Feshbach resonances in an optical lattice

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We present a theory for ultracold atomic gases in an optical lattice near a Feshbach resonance. In the single-band approximation the theory describes atoms and molecules that can both tunnel through the lattice. Moreover, an avoided crossing between the two-atom and the molecular states occurs at every site. We determine the microscopic parameters of the generalized Hubbard model that describes this physics, using the experimentally known parameters of the Feshbach resonance in the absence of the optical lattice. As an application we also calculate the zero-temperature phase diagram of an atomic Bose gas in an optical lattice.

I. INTRODUCTION

In the last few years there has been much excitement in the field of ultracold atomic gases. To a large extent this is due to two recent experimental developments. The first is the use of so-called Feshbach resonances in the collision of two atoms, and the second is the use of an optical lattice. Both developments have led to an unprecedented control over the physically relevant parameters of the atomic gas that can be used to explore strongly correlated regions of its phase diagram. In this paper we propose to combine these two developments and study an atomic gas in an optical lattice near a Feshbach resonance.

A more specific motivation for studying Feshbach resonances in an optical lattice is that recently it has been shown that in an atomic Bose gas near a Feshbach resonance a quantum phase transition occurs between a phase with only a molecular condensate (MC) and a phase with both an atomic and a molecular condensate (AC+MC) [1,2]. The experimental observation of this quantum Ising transition is, however, complicated by the fact that in a harmonic trap the fast vibrational relaxation of Feshbach molecules consisting of two bosonic atoms appears to prevent the creation of a molecular condensate in that case [3]. In an optical lattice with a low filling fraction molecule-molecule and atom-molecule collisions can essentially be neglected and we expect this problem to be much less severe.

Having this particular application in mind, we from now on focus on atomic Bose gases. However, our results can be immediately generalized to the case of a two-component Fermi gas or even an atomic Bose-Fermi mixture in an optical lattice. Moreover, we consider only such low filling fractions that it is justified to neglect the possibility of having three or more atoms per lattice site. The reason for this restriction is that in this case we have at most two atoms per site and the effect of the resonant interactions between the atoms can be incorporated into the theory exactly. The latter was shown previously to be very important for arriving at a

quantitatively accurate description of a harmonically trapped atomic gas near a Feshbach resonance [4]. How this can be achieved also in an optical lattice is discussed next.

II. GENERALIZED HUBBARD MODEL

We consider the experimentally most interesting case of a deep optical lattice in which the on-site potential is, for low energies, well approximated by an isotropic harmonic potential with energy splitting $\hbar\omega$ and the tunneling energy t_a for atoms between sites obeys $t_a \ll \hbar\omega$. For two atoms on a single site the two-channel Feshbach problem in the relative coordinate, after splitting off the center-of-mass motion, is then given by the Schrödinger equation

$$\begin{pmatrix} H_0 + V_{aa} & V_{am} \\ V_{am} & \delta_B \end{pmatrix} \begin{pmatrix} |\psi_a\rangle \\ |\psi_m\rangle \end{pmatrix} = E \begin{pmatrix} |\psi_a\rangle \\ |\psi_m\rangle \end{pmatrix}. \tag{1}$$

Here the noninteracting atomic Hamiltonian is $H_0 = -\hbar^2\nabla_{\mathbf{r}}^2/m + m\omega^2\mathbf{r}^2/4$. The bare detuning is denoted by δ_B, $\mathbf{r}$ is the relative coordinate between the atoms, and m is the atomic mass. The nonresonant or background atom-atom interaction is V_{aa} and the atom-molecule coupling is denoted by V_{am}. In the first instance only the relative part is relevant, since only this part is affected by the interactions between the atoms. The center-of-mass part determines the tunneling. From Eq. (1) we obtain the following equation for the molecules:

$$\langle \psi_m | V_{am} \frac{1}{E - H_0 - V_{aa}} V_{am} | \psi_m \rangle = E - \delta_B, \tag{2}$$

where $|\psi_m\rangle$ is the bare molecular wave function. Note that in the above we have implicitly taken the extent of this wave function to be so small that its energy is not affected by the optical lattice, which is well justified in practice. Because for most atoms we also have that $|V_{aa}| \ll \hbar\omega$, we can neglect in the atomic propagator V_{aa} compared to H_0. Moreover, the eigenstates $|\phi_n\rangle$ of H_0 with energy $E_n = (2n+3/2)\hbar\omega$ that are relevant for an s-wave Feshbach resonance can be written in terms of the generalized Laguerre polynomials as $\langle \mathbf{r}|\phi_n\rangle = e^{-\mathbf{r}^2/4l^2}L_n^{1/2}(\mathbf{r}^2/2l^2)/(2\pi l^2)^{3/4}[L_n^{1/2}(0)]^{1/2}$. Here $l = \sqrt{\hbar/m\omega}$ is

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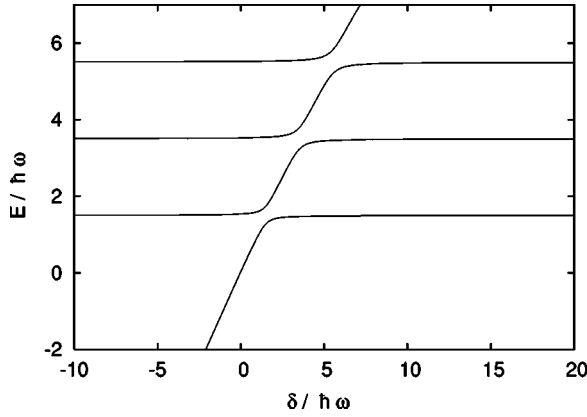
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FIG. 1. The relative energy levels of the atom-molecule system as a function of the detuning δ. This figure was calculated for $g^2/\sqrt{2}\pi l^3(\hbar\omega)^2 = 0.1$.
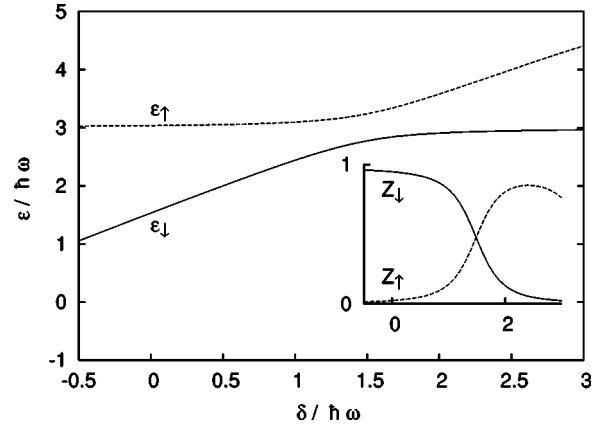

FIG. 2. Details of the physical content of our theory. We show the avoided crossing between the molecular level and the lowest two-atom trap state. The inset shows the probability Z_σ as a function of the detuning δ. This figure was calculated for $g^2/\sqrt{2}\pi l^3(\hbar\omega)^2 = 0.1$ Note that the center-of-mass contribution to the energy has been taken into account here.

the harmonic oscillator length. Using these states Eq. (2) can be rewritten as

$$\sum_n \frac{|\langle \psi_m | V_{am} | \phi_n \rangle|^2}{E - E_n} = E - \delta_B. \tag{3}$$

Using also the usual pseudopotential approximation, we have that $\langle \mathbf{r} | V_{am} | \psi_m \rangle = \sqrt{2}g\delta(\mathbf{r})$, where the atom-molecule coupling $g = \hbar\sqrt{2\pi a_{bg}\Delta B\Delta\mu/m}$ depends on the background scattering length a_{bg}, the width of the resonance ΔB, and the difference in magnetic moments $\Delta\mu$ of the relevant Feshbach resonance [4]. From this we then find that the energy of the molecules obeys

$$E - \delta_B = 2g^2\sum_m \frac{\phi_m^*(0)\phi_m(0)}{E - E_m} = g^2\left[\frac{G(E)}{\sqrt{2}\pi l^3\hbar\omega} - \lim_{r\to 0}\frac{m}{2\pi\hbar^2 r}\right]. \tag{4}$$

The function $G(E)$ is the ratio of two gamma functions $G(E) = \Gamma(-E/2\hbar\omega + 3/4)/\Gamma(-E/2\hbar\omega + 1/4)$. The divergence in Eq. (4), which was first obtained by Busch *et al.* in the context of a single-channel problem [6], can be dealt with by using the following renormalization procedure. The right-hand side of Eq. (4) can be interpreted as the self-energy of the molecules $\hbar\Sigma_m(E)$. The divergence in the self-energy is energy independent and is related to an ultraviolet divergence that comes about because we have used pseudopotentials. To deal with this divergence we have to use the renormalized detuning instead of the bare detuning. The former is defined as $\delta = \delta_B - \lim_{r\downarrow 0}mg^2/2\pi\hbar^2 r$, where $\delta = \Delta\mu(B - B_0)$ is determined by the experimental value of the magnetic field B_0 at resonance. Note that, as expected, the required subtraction is exactly equal to the one needed in the absence of the optical lattice. In the latter case we have to subtract $2g^2\int d\mathbf{k}\, m/\hbar^2\mathbf{k}^2(2\pi)^3$ [4,5], which can be interpreted as $\delta = \delta_B - \lim_{\mathbf{r}\downarrow 0}2g^2\int d\mathbf{k}\, e^{i\mathbf{k}\cdot\mathbf{r}}m/\hbar^2\mathbf{k}^2(2\pi)^3$. In this manner we obtain the relative energy levels of the dressed molecules as a function of the experimental detuning that is shown in Fig. 1.

From this figure we see that for very negative detuning the molecular state lies below the ground state of the on-site microtrap and the bound-state energy is well approximated

by the detuning. As it approaches the ground-state level of the trap there is an avoided crossing and as a result the lowest trap state is shifted upward. If the avoided crossings between the molecular level and subsequent trap states do not strongly overlap, the system can be well described by considering only the lowest trap state. The overlap between the avoided crossings is determined by the strength of the atom-molecule coupling and can be neglected if $g^2/\sqrt{2}\pi l^3(\hbar\omega)^2 \ll 1$. In this paper we restrict ourselves to a single-band approximation, although the generalization to the multiband situation is straightforward. This means that we only take into account the wave functions of the molecular state and the ground state of the on-site microtrap. In that case only two energy levels are of importance when there are two atoms on a lattice site. We denote these levels by $\epsilon_\uparrow$ and $\epsilon_\downarrow$ and their behavior as a function of detuning is shown in Fig. 2.

The effective atom-molecule coupling in the optical lattice is given by $g' = g[\int d\mathbf{x}|\psi_0(\mathbf{x})|^4]^{1/2} = g/(2\pi l^2)^{3/4}$, where $\psi_0(\mathbf{x})$ is the Wannier function in the lowest band of the optical lattice. The effective atom-atom interaction is now given by $U_{eff} = U_{bg} - 2(g')^2/(\delta - 3\hbar\omega/2)$, where the background on-site interaction strength $U_{bg} = (4\pi a_{bg}\hbar^2/m)\int d\mathbf{x}|\psi_0(\mathbf{x})|^4 = \sqrt{2/\pi}\hbar\omega(a_{bg}/l)$. It is interesting to note that in order for the single-band approximation to be valid we do not need to have that $U_{eff} \ll \hbar\omega$ because the on-site two-atom problem has been solved exactly. In Fig. 2 we also show a close-up of the avoided crossing and the wave-function renormalization factors Z_σ that give the amplitude of the closed-channel part of the molecules in the state $|\psi_\sigma\rangle$. Explicitly, we thus have in the single-band approximation that

$$|\psi_\uparrow\rangle = \sqrt{Z_\uparrow}|\psi_m\rangle - \sqrt{1 - Z_\uparrow}|\psi_0\psi_0\rangle,$$

$$|\psi_\downarrow\rangle = \sqrt{Z_\downarrow}|\psi_m\rangle + \sqrt{1 - Z_\downarrow}|\psi_0\psi_0\rangle. \tag{5}$$

The probability Z_σ is determined by the self-energy of the molecules through the relation $Z_\sigma = 1/[1 - \partial\hbar\Sigma_m(E)/\partial E]$ [2].

Note that in Fig. 2 the probability $Z_\uparrow$ already shows the effect of the avoided crossing at a detuning of about $3\hbar\omega$. As long as the single-band approximation is valid this will, however, not affect any of the results because the two-atom state that is involved in this avoided crossing will not be populated.

Combining the above we thus find a generalized Hubbard Hamiltonian that is given by

$$
H = - t_a \sum_{\langle i,j\rangle} a_i^\dagger a_j - t_m \sum_\sigma \sum_{\langle i,j\rangle} b_{i,\sigma}^\dagger b_{j,\sigma} + \sum_\sigma \sum_i (\epsilon_\sigma - 2\mu) b_{i,\sigma}^\dagger b_{i,\sigma}
$$
$$
+ \sum_i (\epsilon_a - \mu) a_i^\dagger a_i + \frac{U_{bg}}{2} \sum_i a_i^\dagger a_i^\dagger a_i a_i
$$
$$
+ g' \sum_\sigma \sum_i \sqrt{Z_\sigma} (b_{i,\sigma}^\dagger a_i a_i + a_i^\dagger a_i^\dagger b_{i,\sigma}). \tag{6}
$$

Here t_a and t_m are the tunneling amplitudes for the atoms and the molecules, respectively, and $\langle i,j\rangle$ denotes a sum over nearest neighbors. The operators $a_i^\dagger$ and a_i correspond to the creation and annihilation operators of a single atom at site i, respectively. The operators $b_{i,\sigma}^\dagger$ and $b_{i,\sigma}$ correspond to the creation and annihilation operators of the dressed molecules at site i, respectively. Also $\epsilon_a = 3\hbar\omega/2$ is the on-site energy of a single atom. In the tight-binding limit the hopping amplitudes can be conveniently expressed in terms of the lattice parameters as [7]

$$
t_{a,m} = \frac{\hbar\omega}{2}\left[1 - \left(\frac{2}{\pi}\right)^2\right]\left(\frac{\lambda}{4l_{a,m}}\right)^2 e^{-(\lambda/4l_{a,m})^2}. \tag{7}
$$

Here λ is the wavelength of the light used to create the optical lattice and $l_m\sqrt{2} = l_a = l$. Note that, as expected, we have that $t_m \propto t_a^2/\hbar\omega \ll t_a$. Note also that our harmonic approximation to the on-site potential in principle slightly underestimates the hopping parameter. A more accurate determination of these parameters would involve the calculation of the appropriate Wannier functions. The chemical potential μ is added because we perform our next calculations in the grand-canonical ensemble.

III. PHASE DIAGRAM

To find the mean-field phase diagram of a Bose gas in an optical lattice, we consider at sufficiently negative detuning the phase with only a Bose-Einstein condensate of molecules and perform a quadratic expansion of the Hamiltonian in the fluctuations of the molecular annihilation operator $\mathbf{b}_{k,\sigma}$ around the nonzero expectation value $\langle b_{k,\sigma}\rangle = \sqrt{n_{mc}}\delta_{k,0}\delta_{\sigma,\downarrow}$. The effective Hamiltonian is then diagonalized by a Bogoliubov transformation and from the result we determine the equation of state of the gas as a function of the detuning δ and the temperature $T \equiv 1/k_B\beta$. For the equation of state for the total filling fraction we find (cf. Ref. [2]) $n = n_a + 2\Sigma_\sigma n_m^\sigma$ with the molecular filling fractions obeying

$$
n_m^\downarrow = n_{mc} + \frac{1}{N_s}\sum_{k\neq 0}\frac{1}{e^{\beta\hbar\omega_{k,\downarrow}}-1},
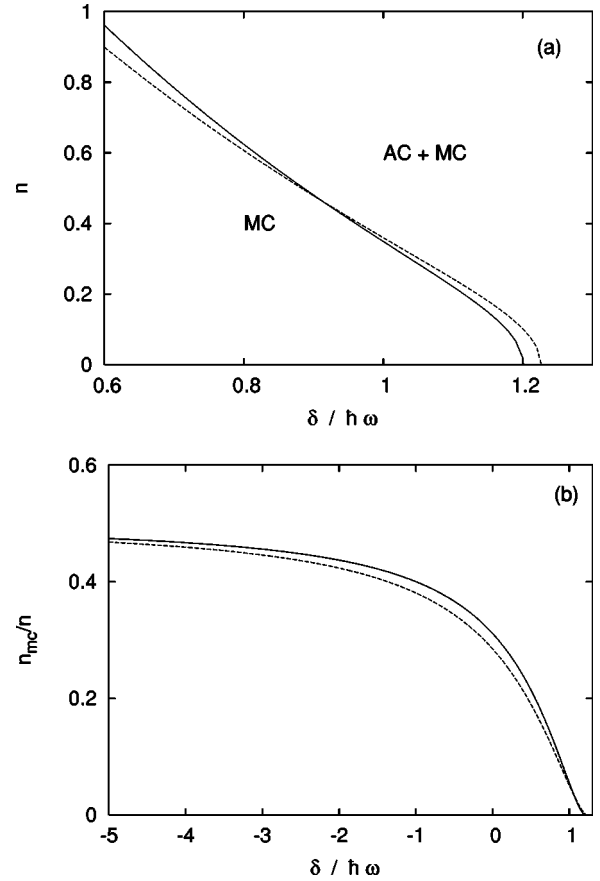$$

FIG. 3. Zero-temperature phase diagram as a function of the filling fraction per site and the detuning δ in units of $\hbar\omega$. The different curves that separate the MC and the AC+MC phases correspond to values of $g'/\hbar\omega = 0.10$ (full curve) and $g'/\hbar\omega = 0.12$ (dashed curve), respectively. In both cases we have taken ω to be 10^4 rad/s.

$$
n_m^\uparrow = \frac{1}{N_s}\sum_k \frac{1}{e^{\beta\hbar\omega_{k,\uparrow}}-1}, \tag{8}
$$

and the atomic filling fraction

$$
n_a = \frac{1}{N_s}\sum_k\left\{\frac{2\epsilon_k^a - \epsilon_m}{2\hbar\omega_k}\frac{1}{e^{\beta\hbar\omega_k}-1} + \frac{2\epsilon_k^a - \epsilon_m - 2\hbar\omega_k}{4\hbar\omega_k}\right\}. \tag{9}
$$

Moreover, we have that N_s is the total number of sites in the lattice, $\epsilon_k^a = -2t_a\Sigma_{j=1}^3\cos(k_j\lambda/2) + \epsilon_a$, $\epsilon_{k,\sigma}^m = -2t_m\Sigma_{j=1}^3\cos(k_j\lambda/2) + \epsilon_\sigma$, and $\hbar\omega_{k,\sigma} = \epsilon_{k,\sigma}^m + \epsilon_m$ is the molecular dispersion. Likewise we find that $\hbar\omega_k = [(\epsilon_k^a - \epsilon_m/2)^2 - 4g'^2 Z_\downarrow n_{mc}]^{1/2}$ is the atomic Bogoliubov dispersion with $\epsilon_m = \epsilon_\downarrow - zt_m$ equal to twice the chemical potential and z the number of nearest neighbors.

The critical temperature for the Bose-Einstein condensation of the molecules follows from the condition $n_{mc}=0$. The location of the Ising quantum phase transitions follows from the zero-momentum instability in the atomic Bogoliubov dispersion when the detuning $\epsilon_m = -4g'\sqrt{Z_\downarrow}\sqrt{n_{mc}} + 2\epsilon_a - 2zt_a$. In Fig. 3(a) we show the results for this condition as a function

of the total filling fraction and detuning. Note that in the limit of vanishing density the quantum critical point is determined by the ideal gas condition for Bose-Einstein condensation, i.e., $\mu = \epsilon_m/2 = \epsilon_a - zt_a$. From this condition it follows that for low enough filling fractions the location of the quantum phase transition shifts to higher detuning with increasing strength of the atom-molecule coupling. On the other hand at large negative detuning a larger value of the atom-molecule coupling implies a larger quantum depletion and hence a smaller molecular condensate fraction. This effect shifts the Ising transition to lower detuning.

For completeness we would like to point out that at $n = 1$ the phase diagram can also contain a Mott-insulator phase [9]. This phase can occur at sufficiently large positive detuning such that $U_{eff}/zt_a \geq 3 + 2\sqrt{2}$ [7,8]. In contrast to the quantum Ising transition, this transition has already been observed experimentally by Greiner *et al.* [10] after the theoretical prediction by Jaksch *et al.* [11]. Its existence does not rely on the presence of the Feshbach resonance and we, therefore, have not included it in the phase diagram in Fig. 3. It is important to realize that this Mott insulator can exist only for repulsive interactions between the atoms, which requires U_{bg} to be positive.

IV. CONCLUSIONS AND DISCUSSION

In summary, we have shown how to determine the microscopic parameters of the generalized Hubbard model in Eq. (6) that describes the physics of resonantly interacting atoms in an optical lattice, using the experimentally known parameters of the Feshbach resonance in the absence of the optical lattice. As an application we also calculated the zero-temperature phase diagram of an atomic Bose gas in an optical lattice in the single-band approximation. By using an optical lattice one can suppress three-body recombination processes that lead to a fast decay of the molecular condensate.

For the single-band approximation to be valid the atom-molecule coupling constant g has to be small enough such that the avoided crossings between subsequent bands do not overlap with each other. In some cases, however, this coupling constant can be too large for realistic conditions and the single-band approximation will not hold anymore. In those cases we have to include higher-lying two-atom states. To avoid this complication the atom-molecule coupling g can be made smaller by using a more narrow Feshbach resonance or by using two-photon Raman transitions to convert atoms into molecules [12]. Inclusion of higher-lying two-atom states is, however, easily achieved in our theory by adding more atomic and molecular states into the generalized Hubbard model. In principle, we have to add several dressed molecular states $|\psi_\sigma\rangle$ for each additional atomic band that is required for a sufficiently accurate description of the atomic gas in the optical lattice. More precisely, for M atomic bands we need to include $M^2 + 1$ dressed molecular states into the theory.

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