Quantum Phases in a Resonantly Interacting Boson-Fermion Mixture

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(Received 14 February 2005; published 17 June 2005)

We consider a resonantly interacting boson-fermion mixture of ^{40}K and ^{87}Rb atoms in an optical lattice. We show that by using a red-detuned optical lattice the mixture can be accurately described by a generalized Hubbard model for ^{40}K and ^{87}Rb atoms, and ^{40}K-^{87}Rb molecules. The microscopic parameters of this model are fully determined by the details of the optical lattice and the interspecies Feshbach resonance in the absence of the lattice. We predict a quantum phase transition to occur in this system already at low atomic filling fraction, and present the phase diagram as a function of the temperature and the applied magnetic field.

DOI: 10.1103/PhysRevLett.94.230404 PACS numbers: 03.75.−b, 32.80.Pj, 39.25.+k, 67.40.−w

Introduction.—In the past few years experiments have shown that it is possible to realize a quantum degenerate gas of fermionic atoms [1]. Combining such a degenerate Fermi gas with a Bose-Einstein condensate of atoms, it is also possible to obtain a quantum degenerate boson-fermion mixture [2], thus creating a dilute analog of the liquid ^{3}He-^{4}He mixture. The recent observation of interspecies Feshbach resonances in a boson-fermion mixture [3,4] opens up even richer physics, as this couples the fermionic and bosonic atoms to a third species, namely, the fermionic heteronuclear molecules. An interesting aspect of the resonantly interacting mixture that we address in much more detail in the following is the possibility to reversibly destroy a Bose-Einstein condensate of atoms, by associating the bosonic atoms into fermionic molecules and thus creating a degenerate Fermi gas of dipolar particles. Moreover, the Bose-Einstein condensed phase is very interesting by itself because it contains a macroscopic quantum coherence between the fermionic atoms and molecules. However, in experiments with magnetic or optical traps the molecules quickly decay due to inelastic atom-molecule and molecule-molecule collisions [5]. By loading the degenerate boson-fermion mixture into an optical lattice with a total filling factor less than unity, these collisions can be prevented and the lifetime of the molecules is expected to be dramatically enhanced.

Boson-fermion mixtures in an optical lattice, but in the absence of an interspecies Feshbach resonance, have been the subject of active theoretical investigation lately. In particular, domain boundaries due to a trapping potential [6], lattice symmetry breaking [7], the existence of quantum phases that involve the pairing of fermions with bosons [8], and also unconventional fermion pairing [9,10] have been predicted. It is the main objective of this Letter to generalize these studies to the case of a resonantly interacting boson-fermion mixture. Although our theoretical methods are very general, we consider as a concrete example a mixture of fermionic ^{40}K atoms and the bosonic ^{87}Rb atoms, as this system is now becoming available experimentally [11,12]. A gas consisting of these two atoms is especially promising as their wavelength is relatively close and readily accessible using Ti:sapphire lasers. Furthermore, the mass of ^{40}K is much larger than the mass of the other experimentally available fermionic atom ^{6}Li, which makes it much easier to trap this species in an optical lattice.

In order to analyze the properties of a resonantly interacting boson-fermion mixture most easily, it is convenient to assume that all the species in the optical lattice, i.e., the fermionic atoms, the bosonic atoms, and the fermionic molecules, experience the same on-site trapping frequency. Because the potassium atoms are lighter than the rubidium atoms, the potential for the former should thus be less deep than that for the latter. Moreover, as is shown in the inset of Fig. 1, both the D1 and D2 lines of potassium are blue compared to the D1 and D2 lines of rubidium. As a result, equal on-site trapping frequencies can be achieved only in an optical lattice that is red detuned with respect to all these four transitions. Making use of the fact that the hyperfine

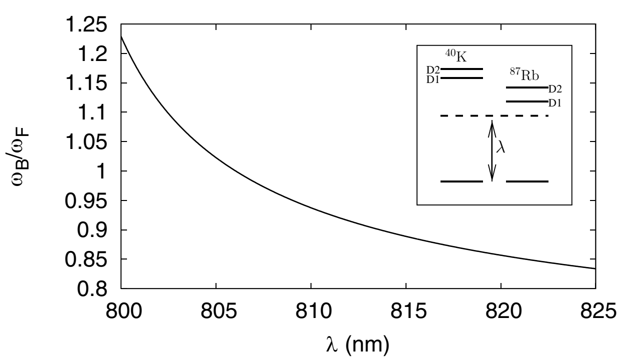

FIG. 1. Ratio of the on-site trap frequencies of the boson ^{87}Rb and the fermion ^{40}K, as a function of the lattice laser wavelength. The inset shows the fine-structure levels of the two atomic species.

structure of the atoms is no longer resolved for the detunings used in optical lattice experiments [13], we have calculated the ratio of the two on-site trapping frequencies as a function of the wavelength of the lattice laser. As can be seen from Fig. 1, using a wavelength of 806 nm ensures that the trapping frequencies for both atomic species are the same. In principle, the polarizability of the molecule is not known. However, recent experiments have shown that for homonuclear molecules, the resulting trap frequency for the molecules is almost the same as that of the atoms [14]. In the following, we make the reasonable assumption that this also holds for the vibrationally highly excited heteronuclear ^{40}K-^{87}Rb molecules of interest to us.

For the particular detuning given above, the on-site trapping frequency is related to the Rabi frequency Ω of the lattice laser by $\omega \equiv \omega_F = \omega_B = 2.1 \times 10^{-5}\ \Omega$. Having to use a red-detuned optical lattice has the disadvantage that the atoms are trapped in the light and not in the dark, which in principle results in a larger decay due to spontaneous emission. We have therefore also calculated this emission rate and find that $\Gamma/\Omega^2 = 1.9 \times 10^{-21}$ s for the optimal wavelength. The lifetime is always longer than 1 s for Rabi frequencies less than 4 GHz ($8\pi \times 10^9$ rad/s), and spontaneous emission can then be safely neglected.

Generalized Hubbard model.—We now consider the many-body aspects of the boson-fermion mixture near a Feshbach resonance. We consider a mixture of ^{40}K and ^{87}Rb that is loaded into a three-dimensional and cubic optical lattice that is sufficiently deep, so that we are allowed to use a tight-binding approximation for the band structure of the single-particle states. Experimentally this requires the Rabi frequency of the lattice laser to be larger than about 1 GHz. For the reasons mentioned above, we consider only low filling fractions, which limits the maximum number of atoms on a single site. As a result, we can neglect atom-molecule and molecule-molecule interactions. Furthermore, for low filling fractions there is also no problem of phase separation of the atomic boson-fermion mixture [15], and it is justified to neglect possible Mott physics in the mixture [16,17].

Under these conditions we have recently derived the theory for resonantly interacting ultracold atomic gases in an optical lattice [18]. Within this theory the two-body Feshbach problem at a single site is solved exactly, which physically leads to a dressing of the molecules and to various avoided crossings in the on-site energy levels of two atoms $\epsilon_\sigma(B)$ as the magnetic field B is swept through the Feshbach resonance. After having solved the on-site problem, the various hopping parameters can be calculated in the tight-binding approximation. In this manner the microscopic parameters of the generalized Hubbard model that describes the boson-fermion mixture near the Feshbach resonance are completely determined by the details of the optical lattice potential and the experimentally known parameters of the Feshbach resonance in the absence of the optical lattice. Ultimately, the mixture is described by the following effective Hamiltonian,

$$\begin{aligned} H = &-t_F \sum_{\langle i,j\rangle} c_i^\dagger c_j - t_B \sum_{\langle i,j\rangle} a_i^\dagger a_j - t_m \sum_\sigma \sum_{\langle i,j\rangle} b_{i,\sigma}^\dagger b_{j,\sigma} \\ &+ \sum_i (\epsilon_a - \mu_F) c_i^\dagger c_i + \sum_i (\epsilon_a - \mu_B) a_i^\dagger a_i \\ &+ \sum_\sigma \sum_i (\epsilon_\sigma - \mu_F - \mu_B) b_{i,\sigma}^\dagger b_{i,\sigma} \\ &+ \frac{U^{\rm BB}}{2} \sum_i a_i^\dagger a_i^\dagger a_i a_i + U_{\rm bg}^{\rm BF} \sum_i a_i^\dagger c_i^\dagger c_i a_i \\ &+ g' \sum_\sigma \sum_i \sqrt{Z_\sigma} (b_{i,\sigma}^\dagger c_i a_i + a_i^\dagger c_i^\dagger b_{i,\sigma}). \end{aligned} \tag{1}$$

Here t_F, t_B and t_m are the tunneling or hopping amplitudes for the fermionic atoms, the bosonic atoms, and the fermionic molecules, respectively. The symbol $\langle i, j\rangle$ denotes a sum over nearest neighbors. The operators $c_i^\dagger$, c_i and $a_i^\dagger$, a_i correspond to the creation and annihilation operators of a single fermionic and bosonic atom at site i, respectively. The operators $b_{i,\sigma}^\dagger$, and $b_{i,\sigma}$ correspond to the creation and annihilation operators of the various dressed molecules at site i that are enumerated by the index σ. Also $\epsilon_a = 3\hbar\omega/2$ is the on-site energy of a single atom. The on-site interaction between two bosons is given by $U^{\rm BB}$, and $U_{\rm bg}^{\rm BF}$ denotes the on-site background interaction between the bosons and the fermions. In the tight-binding limit the hopping amplitudes are for our purposes sufficiently accurately determined in terms of the lattice parameters by [19]

$$t_\nu = \frac{\hbar\omega}{2}\left[1 - \left(\frac{2}{\pi}\right)^2\right]\left(\frac{\lambda}{4l_\nu}\right)^2 e^{-(\lambda/4l_\nu)^2}. \tag{2}$$

Here ν distinguishes the different species in the mixture, i.e., $\nu = F$ for the fermionic atoms, $\nu = B$ for the bosonic atoms, and $\nu = m$ for the molecules. Moreover, λ is the wavelength of the light used to create the optical lattice, and the harmonic oscillator lengths obey $l_\nu = \sqrt{\hbar/m_\nu\omega}$, where m_F, m_B, and $m_m = m_F + m_B$ are the masses of the fermions, bosons, and molecules, respectively. Note that because of the higher mass of the molecules and the desired validity of the tight-binding approximation, we have in general that $t_m \ll t_{F,B} \ll \hbar\omega$. We have also introduced a chemical potential for each atomic species, since it is experimentally possible to control both the filling fraction of the fermions as well as the bosons in the mixture.

Sufficiently close to resonance we can always neglect the on-site interactions $U^{\rm BB}$ and $U_{\rm bg}^{\rm BF}$ compared to the resonant atom-molecule interaction. The strength of the atom-molecule coupling in the lattice is given by $g' = g/(\pi(l_B^2 + l_F^2))^{3/4}$, where $g = \sqrt{2\pi a_{\rm bg}\Delta\mu\Delta B/m_{\rm r}}$ is the bare atom-molecule coupling without the lattice and $m_{\rm r} = m_F m_B/(m_F + m_B)$ is the reduced mass. For the ^{40}K-^{87}Rb mixture with potassium in the hyperfine state $|9/2, -9/2\rangle$

and rubidium in the hyperfine state $|1, 1\rangle$ there occurs a Feshbach resonance at $B_0 = 510$ Gauss for which the parameters that determine g are given by the background scattering length $a_{bg} = 150a_0$ and the width of the resonance $\Delta B = 1$ G [3,20]. The difference in magnetic moments $\Delta\mu$ is equal to 29/22 Bohr magneton in that case. In Fig. 2 we show a close-up of the avoided crossing and the wave function renormalization factors Z_σ that give the probability for the dressed molecules to be in the bare molecular state of this Feshbach resonance. The probability Z_σ is determined by the self-energy of the molecules $\hbar\Sigma_m(E) = (g^2/\pi l_r^3 \hbar\omega) \times \Gamma(-E/2\hbar\omega + 3/4)/\Gamma(-E/2\hbar\omega + 1/4)$, with $\Gamma(z)$ the gamma function, through the relation $Z_\sigma = 1/[1 - \partial\hbar\Sigma_m(E)/\partial E]$ [18]. Note that in Fig. 2 the sum of the probabilities $Z_\downarrow + Z_\uparrow$ does not add up to one. This means that for this relatively broad interspecies Feshbach resonance a single-band approximation is not valid to determine the dressed molecular wave functions. However, a single-band approximation in terms of dressed molecules is always possible for the low filling fractions of interest to us, because the higher-lying on-site dressed molecular states will not be populated as we show now.

Phase diagram.—With the above formalism we next determine the phase diagram for the ^{40}K and ^{87}Rb mixture. For simplicity we consider only equal densities for both atomic species, although the generalization is immediate. We mentioned already that we consider a deep optical lattice for which the hopping strengths of the atoms are small with respect to the level splitting in the on-site microtrap realized by the optical lattice. The hopping strength of the molecules can be completely neglected in this limit, and consequently the band structure for the molecules is essentially flat. At zero temperature the energy $\epsilon_\downarrow$ of the lowest molecular state can, depending on the magnetic field, be either smaller or larger than the sum of the lowest atomic energy levels. As a result, the ground state is either a Fermi sea of ^{40}K-^{87}Rb molecules or a Fermi sea of ^{40}K atoms and a Bose-Einstein condensate of ^{87}Rb atoms. Because of the different symmetries of these ground states there exists a quantum phase transition between these two states that breaks a $U(1)$ symmetry and is in the same universality class as the XY model with dynamical exponent $z = 2$. In the following, we calculate the phase diagram as a function of total filling fraction and temperature by performing a mean-field analysis of the normal state of the Hamiltonian in Eq. (1).

For the equation of state for the total filling fraction we find always that $n = n_F + n_B + 2\Sigma_\sigma n_{m,\sigma}$. In the normal state no condensate exists and the molecular and atomic filling fractions obey $n_{m,\sigma} = (1/N_s)\Sigma_{\mathbf{k}}(e^{\beta\hbar\omega_{\mathbf{k},\sigma}} + 1)^{-1}$, and $n_{F,B} = (1/N_s)\Sigma_{\mathbf{k}}(e^{\beta\hbar\omega_{\mathbf{k},F,B}} \pm 1)^{-1}$, where $\hbar\omega_{\mathbf{k},\sigma} = \epsilon_{\mathbf{k},\sigma} - (\mu_F + \mu_B)$ is the molecular dispersion. The dispersion relations for the fermionic and bosonic atoms are given by $\hbar\omega_{\mathbf{k},F} = \epsilon_{\mathbf{k},F} - \mu_F$ and $\hbar\omega_{\mathbf{k},B} = \epsilon_{\mathbf{k},B} - \mu_B$, respectively. Here $\epsilon_{\mathbf{k},F,B} = -2t_{F,B}\Sigma_{j=1}^3 \cos(k_j\lambda/2) + \epsilon_a$ for the atoms and $\epsilon_{\mathbf{k},\sigma} = \epsilon_\sigma$ for the molecules. The number of sites on the lattice is N_s. We have seen that at zero temperature there is a quantum phase transition between a phase where the ^{87}Rb atoms are Bose-Einstein condensed and a phase with only a Fermi sea of molecules. The quantum critical point is determined by the ideal gas condition for Bose-Einstein condensation, i.e., $\epsilon_\downarrow = 2\epsilon_a - 6(t_B + t_F)$. In the approximation that we can neglect the hopping of the molecules, their band structure is flat and

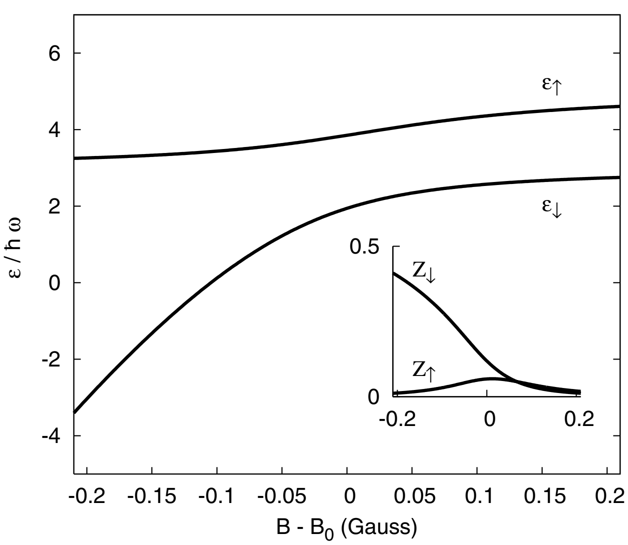

FIG. 2. Details of the physical content of our theory. We show the avoided crossing between the bare molecular level and the lowest two-atom trap state, which results in two dressed molecular states denoted by $|\downarrow\rangle$ and $|\uparrow\rangle$. The inset shows the probability Z_σ as a function of the magnetic field. This figure was calculated for the ^{40}K-^{87}Rb mixture with $\lambda = 806$ nm and $\Omega/2\pi = 1$ GHz.

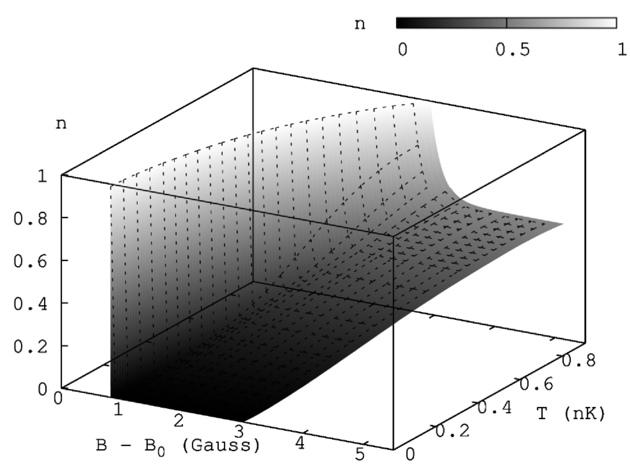

FIG. 3. Critical surface of the ^{40}K and ^{87}Rb mixture as a function of the total filling fraction, magnetic field, and temperature. This figure was calculated for the ^{40}K-^{87}Rb mixture with $\lambda = 806$ nm and $\Omega/2\pi = 1$ GHz.

the quantum critical point is independent of the filling fraction of the molecules. Including the molecular band structure would lead to a critical magnetic field that slowly shifts to lower magnetic fields as the density increases. At nonzero temperatures we can also determine the critical temperature as a function of the detuning and the total filling fraction from the equation of state. The critical surface in Fig. 3 shows how at constant total atomic filling fraction the critical temperature depends on the magnetic field. For large enough magnetic fields there are no molecules and the critical temperature is determined for low densities by the critical temperature of an ideal gas, which is proportional to $n^{2/3}$. Note that the critical temperature always obeys $T_c \ll \hbar\omega/k_B$, which *a posteriori* shows that a single-band approximation for the dressed molecules is, indeed, consistent.

Conclusions and discussion.—In summary, we have shown that by using a red-detuned optical lattice with a wavelength of 806 nm the boson-fermion mixture of ^{40}K and ^{87}Rb atoms can be accurately described by a generalized Hubbard model. Moreover, we have shown that the model contains a quantum phase transition associated with the Bose-Einstein condensation of rubidium. To facilitate the quantitative analysis we have considered the case of equal trapping frequencies for both atomic species. However, the quantum phase transition exists independently of this assumption. Interestingly, the presence of a Bose-Einstein condensate induces also a macroscopic coherence between the fermionic atoms and molecules, because of the specific form of the atom-molecule coupling near a Feshbach resonance. What is especially interesting is that such a coherence cannot be obtained by solely making use of lasers in this case because it involves a quantum coherence between two different species. It would, therefore, be very exciting to observe Rabi oscillations between fermionic atoms and molecules by an appropriate manipulation of the atomic Bose-Einstein condensate density.

Using the known atomic physics of the Feshbach resonance to determine the parameters in the generalized Hubbard Hamiltonian we have calculated the phase diagram for low filling fractions as a function of the applied magnetic field and temperature. Our analysis of the quantum phases of a resonantly interacting Bose-Fermi mixture has been based on mean-field theory. In particular, this implies that we have not considered the attractive finite-range interaction between the fermionic atoms that can be mediated by density fluctuations in the Bose-Einstein condensate [21,22]. In principle, this mechanism can lead to a BCS pairing between the fermionic atoms. However, for the spin-polarized mixture discussed here this pairing must take place in a p-wave channel, which is expected to have a very small critical temperature at small filling fractions. We, therefore, do not consider this interesting possibility in detail here and leave that to future investigations.

This work is supported by the Stichting voor Fundamenteel Onderzoek der Materie (FOM) and by the Nederlandse Organisatie voor Wetenschaplijk Onderzoek (NWO).

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