Feshbach resonances in Optical Lattices

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ABSTRACT

We present the theory for ultracold atomic gases in an optical lattice near a Feshbach resonance. In the single-band approximation the theory describes atoms and molecules which 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.

A: Solution for a single site

For two atoms on a single site the two-channel Feshbach problem in the relative coordinate, after splitting of the center-of-mass motion, is given by the Schrödinger equation:

$$\begin{pmatrix} H_0+V_{\rm aa} & V_{\rm am} \\ V_{\rm am} & \delta_B \end{pmatrix} \begin{pmatrix} |\psi_{\rm a}\rangle \\ |\psi_{\rm m}\rangle \end{pmatrix} = E \begin{pmatrix} |\psi_{\rm a}\rangle \\ |\psi_{\rm m}\rangle \end{pmatrix}.$$

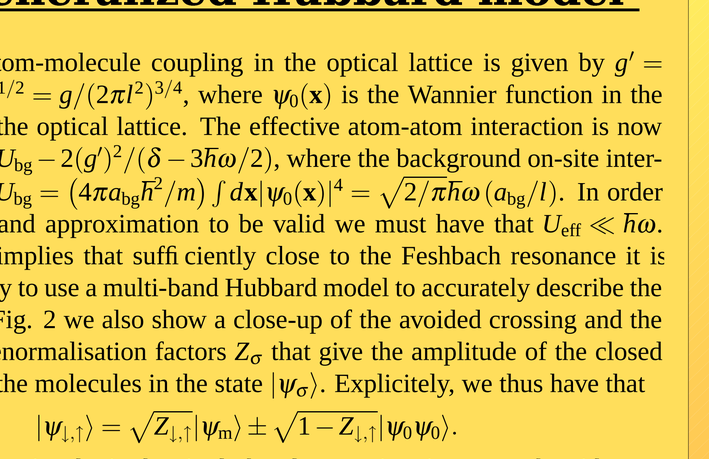
Here the noninteracting atomic Hamiltonian is $H_0 = -\hbar^2\nabla_{\mathbf{r}}^2/m + m\omega^2\mathbf{r}^2/4$. The bare detuning is denoted by $\delta_{\rm B}$, $\mathbf{r}$ is the relative coordinate between the atoms and m is the atomic mass. The nonresonant or background atom-atom interaction is $V_{\rm aa}$ and the atom-molecule coupling is denoted by $V_{\rm am}$. In 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 the above equation we obtain the following equation for the molecules

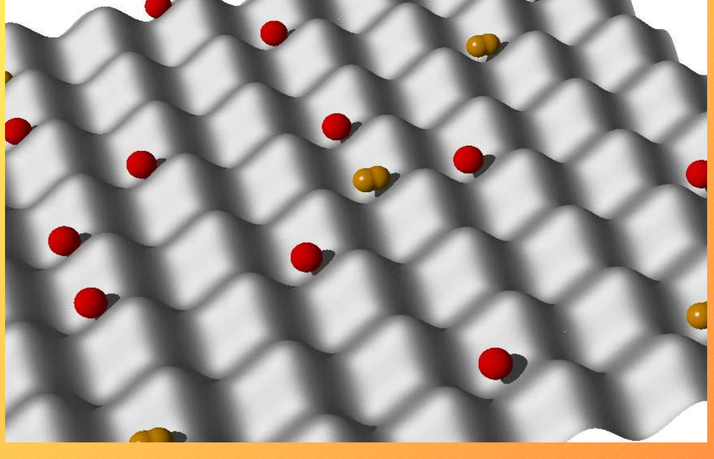
$$\langle\psi_{\rm m}|V_{\rm am}\frac{1}{E-H_0-V_{\rm aa}}V_{\rm am}|\psi_{\rm m}\rangle = E-\delta_{\rm B},$$

where $|\psi_{\rm m}\rangle$ is the bare molecular wavefunction. Note that in the above we have implicitely taken the extend of this wavefunction to be so small that its energy is not affected by the optical lattice, which is well justified in practice. From this we then find that the energy of the molecules obeys

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

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 the selfenergy 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.





Top left: For suffi ciently negative detuning there is a quantum phase transitior to a phase with only a Bose Einstein condensate of dressed molecules. These molecules have a large bare molecule amplitude.
Top right: Above the QPT are mainly dressed molecules that have a large bare molecule amplitude. There are very few single atoms.
Bottom: For large positive detuning there are primarily single Bose condensed atoms and only a few dressed molecules that have a small bare molecule amplitude.

B: Generalized Hubbard model

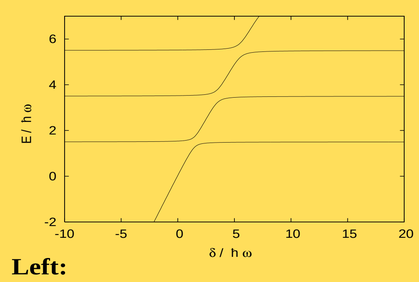
The effective atom-molecule coupling in the optical lattice is given by $g' = g(\int d\mathbf{x}|\psi_0(\mathbf{x})|^4)^{1/2} = g/(2\pi l^2)^{3/4}$, where $\psi_0(\mathbf{x})$ is the Wannier function in the lowest band of the optical lattice. The effective atom-atom interaction is now given by $U_{\rm eff} = U_{\rm bg} - 2(g')^2/(\delta - 3\hbar\omega/2)$, where the background on-site interaction strength $U_{\rm bg} = \left(4\pi a_{\rm bg}\hbar^2/m\right)\int d\mathbf{x}|\psi_0(\mathbf{x})|^4 = \sqrt{2/\pi}\hbar\omega\,(a_{\rm bg}/l)$. In order for the single-band approximation to be valid we must have that $U_{\rm eff} \ll \hbar\omega$. This condition implies that suffi ciently close to the Feshbach resonance it is always necessary to use a multi-band Hubbard model to accurately describe the atomic gas. In Fig. 2 we also show a close-up of the avoided crossing and the wavefunction renormalisation factors Z_σ that give the amplitude of the closed channel part of the molecules in the state $|\psi_\sigma\rangle$. Explicitely, we thus have that

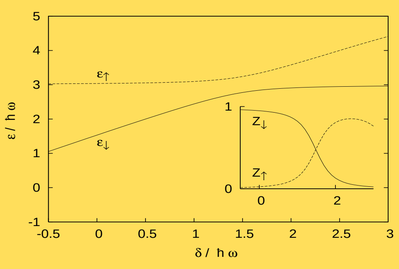
$$|\psi_{\downarrow,\uparrow}\rangle = \sqrt{Z_{\downarrow,\uparrow}}|\psi_{\rm m}\rangle \pm \sqrt{1-Z_{\downarrow,\uparrow}}|\psi_0\psi_0\rangle.$$

As mentioned previously, in the single-band approximation σ can be either up or down. The probability Z_σ is determined by the selfenergy of the molecules through the relation $Z_\sigma = 1/(1-\partial\hbar\Sigma_{\rm m}(E)/\partial E)$. Combining the above we thus find a generalized Hubbard Hamiltonian that is given by

$$\begin{aligned} H = &-t_a\sum_{\langle i,j\rangle} a_i^\dagger a_j - t_m\sum_\sigma\sum_{\langle i,j\rangle} b_{i,\sigma}^\dagger b_{j,\sigma} + \sum_\sigma\sum_i (\varepsilon_\sigma - 2\mu)\, b_{i,\sigma}^\dagger b_{i,\sigma} + \sum_i(\varepsilon_{\rm a}-\mu)a_i^\dagger a_i \\ &+\frac{U_{\rm bg}}{2}\sum_i a_i^\dagger a_i^\dagger a_i a_i + g'\sum_\sigma\sum_i\sqrt{Z_\sigma}\left(b_{i,\sigma}^\dagger a_i a_i + a_i^\dagger a_i^\dagger b_{i,\sigma}\right). \end{aligned}$$

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 neighbours. Also $\varepsilon_{\rm a} = 3\hbar\omega/2$ is the on-site energy of a single atom.





Left:
The relative energy levels of the atom-molecule system as a function of the detuning δ. Both figures was calculated for $g^2/\sqrt{2}\pi l^3(\hbar\omega)^2 = 0.1$ 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 $g^2/\sqrt{2}\pi l^3(\hbar\omega)^2 \ll 1$. Here we restrict ourselves to a single-band approximation, although the generalization to the multi-band situation is straightforward.
Right:
A close-up of the avoided crossing and the wavefunction renormalisation factors Z_σ that give the amplitude of the closed channel part of the molecules in the state $|\psi_\sigma\rangle$. Note that 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.

C: Application to the Bose Gas

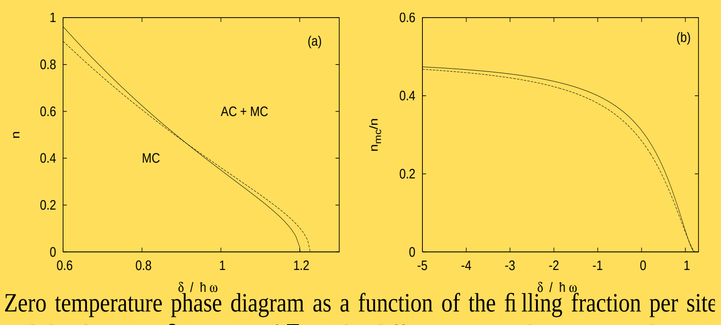
To find the mean-field phase diagram of a Bose gas in an optical lattice, we consider at suffi ciently negative detuning the phase with only a Bose-Einstein condensate of molecules and perform a quadratic expansion of the Hamiltonian in the fluctuations of the molecular annihilation operator $b_{\mathbf{k},\sigma}$ around the nonzero expectation value $\langle b_{\mathbf{k},\sigma}\rangle = \sqrt{n_{\rm mc}}\delta_{\mathbf{k},\mathbf{0}}\delta_{\sigma,\downarrow}$. 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 $n = n_{\rm a} + 2\sum_\sigma n_{\rm m}^\sigma$ with the molecular filling fractions obeying

$$\begin{aligned} n_{\rm m}^\downarrow &= n_{\rm mc} + \frac{1}{N_s}\sum_{\mathbf{k}\neq\mathbf{0}}\frac{1}{e^{\beta\hbar\omega_{\mathbf{k},\downarrow}}-1}, \\ n_{\rm m}^\uparrow &= \frac{1}{N_s}\sum_{\mathbf{k}}\frac{1}{e^{\beta\hbar\omega_{\mathbf{k},\uparrow}}-1}, \end{aligned} \qquad (1)$$

and the atomic filling fraction

$$\begin{aligned} n_{\rm a} = \frac{1}{N_s}\sum_{\mathbf{k}}\Bigg\{&\frac{2\varepsilon_{\mathbf{k}}^{\rm a}-\varepsilon_{\rm m}}{2\hbar\omega_{\mathbf{k}}}\frac{1}{e^{\beta\hbar\omega_{\mathbf{k}}}-1} \\ &+\frac{2\varepsilon_{\mathbf{k}}^{\rm a}-\varepsilon_{\rm m}-2\hbar\omega_{\mathbf{k}}}{4\hbar\omega_{\mathbf{k}}}\Bigg\}. \end{aligned} \qquad (2)$$

Moreover, we have that N_s is the total number of sites in the lattice, $\varepsilon_{\mathbf{k}}^{\rm a} = -2t_{\rm a}\sum_{j=1}^3\cos(k_j\lambda/2) + \varepsilon_{\rm a}$, $\varepsilon_{\mathbf{k},\sigma}^{\rm m} = -2t_{\rm m}\sum_{j=1}^3\cos(k_j\lambda/2) + \varepsilon_\sigma$, and $\hbar\omega_{\mathbf{k},\sigma} = \varepsilon_{\mathbf{k},\sigma}^{\rm m} + \varepsilon_{\rm m}$ is the molecular dispersion. Likewise we find that $\hbar\omega_{\mathbf{k}} = [(\varepsilon_{\mathbf{k}}^{\rm a}-\varepsilon_{\rm m}/2)^2 - 4g'^2Z_\downarrow n_{\rm mc}]^{1/2}$ is the atomic Bogoliubov dispersion with $\varepsilon_{\rm m} = \varepsilon_\downarrow - zt_{\rm m}$ equal to twice the chemical potential and z is the number of nearest neighbours.



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. 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., $\mu = \varepsilon_{\rm m}/2 = \varepsilon_{\rm a} - zt_{\rm a}$. 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.