Quantum phases in a resonantly-interacting Bose-Fermi mixture

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Introduction. — In the last 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 Bose-Fermi mixture,2 thus creating a dilute analog of the liquid He3-He4 mixture. The recent observation of interspecies Feshbach resonances in a Bose-Fermi mixture3,4 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 atom-molecule and molecule-molecule collision.5 By loading the degenerate Bose-Fermi 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.

Bose-Fermi 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, lattice symmetry breaking,6 the existence of quantum phases that involve the pairing of fermions with bosons7, and also unconventional fermion pairing8 have been predicted. It is the main objective of this Letter to generalize these studies to the case of a resonantly-interacting Bose-Fermi mixture. Although our theoretical methods are very general, we consider as a concrete example a mixture of fermionic 40K atoms and the bosonic 87Rb atoms, as this system is now becoming available experimentally.9 A gas consisting of these two atoms is especially promising as their wavelengths are relatively close and readily accessible using Ti:Sapphire lasers. Furthermore, the mass of 40K is much larger than the mass of the other experimentally available fermionic atom 6Li, which makes it much easier to trap this species in an optical lattice.

In order to analyze the properties of a resonantly-interacting Bose-Fermi mixture most easily, it is convenient 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 only be achieved in an optical lattice that is red detuned with respect to all these four transitions. Making use of the fact that the hyperfine structure of the atoms is no longer resolved for the detunings used in optical lattice experiments10, 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 atoms11. In the following, we make the reasonable assumption that this also holds for the heteronuclear 40K-87Rb 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 ω ≡ ωF = ωB = 2.1 · 10−5 Ω. 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 $\Gamma / Q^2 = 1.9 \times 10^{-21}$ s
for the optimal wavelength. Clearly the lifetime is always
longer than one second for realistic Rabi frequencies less
than 4 GHz, and spontaneous emission can thus be safely
neglected.

Generalized Hubbard model. — We now consider the
many-body aspects of the Bose-Fermi mixture near a Fesh-
hbach 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 struc-
ture of the single-particle states. Experimentally this re-
quires 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 in-
teractions. Furthermore, for low filling fractions there is
also no problem of phase separation of the atomic Bose-
Fermi mixture \cite{12} and it is justified to neglect possible
Mott physics in the mixture \cite{13,14}.

Under these conditions we have recently derived the
theory for resonantly-interacting ultracold atomic gases in
an optical lattice \cite{15}. 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 calcu-
lated in the tight-binding approximation. In this man-
ner the microscopic parameters of the generalized Hub-
bard model that describes the Bose-Fermi mixture near
the Feshbach resonance are completely determined by the
details of the optical lattice potential and the experiment-
ally known parameters of the Feshbach resonance in the
absence of the optical lattice. Ultimately, the mixture is
described by the following effective hamiltonian,

\begin{equation}
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_i b_{i,\sigma}^\dagger b_{i,\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^{BB}}{2} \sum_i a_i^\dagger a_i a_i^\dagger a_i + \frac{U^{BF}}{2} \sum_i a_i^\dagger c_i^\dagger c_i a_i
+ g \sum_{\sigma} \sum_i \sqrt{Z_{\sigma}} \left( b_{i,\sigma}^\dagger c_i a_i + a_i^\dagger c_i^\dagger b_{i,\sigma} \right).
\end{equation}

Here $t_F$, $t_B$ and $t_m$ are the tunneling or hopping am-
plitudes 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, $a_i^\dagger$, $a_i$ correspond to the creation and annihila-
tion 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 $i$. Also $\epsilon_\sigma = 3h\omega / 2$ is
the on-site energy of a single atom. The on-site interaction
between two bosons is given by $U^{BB}$, and $U^{BF}$ denotes
the on-site background interaction between the bosons
and the fermions. In the tight-binding limit the hopping
amplitudes can be conveniently expressed in terms of the
lattice parameters as \cite{16}

\begin{equation}
t_\nu = \frac{\hbar \omega}{2} \left( 1 - \left( \frac{2}{\pi} \right)^2 \right) \left( \frac{\lambda}{4\ell_r} \right)^2 e^{-(\lambda / 4\ell_r)^2}. \tag{2}
\end{equation}

Here $\nu$ 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, $\lambda$ is the
wavelength of the light used to create the optical lattice,
and the harmonic oscillator lengths obey $\ell_r = \sqrt{\hbar / 2\mu \omega}$,
where $m_F$, $m_B$, and $m_m = m_F + m_B$ are the masses
of the fermions, bosons, and molecules, respectively. As
expected, we have in general that $t_m \ll t_{F,B} \ll \hbar \omega$.

Note that we have 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.

Close to resonance we can neglect the on-site interactions. The strength of the atom-molecule coupling in the lattice is given by \( g' = g/(\pi (l_0^2 + l_0^2))^{3/4} \), where \( g = \sqrt{2\pi \alpha_{bg} \Delta \mu \Delta B / m} \) is the bare atom-molecule coupling without the lattice and \( m = m_F m_B / \left( m_F + m_B \right) \) 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 \( g \) given by the background scattering length \( a_{bg} = 150 \) a\( \text{o} \) and the width of the resonance \( \Delta B = 1 \) Gauss.\(^3\)\(^4\)\(^9\). The difference in magnetic moments \( \Delta \mu \) is equal to 29.2 Gauss \( \Delta B / \pi a \). The difference in magnetic moments \( \Delta \mu \) is equal to 29.2 Gauss \( \Delta B / \pi a \). The probability \( Z_\sigma \) is determined by the selfenergy of the molecules \( \hbar \Sigma_m(E) = (g^2 / \pi l_0^2 \hbar \omega) \cdot \Gamma(-E/2\hbar \omega + 3/4)/\Gamma(-E/2\hbar \omega + 1/4) \), with \( \Gamma(z) \) the gamma function, through the relation \( Z_\sigma = 1 / (1 - \partial \Sigma_m(E) / \partial E) \).\(^{15}\) Note that in Fig. 2 the sum of the probabilities \( Z_\uparrow + Z_\downarrow \) 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 wavefunctions. 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 onsite 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 is in the same universality class as the XY model. 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

\[
n = n_F + n_B + 2 \sum_{\sigma} n_{m,\sigma}.
\]

In the normal state the molecular filling fractions obey

\[
n_{m,\sigma} = \frac{1}{N_s} \sum_k \frac{1}{e^{\hbar \omega_{k,\sigma} / \beta} + 1},
\]

where \( \hbar \omega_{k,\sigma} = \epsilon_{k,\sigma} - \left( \mu_F + \mu_B \right) \) is the molecular dispersion. The atomic filling fractions are given by

\[
n_F = \frac{1}{N_s} \sum_k \frac{1}{e^{\hbar \omega_{k,F} / \beta} + 1},
\]

\[
n_B = \frac{1}{N_s} \sum_k \frac{1}{e^{\hbar \omega_{k,B} / \beta} - 1},
\]

where \( \hbar \omega_{k,F} = \epsilon_{k,F} - \mu_F \) and \( \hbar \omega_{k,B} = \epsilon_{k,B} - \mu_B \) are the dispersion relations for the fermionic and the bosonic atoms, respectively. Here \( \epsilon_{k,F,B} = -t_{F,B} \sum_{j=1}^3 \cos \left( k_j x / 2 \right) + \epsilon_a \) for the atoms and \( \epsilon_{k,\sigma} = \epsilon_\sigma \) for the molecules. 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., \( \epsilon_\downarrow = 2 \epsilon_a - 6(t_F + t_B) \). In the approximation that we can neglect the hopping of the molecules, their band structure is flat and 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.

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**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. The inset shows the probability \( Z_\sigma \) as a function of the magnetic field. This figure was calculated for the \(^{40}\)K-\(^{87}\)Rb mixture with \( \lambda = 806 \) nm and \( \Omega = 1 \) GHz.
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 phase diagram 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 $T_c \propto \hbar \omega / k_B$, which a posteriori shows that a single-band approximation for the dressed molecules is indeed appropriate.

Conclusions and Discussion. — In summary we have shown that by using a red-detuned optical lattice with a wavelength of 806 nm the Bose-Fermi mixture of $^{40}\text{K}$ and $^{87}\text{Rb}$ 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. 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 critical surface 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. 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.

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FIG. 3: Phase diagram of the $^{40}\text{K}$ and $^{87}\text{Rb}$ mixture as a function of the total filling fraction, magnetic field and temperature. This figure was calculated for the $^{40}\text{K}$–$^{87}\text{Rb}$ mixture with $\lambda = 806$ nm and $\Omega = 1$ GHz.