Extended molecules and geometric scattering resonances in optical lattices

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We develop a theory describing neutral atoms scattering at low energies in an optical lattice. We show that for a repulsive interaction, as the microscopic scattering length increases, the effective scattering amplitude approaches a limiting value which depends only on the lattice parameters. In the case of attractive interaction a geometric resonance occurs before reaching this limit. Close to the resonance, the effective interaction becomes repulsive and supports a weakly bound state, which can extend over several lattice sites.

Recent advances in cooling and trapping of cold atomic gases (see [1] for a review) have led to the experimental realization of optically trapped lattices gases [2, 3]. For a dilute gas and at low energies all physical properties of such gases can be expressed in terms of the two-body scattering amplitude [4]. It is well established that confinement of a gas in one or more spatial dimensions can strongly modify the collisional properties of atoms, and can even induce geometric resonances [5, 6, 7, 8]. In an optical lattice related phenomena should occur when, (i) the microscopic free-space scattering length becomes comparable to the size of a single lattice well; a situation readily obtained by combining Feshbach or shape resonances with optical trapping techniques [9, 10, 11, 12, 13]; and (ii) the tunneling between the neighboring lattice sites is sufficiently small. Below we give a theoretical analysis of the modification of neutral atoms scattering at low energies in an optical lattice. This serves as the basis of writing down an effective (long wavelength) field theory of a dilute optical lattice. This serves as the basis of writing down an effective field theory of a dilute optical lattice. This serves as the basis of writing down an effective field theory of a dilute optical lattice.

We turn now to a discussion of two-body scattering in an optical lattice. The particles interact via a short range interatomic potential \( U(r) \) depending only on the relative coordinate \( r \). The range \( r_0 \) of this potential is assumed to be small compared to the lattice spacing and to the size \( l_0 \) of the ground state wavefunction in an individual well. In addition, the lattice spacing is assumed to be small relative to the de Broglie wavelength of the incoming particle. The particles move in a 3D optical lattice created by counterpropagating laser beams. The resulting periodic potential is characterized by a depth \( V_0 \) and lattice spacing \( d \), which are assumed to be equal for all spatial direction. Close to these minima, the potential can expanded as

\[
V = \frac{M\omega^2}{2} \delta R^2 + \frac{\mu \omega^2}{2} \delta r^2, \tag{2}
\]

where \( \delta R \) and \( \delta r \) are the deviation of the center-of-mass and the relative coordinates \( R = (x_1 + x_2)/2 \) and \( r = x_2 - x_1 \) from their potential minimum positions. Here, \( x_1 \) and \( x_2 \) are the positions of the particles and \( \mu = m/2 \) and \( M = 2m \) are the reduced and the total mass, respectively. Moreover, the curvature within a single lattice site is given by \( \omega^2 = V_0/\rho d^2 \). From here on we will use units such that \( \hbar = m = 1 \).

In such a periodic potential, the two-body wavefunction \( \Psi(x_1, x_2) \) is characterized by certain quasimomenta \( Q \) and \( q \) of the center of mass and the relative motion, as well as by band indices \( S \) and \( s \). Using the fact that the lattice potential is approximately separable (compare Eq. (2)), we can expand the two-body wavefunction in a set of basis functions [4, 14],

\[
\Psi_{Qq}^{(Ss)} = \sum_{N,n} e^{i(Q_{R_N} + i(q_{R_n})} W_S(R - R_N) w_s(r - r_n), \tag{3}
\]

where \( e_{\epsilon_p} \) is the relative energy, and \( m_s \) is the band mass. The main results are: (i) For repulsive interaction, when the microscopic scattering length \( a \) increases, the effective scattering amplitude remains finite and continuously approaches a universal limit, which only depends on the optical lattice parameters. (ii) In the case of an attractive interaction a geometric resonance in the effective scattering amplitude, similar to the resonances found in \[1, 8\], occurs before the universal limit is reached. In addition, after crossing the resonance the effective interaction becomes repulsive and weakly bound states result close to the resonance. This predicts the existence of large lattice induced molecules which can extend over several lattice sites, which - by analogy with the Wannier-Mott excitons in semiconductors [14] - will be referred to below as Wannier-Mott molecules. The parameters effective mass \( m_a \) and scattering length \( a_{\text{eff}} \) appearing in \[1, 8\] are the relevant parameters for the long wavelength effective field theory describing the dilute lattice gas.
where $W$ and $w$ are Wannier functions. Within the TBM the functions $W$ and $w$ coincide with the stationary states of the Hamiltonian $H$. The wavefunctions of the relative motion (Bloch waves) are characterized by the quasimomentum $q$, the band index $s$ and the energy $\epsilon_{sq} = \epsilon_s - t_s \cos(qd)$, where $t_s = \sqrt{D_s \omega / \pi}$, and $D_s \ll 1$ is the WKB tunneling exponent between the neighboring wells, and $\epsilon_s$ are the energies of states $s$ in isolated wells. For sufficiently small momenta the dispersion relation can be approximated as $\epsilon_{sq} \approx \epsilon_s + q^2 / m_s$, where $m_s = 2t_s d^2$ is the effective mass. In the TBM, $l_0 \lesssim d$, the tunneling coefficient is small and hence $m_s \gg 1$. The asymptotic form of the relative part of the two-body wavefunction far from the region around $r = 0$ where the interaction potential acts, can be written as

$$\Psi(r) = \sum_{n} w_s(r-r_n)e^{i(q \cdot r_n)} +$$

$$- \sum_{s'f} \frac{m_s f_{s's'}}{4\pi r_n} e^{i q_s r_n} w_{s'}(r-r_n),$$

(4)

where $f_{s's'}$ is the $s$-wave scattering amplitude, and $q_{s'} = \sqrt{m_s (\epsilon_{sp} - \epsilon_{s'0})}$. This definition ensures that in the continuum case $f = 4\pi a / m_s$, where $a$ is the free space two-body scattering length and $m_s = m$. Since the interparticle interaction $U(r)$ is very short-range, we can use free (Bloch) solutions for the relative motion everywhere apart from the immediate vicinity of $r = 0$. To calculate the effective scattering amplitude we closely follow the method suggested in [7, 8]. The most general solution of the free Schroedinger equation for $r \neq 0$ for a given energy $\epsilon$, which also contains the incoming wave is

$$\Psi(r) = \sum_{n} w_s(r-r_n)e^{i(q \cdot r_n)} + AG(r, 0),$$

(5)

where $A$ is an arbitrary constant. Here the first term describes the incoming wave, whereas the second term gives the scattered waves. The Green function is given by its usual expression

$$G(r, r') = \sum_{s'q,s,n,n'} \frac{w_s(r-r_n)w_{s'}(r'-r_n')e^{i(q \cdot r_n-r_n')}}{\epsilon_{sp} - \epsilon_{s'q} + i0}. $$

(6)

For sufficiently large $r$ we can expand $\epsilon_{sq}$ up to second order around $q = 0$ and integrate over $q$

$$G(r, 0) = -\frac{m_s V}{4\pi} \sum_{s', r_n} \exp \frac{i(q_{s'} r_n)}{r_n} w_{s'}(r-r_n)w_{s'}(0).$$

(7)

where $V$ is the volume of the system. If $\epsilon_{s'0}$ > $\epsilon_{sp}$ then the corresponding partial wave does not propagate to $r \to \infty$, $q_{s'}$ is imaginary, and the channel $s'$ is closed. Comparing Eqs. (4), (5) and (7) we identify the scattering amplitude

$$f_{s's'}(p, q') = A(\epsilon_{sp})V w_{s'}(0)\delta_{ss'},$$

The coefficient $A$ can be found by considering the short distance asymptotics of the solution [5]. Indeed, at small distances $r \ll l_0$ the wavefunction of the relative motion should match the solution of the two-body scattering problem in 3D [15]:

$$\Psi(r) \to B(1 - \frac{a}{r}),$$

(8)

where $B$ is a constant. The scattering length $a$ takes into account all the processes occurring at distances of order $r_0 \ll l_0 d$. In particular, $a$ may contain the effect of Feshbach [10] or shape resonances [17], provided that the size of the molecular bound state is sufficiently small.

We consider incoming particles at low energies so that the scattering occurs in the lowest Bloch band $s = 0$. Taking the limit both $r, r' \to 0$ in the Eq. (6) we find

$$G(r, r') \to 0 \sum_{s,q} \frac{w_s(r)w_s(r')}{\epsilon_{op} - \epsilon_{sq} + i0}. $$

(9)

As it is well known the Green function is singular when $r' \to r$ and can be represented as

$$G(r, r') \to -\frac{1}{4\pi |r-r'|} + \mathcal{F}(\epsilon),$$

(10)

where $\mathcal{F}$ is the regular part of the Green function. The singular part comes from the direct classical trajectory connecting the points $r, r'$, which has a universal character. The regular part consists of the contribution of recurrent trajectories and depends strongly on the details of the confining potential.

The only resonance in the denominator of Eq. (9) occurs for the $s = 0$ contribution. We should therefore study this term separately by writing $G = G_0 + G'$, where the function $G_0$ is not singular, and

$$G_0 = \sum_{q} \frac{w_0(0)w_0(0)}{\epsilon_{0p} - \epsilon_{0q} + i0}. $$

(11)

The TBM wavefunctions can be represented as $w_s = Z_s \psi_s(r)$ where $\psi_s$ is the wave function of the oscillator in a state $s$, and $Z_s$ is a normalization factor ($Z_s^2 = N^{-1}$, where $N$ is the number of the lattice sites). Substituting the wavefunctions in Eq. (11), we find for the imaginary part of $G_0$:

$$\text{Im} \ G_0(p) = -i \frac{m_s}{4\pi} d^3 |\psi_0(0)|^2 p.$$  

(12)

The real part is given by the principle value

$$\text{Re} \ G_0(p \to 0) = -\frac{2\ln 2 |\psi_0(0)|^2}{\pi l_0}. $$

(13)

The remaining terms in Eq. (9) can be analyzed in the WKB approximation. In a spherically symmetric harmonic trap the spectrum of the excitations is $\epsilon_s =
The imaginary part in Eq. (14) is required by the optical theorem [12] and does not imply any inelastic process (apart from those possibly contained in Ima). Depending on the sign $a_{\text{eff}}$ the poles of the scattering amplitude give rise either to bound or to virtual states in the effective potential as a result of the interplay of the interparticle interaction and the lattice potential. An interesting possibility arises when the microscopic scattering length $a$ is negative and its absolute value is slightly larger than the resonance value $l_\ast$. In this case the effective interaction is repulsive and is characterized by a very large and positive scattering length

$$a_{\text{eff}}^+ = l_\ast \beta m_s.$$  

Accordingly, the scattering amplitude [14] has a pole at $|p| = p_s$ corresponding to a bound state with a binding energy

$$|\epsilon_s| = \frac{p_s^2}{m_s(\alpha_{\text{eff}}^+)^2} = \frac{1}{m_s(a_{\text{eff}}^+)^2}.$$  

The size of such a dimer is $\xi \sim a_{\text{eff}}^+$ and must be very large: $\xi \gg d$ so that the bound state of the two particles can extend over many lattice sites, and thus should be referred to as “Wannier-Mott” molecules in analogy to the Wannier-Mott excitons in semiconductors [14], where bound states of electron and holes can very large compared with the lattice constant.

Note that in the TBM $l_\ast \ll l_0$ and, therefore, the geometric resonance $|a| \sim l_\ast$ can occur at realistic values of the microscopic scattering length $a$. Because the rate of 3-body recombination scales as $a_{\text{eff}}^+$ the spontaneous formation of these molecules should be facilitated in the limit that the effective scattering length becomes large. However, at the same time, in this limit the binding energy is very small and a reasonable fraction of bound atoms can only be expected at temperatures $T \ll |\epsilon_s|$. A possible way of detecting these extended and weakly bound Wannier-Mott molecules arises if they are
composed of fermionic atoms in different internal states. When the trapping potentials for the separate states are tilted in opposite directions, the unbound atoms experience a force and will move in one or the other direction, depending on their internal state, whereas the molecules experience zero net force. If the potential gradient difference exceeds a certain critical value related to the binding energy, the molecules dissociate and the remaining atoms are released.

The limiting value of the 2-body scattering amplitude $f_{00}(0)$ is of particular importance for condensed matter calculations

$$f_{00}(0) = \frac{4\pi a_{\text{eff}}}{m_s} = \frac{4\pi\beta}{a^{-1} + l_s^{-1}},$$

and determines the effective interaction strength $\tilde{U} \equiv f_{00}(0)$ for a dilute lattice gas. For example, in the case of a Bose-condensed lattice gas the chemical potential is given by $\tilde{U}/n$, where $n$ is the density of the condensed particles $20$. Similarly, in a system of interacting fermions with an attractive interaction ($\tilde{U} < 0$) the critical temperature of the BCS transition is

$$T_c = \frac{8\exp(\gamma - 2)}{\pi}\epsilon_F \exp\left(-2\pi^2/p_F|\tilde{U}|\right),$$

where $\epsilon_F = p_F^2/2m_s$ is the Fermi energy. An increase of the absolute value of the scattering length leads to a resonance in the effective interaction potential and causes the latter to change from an attractive to a repulsive interaction at $|a| = l_s$. Note however, that close to the resonance the imaginary and energy dependent part of the scattering amplitude cannot be neglected and Eq. (10) loses its validity. A further increase of $|a|$ leads to a repulsive interaction which destroys the BCS ground state and results in the formation of dimers. Since the latter are bosons, at sufficiently small temperatures a BEC of dimers can be created. This possibility is related to the ongoing discussion of the BCS-to-BEC crossover in strongly interacting Fermi-gases with attractive interaction $22$. We note that the BEC of large molecules provides an example of a superfluid ground state for a system of interacting fermions with effective repulsion. This possibility is related to the reported BEC of excitons in semiconductors $23$.

In summary, we have derived an analytical expression for the scattering amplitude as a function of the free space scattering length and the parameters of the confining optical potential for small energies. For a repulsive interaction, as the microscopic scattering length increases, the effective scattering amplitude grows and continuously approaches a universal limit. In the case of attractive interaction, increasing the scattering length leads to a geometric resonance occurring before the universal limit is reached. Close to the resonance, when the effective interaction becomes repulsive, it supports a weakly bound Wannier-Mott molecule which can extend over several lattice sites.

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