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Quantum phase transitions in the Fermi–Bose Hubbard model

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We propose a multiband Fermi-Bose Hubbard model with on-site fermion-boson conversion and general filling factor in three dimensions. Such a Hamiltonian models an atomic Fermi gas trapped in a lattice potential and subject to a Feshbach resonance. We solve this model in the two-state approximation for paired fermions at zero temperature. The problem then maps onto a coupled Heisenberg spin model. In the limit of large positive and negative detuning, the quantum phase transitions in the Bose Hubbard and paired-Fermi Hubbard models are correctly reproduced. Near resonance, the Mott states are given by a superposition of the paired-fermion and boson fields and the Mott-superfluid borders go through an avoided crossing in the phase diagram.

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The experimental investigation of cold atomic gases is proceeding rapidly. Both bosons and fermions have been brought to quantum degeneracy [1,2]. They have been trapped in the sinusoidal lattice potential created by an optical standing wave of two counterpropagating lasers [3,4]. In the tightly bound regime of this potential, the Bose Hubbard Hamiltonian has proven to be a useful model to describe the transition from a superfluid, in which the atoms are delocalized, to a Mott insulator, which has an integer number of atoms at each lattice site [5–8]. Recently, the successful implementation of Feshbach resonances in degenerate Fermi gases has enabled the experimental study of the BardeenCooper-Schrieffer (BCS) to Bose-Einstein condensate (BEC) crossover in the continuum, a long-standing theoretical problem [9,10]. Initial evidence of a new superfluid state has been found in the strongly interacting regime [11]. It is a logical next step to study such a crossover in an atomic Fermi gas trapped in a lattice potential [4].

In this letter, we investigate the BCS-BEC crossover in the context of the Fermi–Bose Hubbard Hamiltonian (FBHH), motivated by this vigorous experimental activity. Hubbard models have proven useful in experiments on BECs [5,8] and are expected to be equally relevant for fermions [4,12]. A phenomenological fermion-boson conversion term in a simplified FBHH was first suggested in the context of high-temperature superconductors [13], while FBHH's without conversion have been treated in the context of cold quantum gases [14]. In contrast, the model we shall study includes the possibility of both classical and quantum phase transitions [7] in the Fermi and Bose Hubbard limits, as well as a conversion term. In addition, we allow the fermions to occupy multiple bands, so that the filling factor is not constrained. In contrast to high-T_c [13], fermion-boson conversion is a real physical process in cold quantum gases, where a Feshbach resonance is used to coherently transfer fermionic atoms into a bound two-atom bosonic state, as illustrated in Fig. 1.

The effect of the conversion term is to lock the order parameter of the fermions and bosons together. It thus leads to a reduction in the number of quantum phases from four to two. The main reason we introduce a bosonic field is to describe the the BCS-BEC crossover: The attractive Fermi Hubbard Hamiltonian, even in the paired fermion limit, does not map simply onto the repulsive Bose Hubbard Hamiltonian [15]. After proposing this new FBHH, we solve it in detail in the limit of on-site paired fermions [15] in the two-state approximation at zero temperature for a filling of from zero to two fermions per site. The on-site paired-fermion limit corresponds to the experimentally realizable case of a strongly confining potential and/or strong interactions. In this limit, the FBHH maps isomorphically onto a coupled Heisenberg spin model, or coupled magnets.

Consider the FBHH in the grand canonical ensemble,

$$H = H_f + H_b + H_{fb}, \tag{1}$$

$$H_b \equiv - J_b \sum_{\langle i,j\rangle} (b_i^\dagger b_j + b_i b_j^\dagger) + \frac{1}{2} V_b \sum_i n_i^b (n_i^b - 1) - \mu_b \sum_i n_i^b, \tag{2}$$

$$H_f \equiv - J_f \sum_{\langle i,j\rangle,s,m,m'} (f_{ism}^\dagger f_{jsm'} + f_{ism} f_{jsm'}^\dagger) - \frac{1}{2} V_f \sum_{i,m,m'} n_{i\uparrow m}^f n_{i\downarrow m'}^f - \sum_{i,s,m} (\mu_f - E_m) n_{ism}^f, \tag{3}$$

$$H_{fb} \equiv g \sum_i (b_i^\dagger f_{i\uparrow} f_{i\downarrow} + b_i f_{i\downarrow}^\dagger f_{i\uparrow}^\dagger) + \frac{V_{fb}}{2} \sum_{i,s,m} n_i^b n_{ism}^f. \tag{4}$$

Equations (2) and (3) are the usual repulsive Bose Hubbard and multiband attractive Fermi Hubbard Hamiltonians for a uniform lattice, and Eq. (4) is the fermion-boson coupling. The symbol $\langle i,j\rangle$ denotes nearest neighbors, while the indices $s \in \{\uparrow,\downarrow\}$ and m denote the spin state and band number. The hopping or tunneling strengths $J_{f,b}$ and the on-site interaction strengths $V_{f,b}$ are taken as real and positive definite. The band-gap energy of the mth band is E_m. The strength g

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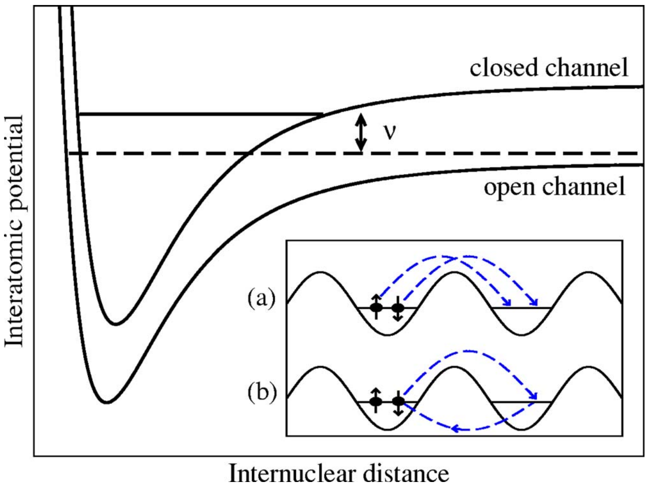

FIG. 1. (Color online) Outer figure: Pairs of fermionic atoms in the open channel are coherently transferred into a closed channel, bosonic state via a Feshbach resonance. Inset: Second order degenerate perturbation theory in the limit $J_f \ll V_f$ leads to two hopping events on the lattice, (a) pair hopping, and (b) a single fermion hopping to an adjacent site and back.

of the interconversion term and V_{fb} of the density coupling may have either sign. The creation and annihilation operators $f^\dagger, f$ and $b^\dagger, b$ satisfy the usual commutation relations for fermions and bosons, respectively. The number operators are defined as $n_i^b = b_i^\dagger b_i$, $n_{ism}^f = f_{ism}^\dagger f_{ism}$. In order to match the physical context of quantum degenerate gases in chemical equilibrium, we require

$$\mu_b = 2\mu_f + \hbar\nu, \tag{5}$$

where ν is the detuning associated with a Feshbach resonance and we set $\hbar = 1$. The conserved quantity

$$n \equiv 2\sum_i n_i^b + \sum_{i,s,m} n_{ism}^f \tag{6}$$

is the total number of fermions. Eliminating μ_b by substituting Eq. (5) into Eqs. (1)–(4), one finds that μ_f multiplies n. One can thus take μ_f as the chemical potential of the coupled system, while ν determines the relative number of bosons and fermions.

The FBHH of Eqs. (1)–(4) models a pseudo-spin-1/2 system of fermions with s-wave interactions, as in experiments [2,4,11]. In practice, the index $s \in \{\uparrow, \downarrow\}$ represents two hyperfine states in the level structure of an effectively fermionic alkali atom, such as ^{40}K or ^{6}Li, scattering near threshold in an open channel. The bosonic field represents a bound closed-channel molecular state, $^{6}Li_2$ or $^{40}K_2$, which is coupled to the fermionic field via a resonance with an unbound open-channel atomic state, called a Feshbach resonance. A schematic is shown in Fig. 1. Note that $V_{f,b}$ and g are not functions of ν. Methods for calculating the parameters V_f, V_b, etc. in Eqs. (2)–(4) from few-body atomic physics have been described in detail elsewhere [17]. Another important assumption is that the pairing of fermions into bosons occurs on-site. This is physically reasonable for present experiments [18].

We consider the limit in which $J_f \ll V_f$, which corresponds to a strongly confining lattice [20]. Since the lattice height is proportional to the intensity of the lasers creating the standing wave, this is straightforward to obtain. Because the on-site interactions are attractive and s wave, and the hopping is taken perturbatively, the fermions form spin-up/spin-down pairs. We also restrict them to be in the lowest band. This is the typical experimental case in three dimensions, where 10^5 to 10^6 fermions are distributed among 100^3 sites. Thus $m=1$ and $n \in [0,2]$, i.e., there are from zero to two fermions, or zero to one Fermi pair, per site. Then, second-order degenerate perturbation theory maps H_f onto a new spin-1/2 system (a quantum XXZ model) [15,16]:

$$H_f' = -J_f' \sum_{\langle i,j \rangle} (\tau_i^+ \tau_j^- - n_i n_j) - \mu_f' \sum_i n_i, \tag{7}$$

where $J_f' \equiv 8J_f^2/V_f$ and $\mu_f' \equiv 2\mu_f + V_f/2$. The operator $\tau_i^+ \equiv (\tau_i^-)^\dagger \equiv f_{i\downarrow}^\dagger f_{i\uparrow}^\dagger$ is a pair creation/annihilation operator and $n_i \equiv \frac{1}{2}(n_{i\uparrow}^f + n_{i\downarrow}^f - 1)$. The perturbative treatment results in two hopping-type events, as is sketched in the inset of Fig. 1: The $\tau_i^+ \tau_j^-$ term corresponds to pair hopping, while the $n_i n_j$ term corresponds to a single fermion hopping to an adjacent site and hopping back.

These operators obey the commutation relation $[\tau_i^\alpha, \tau_j^\beta] = 2i\tau_i^\gamma \epsilon^{\alpha\beta\gamma}\delta_{ij}$, where $\alpha, \beta, \gamma \in \{x, y, z\}$, $\tau_i^\pm \equiv \tau_i^x \pm i\tau_i^y$, and $\tau_i^z \equiv n_i$. Thus, despite the fact that $\tau_i^\pm$ is a creation/annihilation operator for fermion pairs, the τ operators obey the Pauli spin commutation relations, not the bosonic commutation relations. This is one reason why the attractive Fermi Hubbard model does not map simply onto the repulsive Bose Hubbard model, even in the limit of strong interactions. A second reason is that in order to achieve such a mapping, a sum over many bands is required, since the internal energy of bosons composed of two fermions is much greater than the band spacing. In contrast, the FBHH is asymptotically able to represent both the attractive Fermi Hubbard and repulsive Bose Hubbard models in a simple way. It is therefore a good candidate for the study of the BCS-BEC crossover.

In general, a paired-Fermi Hubbard Hamiltonian can act on all number states of the fermions. However, as in Eq. (7), we consider only $n \in [0,2]$, the Hilbert space on which it operates is restricted to two paired-number states. Thus, H_f' is equivalent to the Heisenberg spin Hamiltonian, or a magnet,

$$H_{spin} = -\sum_{i,j} J_{ij} \vec{S}_i \cdot \vec{S}_j - \vec{h} \cdot \sum_i \vec{S}_i, \tag{8}$$

where μ_f' plays the role of the magnetic field h_z. For $T=0$, one therefore expects *coherent* paramagnetic and either ferromagnetic or antiferromagnetic phases. The former correspond to the superfluid phase, while the latter are Mott [19] and charge-density wave (checkerboard) phases. Similarly, the restriction of the Hilbert space on which H_b operates to two number states leads to an isotropic Heisenberg spin Hamiltonian (the quantum XX model [7]). We formulate the two-state approximation for the coupled model as superposition states of the form $|\psi\rangle = \Pi_j |\psi\rangle_j$, where

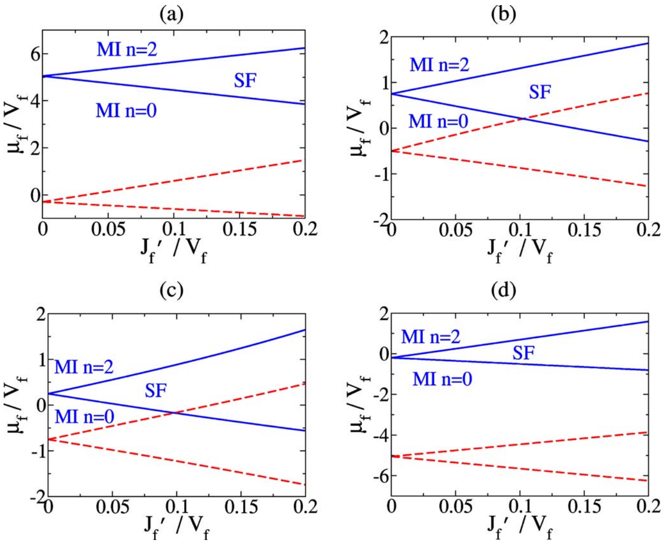

FIG. 2. (Color online) Shown is the phase diagram for detunings (a) $\nu/V_f=-10$, (b) $\nu/V_f=-1$, (c) $\nu/V_f=1/2$, and (d) $\nu/V_f=10$. The blue solid curves show the Mott-superfluid borders, while the red dashed curves show alternate extrema which are maxima (see Fig. 3). SF=superfluid, MI=Mott insulator, n=fermion filling factor.

$$|\psi\rangle_j \equiv |0\rangle_j^b \otimes |0\rangle_j^f \cos\theta_j + \sin(\theta_j) e^{i\phi_j} \times (|1\rangle_j^b \otimes |0\rangle_j^f \cos\chi_j + |0\rangle_j^b \otimes |1\rangle_j^f \sin\chi_j e^{i\alpha_j}). \quad (9)$$

The superscripts b and f refer to Fock states of bosons and Fermi pairs on the jth site.

The two-state approximation is useful in determining the Mott-superfluid borders in the phase diagram. The Mott state is a single number state, while the lowest-order approximation of a superfluid is a superposition of two number states. Therefore, Mott states occur in Eq. (9) for $\theta \in \{0, \pi/2, \pi\}$. The mixing angle χ is determined by the detuning ν in Eq. (5). To determine which phase is energetically favorable one evaluates $E_{\mathrm{gs}} \equiv \langle\psi|H|\psi\rangle$. In addition, we make the uniform approximation $\theta_j=\theta$, $\phi_j=\phi$, $\chi_j=\chi$, $\alpha_j=\alpha$. Then, ϕ does not appear in the ground state energy, while α can only change the sign of g. Setting $g'=\min[g\exp(i\alpha)]$, neither ϕ nor α need be considered to obtain the phase diagram. Note that the uniform approximation leaves out a range of excited many-body states. However, it does obtain two solutions vital to understanding the crossover, one of which is the ground state, as explained below and in Fig. 3. An important point is that the ground state is either coherent paramagnetic (superfluid) or ferromagnetic (Mott). It can be proven that it is not antiferromagnetic (charge-density wave), either by setting the angles to differ by $\pi/2$ on each site, or by making a spin rotation in the Hamiltonian [21].

The Mott-superfluid borders are obtained as follows [22]. The ground-state energy is expanded around the Mott angles $\theta \in \{0, \pi/2, \pi\}$. The zeroth-order term gives the energy. The first-order term is zero, showing that the Mott state is always an extremum. The sign of the second-order term determines whether the Mott state is a maximum or a minimum. Setting this equal to zero, one obtains the Mott-superfluid borders. One must also extremize in the mixing angle χ and determine whether or not it is a maximum. Thus, there are three conditions:

$$\partial^2 E_{\mathrm{gs}}/\partial\theta^2 = 0, \quad (10)$$

$$\partial E_{\mathrm{gs}}/\partial\chi = 0, \quad (11)$$

$$\partial^2 E_{\mathrm{gs}}/\partial\chi^2 > 0. \quad (12)$$

Using conditions (10) and (11) to eliminate χ and Eq. (5) to eliminate μ_b, one finds a quartic equation in μ_f. The coefficients are functions of J_f', J_b, V_f, V_b, $|g'|=|g|$, and ν. We set $V_{fb}=0$ in order to focus on the effect of the fermion-boson conversion term in Eq. (4). The solution to the quartic equation, though lengthy, can be written in closed analytic form. It is best understood when evaluated in limits of the parameters and for particular values of them.

First consider the case $\nu \to \pm\infty$. We assume a bipartite lattice with Z as the number of nearest neighbors. Then, $\chi \in \{0, \pi/2\}$ and one obtains the Mott borders

$$\mu_f/V_f = -1/4 + (Z/2)(1-2\sigma_f)J_f'/V_f, \quad (13)$$

$$\mu_b/V_b = -2\sigma_b Z J_b/V_b, \quad (14)$$

where $\sigma_f \equiv \pm 1$ gives the vacuum/one-Fermi-pair and $\sigma_b \equiv \pm 1$ the vacuum/one-boson Mott states. Equations (13) and (14) correspond to the solutions one finds for $g=0$ in the two-state approximation. For $\nu \to +\infty$, condition (c) shows that Eq. (13) is a minimum and Eq. (14) is a maximum. For

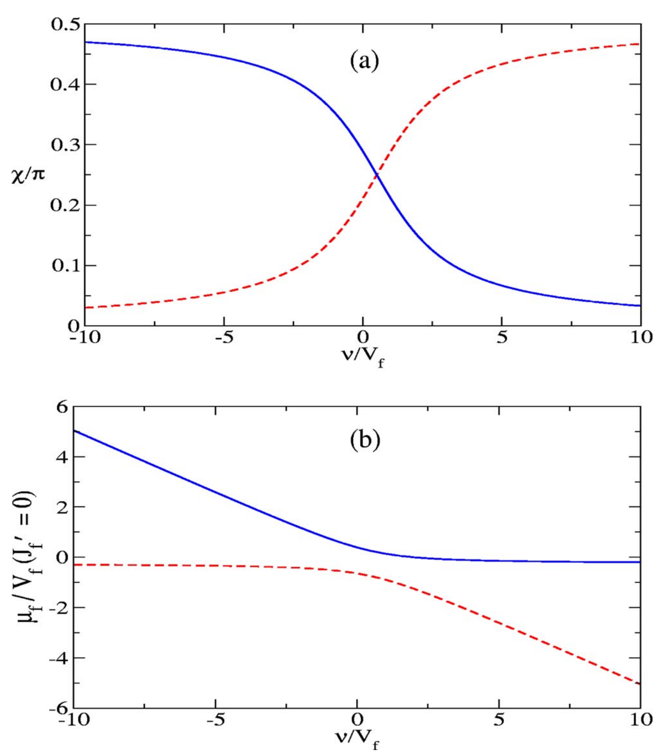

FIG. 3. (Color online) (a) The mixing angle χ as a function of the detuning ν/V_f. (b) The y intercepts in the phase diagram of Fig. 2 go through an avoided crossing as a function of the detuning. Blue solid curves: Energy minima; red dashed curves: energy maxima.

$\nu \to -\infty$, the inverse is the case. Thus, the Bose Hubbard and paired-Fermi Hubbard limits are obtained naturally from the ansatz of Eq. (9) in the limits of large negative and positive detuning. The FBHH we have proposed therefore correctly obtains the endpoints of the BCS-BEC crossover on a lattice.

Next, consider the case of the physically reasonable parameter set $V_b = V_f$, $J_b = J_f'$, with the scaling chosen such that $V_f = 1$. The quartic equation has four roots. Two are complex and therefore physically extraneous. The other two represent an energy minimum and an energy maximum. There is no saddle point. The phase diagram is shown in Fig. 2 for $\nu = -10,\ -1,\ 1/2,\ 10$, and $g = 1$. The results are qualitatively the same for all $g \neq 0$. The point $\nu = 1/2$ is the actual crossover in our model, i.e., the point at which the Mott borders become degenerate. To illustrate this, in Fig. 3(a) is shown the mixing angle χ as a function of ν. Note the appropriate $\nu \to \pm\infty$ limits. In Fig. 3(b) are shown the y intercepts of the Mott phases from the phase diagrams of Fig. 2 as a function of ν. These go through an avoided crossing [10] at $\nu = 1/2$. Smaller values of $|g|$ cause the avoided crossing to become narrower. Similarly, the width of $\chi(\nu)$ in Fig. 3(a) is proportional to $|g|$.

In conclusion, we have proposed a general Fermi-Bose Hubbard model which describes the BCS-BEC crossover on a lattice. Our restriction of the Hilbert space to the lowest band and paired fermions corresponds to the experimentally realizable case of from zero to two fermions per site in three dimensions and a strongly confining lattice. We used a superposition ansatz [Eq. (9)] which is relevant to both broad and narrow Feshbach resonances, i.e., for general coupling g. We found that the paired-Fermi Hubbard and Bose Hubbard phase diagrams appear naturally and asymptotically for large positive and negative detuning. We also showed that the Mott phases of the dressed fermion and boson fields go through an avoided crossing as the system approaches resonance.

Note added in proof: At the time of publication, two preprints appeared [F. Zhou, e-print cond-mat/050740 (2005); R. B. Diener and T.-L. Ho, e-print cond-mat/0507253 (2005)] which present solutions to more general parameter regimes of Eqs. (1)–(4) than the ones we have described herein.

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