identical (at most one boson or one fermion per lattice site). Notice that the suppression of the hopping terms is exponential. Moreover, since $\tilde{V}_B^{(i)}=\tilde{V}_F^{(i)}$ for all lattice sites i, larger the value of $\tilde{V}_0$, more symmetric the role of bosons and fermions. There are then many ground states that are degenerate in energy with respect to any permutation of lattice sites, as long as all particles are located around the minimum of the confining external potential $\tilde{V}_B^{(0)}=\tilde{V}_F^{(0)}=0$. These degenerate configurations will be given by all possible symmetric and nonsymmetric fermion and boson distributions in a region around the center of the lattice, with every site of the region occupied by one and only one particle. Such possible configurations are, for example, checkerboard alternating patterns of bosons and fermions, or Mott bosonic central configurations with fermionic wings on the sides, or consecutive block crystalline arrangements of variable length of bosons and fermions. In brief, while the Hamiltonian formally retains its mirror-symmetry under reflection of the lattice around its center, the degenerate ground states need not, and spontaneous mirror symmetry breaking occurs. At the same time, complete boson-fermion exchange symmetry sets on. No ground state is *a priori* favored compared to any other: any random pattern of consecutive bosons and fermions located around the minimum of the external trapping potential is a legitimate ground state. Figure 8 shows representative on-site bosonic densities in the regime of large values of $\tilde{V}_0$ around $\tilde{V}_0=50$ for the case of boson-boson and boson-fermion repulsion in a system composed of five bosons and

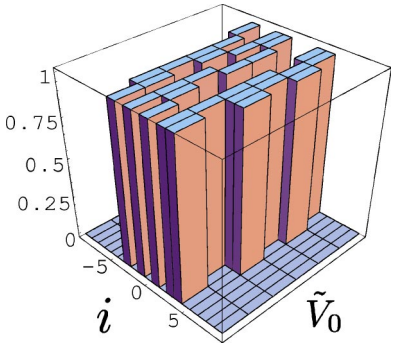

FIG. 8. The disordered pattern of bosonic ground-state distributions for repulsive boson-boson and boson-fermion interactions for large values of $\tilde{V}_0$ around $\tilde{V}_0 = 50$.

five fermions: at each value of the lattice potential strength, a particular state is selected from the set of those with same energy. Each vanishing value of the on-site bosonic density means that exactly one fermion has filled that particular lattice site. The large value chosen for $\tilde{V}_0$ allows one to clearly stress the random nature of the configuration patterns even for very small changes of the lattice potential strength, whereas degeneracy and disorder can set in already at lower values of the lattice depth, depending on the tuning of the harmonic oscillator and scattering lengths (see below). The degenerate states are separated by energy barriers. The system is nonergodic, and hysteresis should be observed: what particular state is chosen, depends on the exact mechanism of preparation of the system and of loading of the mixture into the optical lattice.

The criterion for the onset of degeneracy and nonperiodic ground states in the bulk region around the center of the lattice and of the trapping potential is easily identified, by looking at the relative importance of the trapping on-site energy with respect to the on-site boson or fermion interaction energy. For instance, to allow for the fermionic behavior of the boson on-site occupation numbers (either 0 or 1) one must require that the energy is lower, having one boson at the edge of the bulk central region rather than having it sitting on top of another boson at the center of the lattice:

$$\tilde{U}_{BB} > \tilde{V}_B \quad [i = (N_B + N_F)/2]. \tag{56}$$

The analogous condition for the Bose-Fermi on-site interaction is:

$$\tilde{U}_{BF} > \tilde{V}_{B/F} \quad [i = (N_B + N_F)/2]. \tag{57}$$

For smaller values of $\tilde{V}_0$, the boson hopping contribution will become more and more important. A representative situation of this intermediate regime is depicted in Figs. 2 and 3: here, the repulsion between bosons and fermions is strong enough to allow for phase separation, while the nonnegligible hopping terms still favor configurations where bosons have bosons as nearest neighbors. The transition to degeneracy and disorder, exact in the limit of infinite lattice depth, is a peculiar feature of Bose-Fermi mixtures and it should hold in general for any multicomponent Bose or Fermi dilute atomic system loaded in a deep optical lattice at zero temperature, provided that intercomponent interactions are repulsive and the on site confining potentials coincide for the different components. It clearly cannot take place in a single-component system, say a pure single-component Bose gas, where only a SF-MI transition occurs [7]. The rather complex and rich interplay between ordered and disordered configurations of Bose-Fermi mixtures in very deep optical lattices will be considered in more detail elsewhere.

VI. SUMMARY AND OUTLOOK

In conclusion, we have studied the zero-temperature properties of a mixture of weakly interacting gases of neutral bosonic and fermionic atoms loaded in one-dimensional optical lattices and confined by harmonic trapping potentials. We have derived a single-band Bose-Fermi Hubbard Hamiltonian, and performed some mean-field studies of the zero-temperature phase diagram. We have considered the case of a quasifree fermion sea acting on the bosons, which have been treated in their full dynamical range. We have always worked in the approximation of *s*-wave boson-boson and boson-fermion contact interactions. According to the different possible combinations of intraspecies and interspecies attractive and repulsive interactions, the system displays a rich phase structure, including the onset of a SF-MI transition in the boson sector, and a simultaneous transition to demixing in the boson-fermion sector. The optical lattice potential plays a crucial role, allowing to tune the system into regimes of strong boson-boson and boson-fermion couplings as the lattice depth is increased. For very deep lattices the system displays a remarkable transition to a multiply degenerate phase in which all possible permutations of configurations with one bosonic or fermionic atom per site are legitimate ground states. The transition is related with breaking of the lattice mirror symmetry for very large values of the lattice depth. This peculiar disordered pattern of degenerate ground-state configurations separated by very large barriers is somehow reminiscent of the behavior of classical disordered systems, such as glasses and spin glasses, but it takes place in a quantum system at zero temperature.

The setting that has been investigated in detail in the present paper can be extended in various ways. Certainly a larger number of bosons and fermions have to be considered in order to obtain a more realistic description of the system. While our previous analytical findings are applicable to any numbers of atoms, in order to extend the numerical calculations to larger numbers more powerful numerical methods have to be introduced. So far, Monte Carlo simulations with a fairly large number of particles have been carried out only for an inhomogeneous Bose-Hubbard model [38]. The authors have also speculated that the qualitative phase diagram does not depend on the dimensionality of the system.

In order to extend the work presented in this paper to the case of interacting fermions, one may either allow for different fermionic species in magnetic traps or for spin-unpolarized identical fermions in optical traps. Exchange-correlation effects that are already included in the Gutzwiller Ansatz for the bosons will then become important for the

fermions as well [39]. In this way, the Bose-Fermi interaction has to be consistently incorporated beyond the mean-field level. In the present paper, the mean-field treatment of the Bose-Fermi interaction is consistent, since we only included the fermions in a mean-field and LDA prescription.

At the opposite extreme, one can consider the fermions to be static impurities for the bosons, as very recently discussed by Vignolo and Akdeniz, and Jest [40]. Recently, Buchler and Blatter reported on the induced boson-boson interaction due to the fermions for mixtures loaded in a 2D lattice [41].

Besides these fundamental theoretical aspects related to the theory of quantum phase transitions and the statistical mechanics of complex systems, ultracold Bose-Fermi mixtures in an optical lattice qualify for potential applications in the physics of quantum information. As with systems involving either bosons or fermions which have been studied so far [18,17,21,19,16], mixtures could be used for the preparation of multiparticle entangled states [16], such as cluster states or certain instances of graph states [42], as well as for the implementation of quantum gates. With bosons and fermions serving two different purposes, Bose-Fermi mixtures could in fact allow for new possibilities of quantum information processing in optical lattices. The fermions would be suitable for storage of quantum information due to their noninteracting behavior, whereas the bosons could be used to let the systems interact and perform operations.

In turn, the study of such coupled quantum systems exhibiting collective phenomena with the methods of the theory of multiparticle entanglement is an attractive investigation in its own right. The aim here is not to use the coupled system to prepare strongly entangled systems that form the starting point for applications in quantum information processing. Instead, the motivation of such investigations is to go beyond conventional methods to characterize the natural correlations present in the distributed system at zero temperature [43–46]. The quantitative theory of entanglement, which abstracts from the actual physical realization of a Bose-Fermi Hubbard model, could provide the tools to understand how global properties emerge here from quantum correlations between the elementary constituents.

ACKNOWLEDGMENTS

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