Atomic Bose-Fermi Mixtures in an Optical Lattice

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A mixture of ultracold bosons and fermions placed in an optical lattice constitutes a novel kind of quantum gas, and leads to phenomena, which so far has been discussed neither in atomic physics, nor in condensed matter physics. We discuss the phase diagram at low temperatures, and in the limit of strong atom-atom interactions, and predict the existence of quantum phases that involve pairing of fermions with one or more bosons, or, respectively, bosonic holes. The resulting composite fermions may form, depending on the system parameters, a normal Fermi liquid, a density wave, a superfluid liquid, or an insulator with fermionic domains. We discuss the feasibility for observing such phases in current experiments.

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Since the first observation of Bose-Einstein condensation (BEC) in atomic vapors [1], atomic physics has been constantly approaching research topics traditionally associated with condensed matter physics, such as the analysis of superfluidity in BEC [2], or the ongoing intensive search for the Bardeen-Cooper-Schrieffer (BCS) superfluid transition in ultracold atomic Fermi gases [3,4]. Recently, striking experimental developments have driven a rapidly growing interest on strongly correlated systems in atomic physics. In this sense, the control of the interatomic interactions via Feshbach resonances [5] has become particularly interesting, opening the way towards strongly interacting gases [6]. Additionally, strong correlations are predicted to play a dominant role in low-dimensional systems, such as 1D Bose gases (Tonks-Girardeau regime) [7], 1D Fermi systems (Luttinger liquid) [8], or rapidly rotating 2D gases, where the physics resembles that of fractional quantum Hall effect [9].

The recent observation of the superfluid (SF) to Mott insulator (MI) transition in ultracold atoms in optical lattices [10], predicted in Ref. [11], constitutes up to now the most spectacular example of phenomena related to strongly correlated atomic gases. In this experiment (performed with ^{87}Rb atoms), by changing the laser intensity and/or detuning, one can control the tunneling to neighboring sites as well as the strength of the on-site repulsive interactions, and therefore one is able to switch between the SF phase (dominated by the tunneling) and the MI phase with a fixed number of atoms per site [10].

The possibility of sympathetic cooling of fermions with bosons has led to several recent experiments on trapped ultracold Bose-Fermi mixtures [4]. So far, temperatures $T \sim 0.05T_F$ have been obtained, where T_F is the Fermi temperature at which the Fermi gas starts to exhibit quantum degeneracy (typically of the order of 10 μK). Although the main goal of these experiments is to achieve the BCS transition in atomic Fermi gases, several groups recently show a growing interest towards the physics of ultracold Bose-Fermi mixtures themselves, including the analysis of the ground-state properties, stability, excitations, and the effective Fermi-Fermi interaction mediated by the bosons [12]. Additionally, new experimental developments have attracted the attention towards the behavior of these mixtures in 1D geometries [13] and optical lattices [14,15].

In this Letter, we investigate a Bose-Fermi lattice gas, i.e., a mixture of ultracold bosonic and fermionic atoms in an optical lattice. This system is somewhat similar to the Bose lattice gas of Ref. [10], yet much more complex and with a richer behavior at low temperatures. We discuss the limit of strong atom-atom interactions (strong-coupling regime) at low temperatures. Our main prediction concerns the existence of novel quantum phases that involve pairing of fermions with one or more bosons, or, respectively, bosonic holes, depending on the sign of the interaction between fermions and bosons [16]. The resulting composite fermions may form a normal Fermi liquid, a density wave, a superfluid, or an insulator with fermionic domains, depending on the parameters characterizing the system. At the end of this paper, we discuss the experimental feasibility of the predicted phases.

The lattice potential is practically the same for both species in a ^{7}Li-^{6}Li mixture, and accidentally very similar for the ^{87}Rb-^{40}K case (for detunings corresponding to the wavelength 1064 nm of a Nd:YAG laser [17]). Because of the periodicity of this potential, energy bands are formed. If the temperature is low enough and/or the lattice wells are sufficiently deep, the atoms occupy only the lowest band. Of course, for fermions this is only possible if their number is smaller than the number of lattice sites (filling factor $\rho_F \leq 1$). To describe the system under these conditions, we choose a particularly suitable set of single particle states in the lowest band, the so-called Wannier states, which are localized at each lattice site. The system is then described by the tight-binding Bose-Fermi-Hubbard (BFH) model (for a derivation from a microscopic model, see Ref. [14]), which is a generalization of the fermionic Hubbard model, extensively studied in condensed matter theory (cf. [18]):

$$H_{\mathrm{BFH}} = -\sum_{\langle ij\rangle}(J_B b_i^\dagger b_j + J_F f_i^\dagger f_j + \mathrm{H.c}) + \sum_i\left[\frac{1}{2}Vn_i(n_i-1) - \mu n_i\right] + U\sum_i n_i m_i, \quad (1)$$

where $b_i^\dagger$, b_j, $f_i^\dagger$, and f_j are the bosonic and fermionic creation-annihilation operators, respectively, $n_i = b_i^\dagger b_i$, $m_i = f_i^\dagger f_i$, and μ is the bosonic chemical potential. The fermionic chemical potential is absent in H_{BFH}, since the fermion number is fixed. The BFH model describes (i) nearest neighbor boson (fermion) hopping, with an associated negative energy, $-J_B$ ($-J_F$); in the following we assume $J_F = J_B = J$, while the more general case of different tunneling rates will be analyzed elsewhere; (ii) on-site repulsive boson-boson interactions with an associated energy V; (iii) on-site boson-fermion interactions with an associated energy U, which is positive (negative) for repulsive (attractive) interactions.

In this Letter we are interested in the strong-coupling limit, $J \ll U, V$, which can be easily reached by increasing the lattice intensity. We first analyze the case of vanishing hopping ($J = 0$). For the simplest case of $U = 0$, at zero temperature, the fermions can occupy any available many-body state, since the energy of the system does not depend on their configuration. Bosons on the contrary are necessarily in the MI state with exactly $\tilde{n} = [\tilde{\mu}] + 1$ bosons per site, where $[\tilde{\mu}]$ is the integer part of $\tilde{\mu} = \mu/V$. For small $|U| \neq 0$, the system is only perturbatively affected. However, if $U > 0$ is sufficiently large, $U > \mu - (\tilde{n} - 1)V$, the fermions push the bosons out of the sites that they occupy. Hence, localized composite fermions are formed, consisting of one fermion and the corresponding number of missing bosons (bosonic holes). Similarly, if $U < \mu - \tilde{n}V$, the fermions will attract bosons to their sites, and again localized composite fermions are formed, but now consisting of one fermion and the corresponding number of bosons.

Figure 1(a) shows the phase diagram of the system in the $\alpha - \tilde{\mu}$ plane, where $\alpha = U/V$. Quite generally, for $\tilde{\mu} - [\tilde{\mu}] + s > \alpha > \tilde{\mu} - [\tilde{\mu}] + s - 1$, we obtain that s holes (or, for $s < 0$, $-s$ bosons) form with a single fermion a composite fermion, annihilated by $\tilde{f}_i = \sqrt{(\tilde{n}-s)!/\tilde{n}!}(b_i^\dagger)^s f_i$ $[\sqrt{\tilde{n}!/(\tilde{n}-s)!}(b_i)^{-s} f_i]$. Since the maximal number of holes is limited by $\tilde{n}$, s must not be greater than $\tilde{n}$; it can, on the other hand, attain arbitrary negative integer values, i.e., we may have fermion composites of one fermion and many bosons in the case of very strong attractive interactions, $\alpha < 0$, and $|\alpha| \gg 1$. In Fig. 1(a) the different regions in the phase diagram are denoted with roman numbers I, II, III, IV, etc., which denote the number of particles that form the corresponding composite fermion. Additionally, a bar over a roman number indicates composite fermions formed by one bare fermion and bosonic holes, rather than bosons.

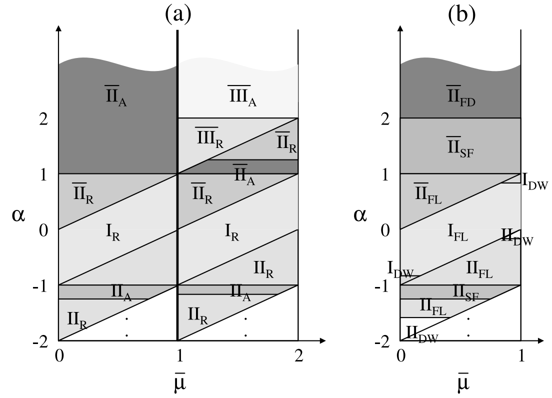

FIG. 1. (a) Phase space as a function of $\tilde{\mu}$ and $\alpha = U/V$. See text for details on the notation. (b) Full phase diagram for the region $0 < \tilde{\mu} < 1$, for $\rho_f = 0.4$ and $J/V = 0.02$. Different phases are present, including fermionic domains (FD), superfluid (SF), Fermi liquid (FL), and density wave phase (DW).

Although our composite fermions neither move nor interact with each other ($J = 0$), the phase diagram is quite complex. As a result, switching on a small, but finite hopping, leads to an amazingly rich physics. The latter can be investigated on the basis of an effective theory for composite fermions, which can be derived using degenerate perturbation theory (to second order in J) along the lines of the derivation of the t-J model (see, e.g., Ref. [18]). Remarkably, the resulting effective model is universal for all the distinct regions in the phase diagram in Fig. 1(a), and the corresponding Hamiltonian

$$H_{\mathrm{eff}} = -J_{\mathrm{eff}}\sum_{\langle ij\rangle}(\tilde{f}_i^\dagger \tilde{f}_j + \mathrm{H.c.}) + K_{\mathrm{eff}}\sum_{\langle ij\rangle}\tilde{m}_i\tilde{m}_j \quad (2)$$

is determined by two effective parameters describing (i) nearest neighbor hopping of composite fermions with the corresponding negative energy $-J_{\mathrm{eff}}$; (ii) nearest neighbor composite fermion-fermion interactions with the associated energy K_{eff}, which may be repulsive (> 0) or attractive (< 0). In Eq. (2) we employ the number operator $\tilde{m}_i = \tilde{f}_i^\dagger \tilde{f}_i$. This effective model is equivalent to that of spinless interacting fermions (cf. [19,20]), and, despite its simplicity, has a rich phase diagram. The coefficient K_{eff} has the universal form

$$K_{\mathrm{eff}} = 2\frac{J^2}{V}\left\{\frac{\tilde{n}(\tilde{n}+1-s)}{1+\alpha-s} + \frac{(\tilde{n}-s)(\tilde{n}+1)}{1-\alpha+s} + \frac{1}{\alpha s} - \tilde{n}(\tilde{n}+1) - (\tilde{n}-s)(\tilde{n}+1-s)\right\}, \quad (3)$$

whereas the dependence of J_{eff} on J, V, and U has different forms in different regions of Fig. 1(a). For example, for $0 < \tilde{\mu} < 1$, $J_{\mathrm{eff}} = J$ (in I), $2J^2/\alpha V$ (in $\overline{\mathrm{II}}$), $4J^2/|\alpha|V$ (in II), etc. The physics of the effective model is determined by the ratio $\Delta = K_{\mathrm{eff}}/2J_{\mathrm{eff}}$, and by the sign of K_{eff}. In Fig. 1(a) the subindex A (R) denotes attractive (repulsive) interactions.

The problem of finding the ground state of the BFH model is then reduced to the analysis of the ground state of the spinless Fermi model (2). In the case of a repulsive effective interaction, $K_{\rm eff} > 0$, and filling fraction close to zero, $\rho_F \ll 1$, or 1, $1 - \rho_F \ll 1$, the ground state of $H_{\rm eff}$ corresponds to a Fermi liquid (a metal), and is well described in the Bloch representation. In the considered cases, the relevant momenta are small compared to the inverse lattice constant (the size of the Brillouin zone). One can thus take the continuous limit, in which the first term in $H_{\rm eff}$ corresponds to a quadratic dispersion with a positive (negative) effective mass for particles (holes), while the second term describes p-wave interactions. The lattice is irrelevant in this limit, and the system is equivalent to a Fermi gas of spinless fermions (for $\rho_F \ll 1$), or holes (for $1 - \rho_F \ll 1$). Remarkably, this gas is weakly interacting for every value of $K_{\rm eff}$, even when $K_{\rm eff} \to \infty$. The latter case corresponds to the exclusion of the sites that surround an occupied site from the space available for other fermions. As a result, the scattering length remains finite, being of the order of the lattice spacing. Therefore, $1 - \rho_F$ (ρ_F) acts as the gas parameter for the gas of holes (particles). This picture can be rigorously justified using the renormalization group approach [20].

The weakly interacting picture becomes inadequate near half filling, $\rho_F \to 1/2$, and for large Δ, where the effects of the interactions between fermions become important, and one expects the appearance of localized phases. A physical insight on the properties of this regime can be obtained by using Gutzwiller ansatz (GA) [21], in which the ground state is a product of on-site states with zero or one composites, $\prod_i(\cos\theta_i/2|1\rangle_i + \sin\theta_i/2e^{\phi_i}|0\rangle_i)$, and which is in fact well suited for describing the states with reduced mobility and, therefore, with small correlations between different sites. Such an approach allows one to determine the boundaries of various quantum phases relatively well in 3D, 2D, and even 1D, but does not provide the correct description of correlations and excitations; these failures become particularly important in 1D, where, strictly speaking, the GA approach is inappropriate. For $K_{\rm eff} > 0$ the GA approach maps $H_{\rm eff}$ onto the classical antiferromagnetic spin model with spins of length 1, $\vec{S}_i = (\sin\theta_i\cos\phi_i, \sin\theta_i\sin\phi_i, cos\theta_i)$ [18]. The corresponding ground state is a spin-flop (canted) antiferromagnet [18,19] with a constant density, provided $\Delta < \Delta_{\rm crit} = (1 + m_z^2)/(1 - m_z^2)$, where the "magnetization per spin" is $m_z = 2\rho_F - 1$. When $\Delta > \Delta_{\rm crit}$, the GA ground state of the classical spin model exhibits modulations of m_z with a periodicity of two lattice constants. We expect that the employed GA formalism predicts the phase boundary $\Delta_{\rm crit}$ accurately for ρ_F close to 1/2. Coming back to the composite fermion picture, we predict thus that the ground state for $\Delta < \Delta_{\rm crit}$ is a Fermi liquid, while for $\Delta > \Delta_{\rm crit}$ it is a density wave. For the special case of half filling, $\rho_F = 1/2$, the ground state is the so-called checkerboard state, with every second site occupied by one composite fermion. One should stress that the GA value of $\Delta_{\rm crit}$ is incorrect for filling factors ρ_F close to 0 or 1. In particular, the GA approach predicts that $\Delta_{\rm crit}$ tends gradually to infinity and the density wave phase gradually shrinks as $\rho_F \to 0$ or 1, i.e. $1 - m_z^2 \to 0$. As discussed above, an analysis beyond the GA approach shows the disappearance of the density wave phase already for a finite nonzero value of $1 - m_z^2$.

The situation is different when the effective interaction is attractive, $K_{\rm eff} < 0$, which in the spin description corresponds to ferromagnetic spin couplings. In the GA approach the ground state for $0 > \Delta \geq -1$ is ferromagnetic and homogeneous. In this description, fixing the fermion number means fixing the z component of the magnetization $M_z = N(2\rho_F - 1)$. When $|\Delta| \ll 1$, and ρ_F is close to zero (1), i.e., low (high) lattice filling, a very good approach to the ground state is given by a BCS ansatz [22], in which the composite fermions (holes) of opposite momentum build p-wave Cooper pairs, $\prod_{\vec{k}}(v_{\vec{k}}|00\rangle_{\vec{k},-\vec{k}} + u_{\vec{k}}|1,1\rangle_{\vec{k},-\vec{k}})$, where $v_{\vec{k}}$ and $u_{\vec{k}}$ are the coefficients of the Bogoliubov transformation. The ground state becomes more complex for arbitrary ρ_F, and for Δ approaching -1 from above. The system becomes strongly correlated, and the composite fermions in the SF phase may build not only pairs, but also triples, quadruples, etc. The situation becomes simpler when $\Delta < -1$. In the spin picture the spins form then ferromagnetic domains with spins ordered along the z axis. In the fermionic language this corresponds to the formation of domains of composite fermions ("domain" insulator). This mean-field result is in fact exact.

Figure 1(b) shows the cases I, II, and $\overline{\rm II}$ for $0 < \mu < 1$, with the predicted quantum phases. The observation of the predicted phases constitutes a challenging, but definitely accessible, goal for experiments. Systems of different dimensionalities are nowadays achievable by controlling the potential strength in different directions [23]. The conditions for the exclusive occupancy of the lowest band, and for $J \ll V, U$, are fulfilled for sufficiently strong lattice potentials, as those typically employed in current experiments [10] (10–20 recoil energies). Additionally, our $T = 0$ analysis is valid for T much lower than the smallest energy scale in our problem, namely, the tunneling rate. This regime is definitely accessible for sufficiently large interactions. In typical experiments, the presence of an inhomogeneous trapping potential leads to the appearance of regions of different phases [11,24], and it is crucial for the observation of MI phases [10]. The inhomogeneity controls thus the bosonic chemical potential, which can also be tailored by changing the number of bosons in the lattice, regulating the strength of the lattice potential, and/or modifying the interatomic interactions by means of Feshbach resonances [5]. We would like also to note that for $J \ll V$, phases I, II, and $\overline{\rm II}$ are easier to study, since the fermions, or composite fermions, attain effective hopping energies that are not too small and can compete with the effective interactions $K_{\rm eff}$. The predicted phases can be detected by using two already widely employed techniques. First, the removal of the confining potentials, and the subsequent presence or absence of interferences in the time of flight image, would distinguish between phase-coherent and incoherent phases. Second, by ramping up abruptly the lattice potential, it is possible to freeze the spatial density correlations, which could be later on probed by means of Bragg scattering. The latter should allow one to distinguish between homogeneous and modulated phases. An independent Bragg analysis for fermions and bosons should reveal the formation of composite fermions.

In this Letter we have shown that the phase diagram for Bose-Fermi lattice gases in the strong-coupling limit is enormously rich and contains several novel types of quantum phases involving composite fermions, which for attractive (repulsive) Bose-Fermi interactions are formed by a fermion and one or several bosons (bosonic holes). The predicted ground-state solutions include delocalized phases (metallic, superfluid), and localized ones (density wave and domain insulator). The remarkable development of the experimental techniques for cold atomic gases allows not only for the observability of the predicted phases, but also for an unprecedented degree of control not available in other condensed matter systems.

In the 1D case, due to the leading role of fluctuations, mean-field theories become inaccurate. In 1D we can, however, use the Wigner-Jordan transformation to convert the effective model into the quantum spin $1/2$ chain, the so-called XXZ model [19], with a fixed magnetization $m_z = \rho_F - 1/2$, whose ground state is known exactly from Bethe ansatz [25,26]. The coefficient characterizing the spin coupling on the x-y plane will then be $J_{\mathrm{eff}}/2$, whereas that in the z direction will be $K_{\mathrm{eff}}/4$.

Finally, we stress that interesting physics is also expected when J is comparable to U and V. For finite J the phase diagrams should be extended to three dimensions by adding the J/V axis, and will develop a lobe structure in the $J/V - \bar{\mu}$ plane, similar to that occurring in MI phases in the Bose-Hubbard model [19]. This analysis, as well as the studies of the excitations in this system, will be the subject of a separate paper.

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[1] M. H. Anderson *et al.*, Science **269**, 198 (1995); K. B. Davis *et al.*, Phys. Rev. Lett. **75**, 3969 (1995).
[2] C. Raman *et al.*, Phys. Rev. Lett. **83**, 2502 (1999); O. M. Moragó *et al.*, Phys. Rev. Lett. **84**, 2056 (2000); M. R. Matthews *et al.*, Phys. Rev. Lett. **83**, 2498 (1999); K. W. Madison, F. Chevy, W. Wohlleben, and J. Dalibard, Phys. Rev. Lett. **84**, 806 (2000); F. S. Cataliotti *et al.*, Science **293**, 843 (2001).
[3] B. deMarco and D. S. Jin, Science **285**, 1703 (1999); K. M. O'Hara *et al.*, Science **298**, 2179 (2002); C. A. Regal and D. S. Jin, Phys. Rev. Lett. **90**, 230404 (2003).
[4] A. G. Truscott *et al.*, Science **291**, 2570 (2001); F. Schreck *et al.*, Phys. Rev. Lett. **87**, 080403 (2001); Z. Hadzibabic *et al.*, Phys. Rev. Lett. **88**, 160401 (2002); G. Modugno *et al.*, Science **297**, 2240 (2002); Z. Hadzibabic *et al.*, Phys. Rev. Lett. **91**, 160401 (2003).
[5] S. Inouye *et al.*, Nature (London) **392**, 151 (1998); S. L. Cornish *et al.*, Phys. Rev. Lett. **85**, 1795 (2000).
[6] E. A. Donley *et al.*, Nature (London) **417**, 529 (2002).
[7] M. Girardeau, J. Math. Phys. (N.Y.) **1**, 516 (1960).
[8] A. Recati, P. O. Fedichev, W. Zwerger, and P. Zoller, Phys. Rev. Lett. **90**, 020401 (2003).
[9] N. K. Wilkin and J. M. F. Gunn, Phys. Rev. Lett. **84**, 6 (2000); B. Paredes, P. Fedichev, J. I. Cirac, and P. Zoller, Phys. Rev. Lett. **87**, 010402 (2001).
[10] M. Greiner *et al.*, Nature (London) **415**, 39 (2002).
[11] D. Jaksch *et al.*, Phys. Rev. Lett. **81**, 3108 (1998).
[12] M. J. Bijlsma, B. A. Heringa, and H. T. C. Stoof, Phys. Rev. A **61**, 053601 (2000); P. Capuzzi and E. S. Hernández, Phys. Rev. A **64**, 043607 (2001); A. Albus, S. A. Gardiner, F. Illuminati, and M. Wilkens, Phys. Rev. A **65**, 053607 (2002); L. Viverit and S. Giorgini, Phys. Rev. A **66**, 063604 (2002); H. Pu, W. Zhang, M. Wilkens, and P. Meystre, Phys. Rev. Lett. **88**, 070408 (2002); X.-J. Liu and H. Hu, Phys. Rev. A **67**, 023613 (2003).
[13] K. K. Das, Phys. Rev. Lett. **90**, 170403 (2003); M. A. Cazalilla and A. F. Ho, Phys. Rev. Lett. **91**, 150403 (2003).
[14] A. Albus, F. Illuminati, and J. Eisert, Phys. Rev. A **68**, 023606 (2003).
[15] H. P. Büchler and G. Blatter, Phys. Rev. Lett. **91**, 130404 (2003).
[16] The formation of composite fermions in gaseous Fermi-Bose mixtures was considered recently for the case of attractive boson-fermion interaction by M. Yu. Kagan, D. V. Efremov, and A. V. Klaptsov, cond-mat/0209481.
[17] R. Grimm, M. Weidemüller, and Y. B. Ovchinnikov, Adv. At. Mol. Opt. Phys. **42**, 95 (2000).
[18] A. Auerbach, *Interacting Electrons and Quantum Magnetism* (Springer, New York, 1994).
[19] S. Sachdev, *Quantum Phase Transitions* (Cambridge University Press, Cambridge, 1999).
[20] R. Shankar, Rev. Mod. Phys. **66**, 129 (1994).
[21] W. Krauth, M. Caffarel, and J.-P. Bouchard, Phys. Rev. B **45**, 3137 (1992); K. Sheshadri *et al.*, Europhys. Lett. **22**, 257 (1993).
[22] See, e.g., P. G. de Gennes, *Superconductivity in Metals and Alloys* (W. A. Benjamin, New York, 1966).
[23] W. Hänsel *et al.*, Nature (London) **413**, 498 (2001); F. Schreck *et al.*, Phys. Rev. Lett. **87**, 080403 (2001); A. Görlitz *et al.*, Phys. Rev. Lett. **87**, 130402 (2001); M. Greiner *et al.*, Phys. Rev. Lett. **87**, 160405 (2001); S. Burger *et al.*, Europhys. Lett. **57**, 1 (2002).
[24] G. G. Batrouni *et al.*, Phys. Rev. Lett. **89**, 117203 (2002).
[25] H. Bethe, Z. Phys. **71**, 205 (1931).
[26] J. D. Johnson, S. Krinsky, and B. M. McCoy, Phys. Rev. A **8**, 2526 (1973).