Formation of Molecules near a Feshbach Resonance in a 1D Optical Lattice

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We study the molecular behavior of two atoms interacting near a Feshbach resonance in the presence of a 1D periodic potential. The critical value of the scattering length needed to produce a molecule and the binding energy at resonance are calculated as a function of the intensity of the periodic potential. Because of the nonseparability of the center of mass and relative motion, the binding energy depends on the quasimomentum of the molecule. This has dramatic consequences on the molecular tunneling properties, which become strongly dependent on the scattering length.

The availability of tunable periodic potentials of an optical nature [1] and the quantum manipulation of the interatomic forces via Feshbach resonances [2] are opening new perspectives in the field of ultracold atomic gases. In the absence of the external potential, molecules can be formed near resonance only for positive values of the *s*-wave scattering length a, the corresponding binding energy being given by the formula $E_b = -\hbar^2/ma^2$, where m is the mass of each atom. These molecules have already been observed experimentally by several groups [3–6].

An interesting problem is the formation of molecules in an optical lattice generated by laser fields. First experimental results have been obtained very recently by the group of Esslinger [7] working with samples of potassium ^{40}K in a tight 2D lattice. From the theoretical front, Fedichev *et al.* [8] have investigated the case of a tight 3D lattice and shown that a bound state can also be formed for negative scattering lengths down to a critical value. Their approach holds for zero quasimomentum and under the assumption that the binding energy is smaller than the width of the lowest Bloch band so that the molecular wave function extends over many lattice sites.

In this Letter, we discuss the formation of molecules in a 1D optical lattice for *arbitrary* values of the scattering length and the laser intensity. If the barriers separating two consecutive wells are very high (high laser intensity), the system behaves as a series of 2D discs which lie at the bottom of the wells and feel a harmonic potential in the direction of the laser field. In this asymptotic regime the two-body problem is significantly simplified by the possibility of separating the center of mass and the relative coordinates of the two interacting atoms [9]. When this condition is violated, many interesting questions can be addressed: What is the critical value of the scattering length required to ensure the formation of a molecule? What is the value of the binding energy of the molecule in the so called unitarity limit where the scattering length approaches an infinite value? What is the dependence of

the binding energy of the molecule on its quasimomentum? How do the tunneling properties (bandwidth and effective mass) of molecules depend on the scattering length? The purpose of this Letter is to provide an explicit answer to these relevant questions.

Let us start by writing the 3D Schrödinger equation for two atoms interacting in the presence of a 1D periodic potential $V_{\text{opt}}(z)$:

$$\left(-\frac{\hbar^2}{m}\nabla^2 - \frac{\hbar^2}{4m}\frac{\partial^2}{\partial Z^2} + V(Z, z) + g\delta(\mathbf{r})\frac{\partial}{\partial r}r\right)\Psi = E\Psi,$$

(1)

where $V(Z, z) = V_{\text{opt}}(z_1) + V_{\text{opt}}(z_2)$ and we have introduced the center of mass and relative coordinates $Z = (z_1 + z_2)/2$ and $\mathbf{r} = \mathbf{r}_1 - \mathbf{r}_2$.

In Eq. (1) the interaction is modeled via an *s*-wave pseudopotential with coupling constant $g = 4\pi\hbar^2 a/m$, where a is the scattering length in vacuum. The solution of Eq. (1) can be written, for $g \neq 0$, as

$$\Psi(\mathbf{r}, Z) = \int dZ' G_E(\mathbf{r}, Z; \mathbf{0}, Z')g\frac{\partial}{\partial r'}[r'\Psi(\mathbf{r}', Z')]_{\mathbf{r}'=0}, \quad (2)$$

where G_E is the free ($g = 0$) Green function associated with Eq. (1). At short distance, the Green function is determined only by the kinetic energy. Neglecting the external potential and setting $E = 0$ in Eq. (1), we find $G_{E=0}(\mathbf{r}, Z; \mathbf{0}, Z') = -(m/8\pi^2\hbar^2)[(Z - Z')^2 + (r/2)^2]^{-1}$. Therefore the Green function has the following expansion:

$$G_E(\mathbf{r}, Z; \mathbf{0}, Z') = -\frac{m}{4\pi\hbar^2 r}\delta(Z - Z') + K_E(Z, Z') + O(r),$$

(3)

where the regular kernel $K_E(Z, Z')$ depends on the external potential and we used the representation of the delta function $\delta(x) = \lim_{r\to 0} r/\pi(r^2 + x^2)$. When inserted into Eq. (2), Eq. implies, for $r \to 0$, the boundary condition $\Psi(\mathbf{r}, Z) \sim (1/r - 1/a)f(Z)$, where $f(Z)$ is a function of

the center of mass position satisfying the integral equation

$$\frac{1}{g}f(Z) = \int dZ' K_E(Z, Z')f(Z'). \quad (4)$$

If the center of mass and the relative motion decouple, the function $f(Z)$ must be an eigenstate of the center of mass Hamiltonian independent of the scattering length. By inserting it into Eq. (4), the dependence on Z factors out and we are left with an algebraic equation yielding the energy as a function of the scattering length. For instance, in the absence of the optical lattice the kernel is given by

$$K_E^0(Z, Z') = \frac{m}{4\pi\hbar^2}\int\frac{dP}{2\pi}e^{iP(Z-Z')}\sqrt{|E| + \hbar^2 P^2/4m}. \quad (5)$$

The lowest energy solution of Eqs. (4) and (5) corresponds to an $f(Z)$ constant and yields $E = -\hbar^2/ma^2$.

For periodic potentials, the kernel has the property $K_E(Z, Z') = K_E(Z + jd, Z' + jd)$, where j is any integer and d is the lattice spacing. This means that the general solution of Eq. (4) has the Bloch form $f(Z) = e^{iQZ}f_Q(Z)$, where $f_Q(Z)$ is a periodic function, Q being the quasimomentum of the molecule. In the following, we restrict our discussion to the lowest bound state given by Eq. (4).

Because of the singular term in Eq. (3), the numerical evaluation of the kernel $K_E(Z, Z')$ from the Green function G_E is not trivial. The latter can be written in the general form

$$G_E(\mathbf{r}, Z; \mathbf{0}, Z') = \sum_{n_1, n_2}\int\frac{d^2\mathbf{k}_\perp}{(2\pi)^2}\int_{-q_B}^{q_B}\frac{dq_1}{2\pi}\frac{dq_2}{2\pi}e^{i\mathbf{k}_\perp\cdot\mathbf{r}}$$
$$\times\frac{\phi_{n_1,q_1}(Z)\phi_{n_2,q_2}(Z)\phi_{n_1,q_1}^*(Z')\phi_{n_2,q_2}^*(Z')}{E - \epsilon_{n_1}(q_1) - \epsilon_{n_2}(q_2) - \hbar^2 k_\perp^2/m},$$
$$(6)$$

where $q_B = \pi/d$ is the Bragg wave vector and $\phi_{n,q}(z_1)$ are the eigenstates of $H_z = -(\hbar^2/2m)d^2/dz_1^2 + V_{opt}(z_1)$ with energies $\epsilon_n(q)$. In the following, the periodic potential will be taken of the form

$$V_{opt}(z_1) = sE_R\sin^2\left(\frac{\pi z_1}{d}\right), \quad (7)$$

as usually provided by two counterpropagating laser beams (optical lattices), where s is the laser intensity, the spacing d being related to the wavelength of the laser fields, and $E_R = \hbar^2\pi^2/2md^2$ is the recoil energy. Since the singular term on the right-hand side of Eq. (3) does not depend on the external potential, we add and substract from G_E the Green function (6) evaluated for $s = 0$. This permits us to write the kernel as $K_E(Z, Z') = \lim_{r\to 0}[G_E(\mathbf{r}, Z; \mathbf{0}, Z') - G_E^0(\mathbf{r}, Z; \mathbf{0}, Z')] + K_E^0(Z, Z')$, with K_E^0 defined in Eq. (5). After these manipulations, the integration over $\mathbf{k}_\perp$ in Eq. (6) converges and can be performed analytically. The remaining summation over band indices and the integration over quasimomentum are done numerically.

We define the binding energy as $E_b(Q) = E(Q) - E_{ref}(Q)$, where $E_{ref}(Q) = 2\epsilon_1(Q/2)$ is the lowest energy state for two noninteracting particles with total quasimomentum Q and ϵ_1 is the dispersion of the lowest Bloch band. With this notation, E_b is always negative for a bound state.

We first discuss the case of zero quasimomentum ($Q = 0$). The binding energy as a function of the inverse scattering length is shown in Fig. 1 for different values of the laser intensity. One can identify three different regimes: the regime of tightly bound molecules for small positive scattering length, an intermediate quasi-2D regime which emerges for large scattering length when the laser intensity is raised, and finally an anisotropic 3D regime occurring at small negative scattering length down to a critical value. We discuss the three regimes separately.

When the binding energy is large with respect to the depth of the lattice ($h^2/ma^2 \gg sE_R$), the periodic potential (7) can be treated as a perturbation and the wave function takes the form $\Psi(\mathbf{r}, Z) = \varphi(Z)\phi_b(r)$, with $\phi_b(r) = (1/\sqrt{2\pi a})e^{-r/a}/r$. Within first order perturbation theory, the effective potential acting on the center of mass of the molecule is given by $U_{eff}(Z) = \int \phi_b^2(r)V(Z, z)d^3\mathbf{r}$, yielding

$$U_{eff}(Z) = sE_R - sE_R\frac{2}{aq_B}\arctan\left(\frac{aq_B}{2}\right)\cos(2q_BZ). \quad (8)$$

We see that the potential (8) depends on the value of the scattering length, unless $aq_B \ll 1$, where $U_{eff}(Z) = 2V_{opt}(Z)$. The binding energy is then given by $E_b = -\hbar^2/ma^2 + E'$, with E' solution of the Schrödinger equation

$$\left[-\frac{\hbar^2}{4m}\nabla_z^2 + U_{eff}(Z)\right]\varphi(Z) = E'\varphi(Z). \quad (9)$$

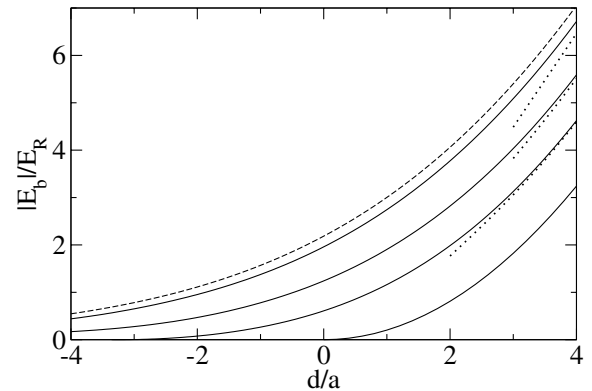The asymptotic behavior based in Eqs. (8) and (9) is

FIG. 1. Binding energy versus inverse scattering length for different values of the laser intensity: from top to bottom, $s = 20, 10, 5, 0$ (solid line). Also shown are the asymptotic behavior for large d/a (dotted line) and the binding energy in harmonic approximation (dashed line) for $s = 20$.

plotted in Fig. 1, with the dotted line for different values of s.

Moving towards the Feshbach resonance and for sufficiently deep lattices, the molecule enters a quasi-2D regime. The two interacting atoms are localized at the bottom of the same optical well, where, to a first approximation, the potential (7) is harmonic with frequency $\omega_0 = 2\sqrt{s}E_R/\hbar$. In this case, the center of mass and the relative motion decouple and the scattering problem can be solved analytically [9,10]. The corresponding result for the binding energy as a function of the inverse scattering length is shown in Fig. 1 for $s = 20$ (dashed line). The interval of values d/a characterizing the 2D regime around resonance ($d/a = 0$) becomes wider and wider as the laser intensity increases.

Finally, for negative and small scattering length, the binding energy is smaller than the atomic bandwidth and the bound state wave function is delocalized over many lattice sites. In this anisotropic 3D regime, the binding energy as a function of the scattering length takes the universal form $1/a - 1/a_{\rm cr} = C\sqrt{|E_b|m^*}/\hbar$, where $a = a_{\rm cr}$ is a function of the laser intensity and corresponds to the critical value of the scattering length needed to form a bound state (see Fig. 2, left panel). Here m^* is the atomic effective mass and $C = C(s)$ is a dimensionless function of the laser intensity. For $s = 0$ one has $C = 1$, while in tight binding limit one finds $C = d/\sqrt{2\pi}\sigma$, where σ is the width of the variational Gaussian ansatz $w(z) = \exp(-z^2/2\sigma^2)/\pi^{1/4}\sigma^{1/2}$ for the Bloch function $\phi_{1,q}(z) \sim \Sigma_\ell e^{iq\ell d}w(z - \ell d)$ [11]. The above result shows that the optical lattice gives rise to an effective shift of the resonance, in analogy with the case of a 3D tight lattice investigated in Ref. [8].

It is interesting to discuss explicitly the behavior of the binding energy at resonance ($1/a = 0$) as a function of the laser intensity. The numerical result is shown in the right panel of Fig. 2 (solid line). For large s the harmonic approximation characterizing the quasi-2D regime gives [9,10] $E_b^{\rm ho}(1/a = 0) = -0.244\hbar\omega_0 = -0.488\sqrt{s}E_R$ (dashed line). The remaining shift ΔE in the binding energy is due to the nonharmonic terms. We have found that the inclusion of such corrections via first order perturbation theory results in an s-independent shift $\Delta E = 0.198E_R$, which well reproduces the full numerical result for $s \gtrsim 10$ (see dots in Fig. 2).

Let us now discuss the solutions of Eq. (4) with finite quasimomentum Q. The dependence of the binding energy on Q is plotted in Fig. 3 for $s = 2.5$ and different values of the scattering length. We see that the modulus of the binding energy increases when Q increases and the effect is more pronounced for a small positive scattering length, where the molecules are tightly bound. An immediate consequence of the above result is that the critical value of the scattering length also depends on quasimomentum. This is illustrated in Fig. 2 where we have also plotted $d/a_{\rm cr}$ for $Q = q_B$ (dashed line).

Another important consequence of the dependence of the binding energy on quasimomentum concerns the tunneling properties of the molecule which acquire a strong dependence on the scattering length. The molecular bandwidth $w = E(q_B) - E(0)$ is plotted in Fig. 4 (left panel) as a function of d/a for $s = 2.5$. We see that w decreases as d/a increases. This can be understood by writing $w = E_b(a, q_B) - E_b(a, 0) + 2\epsilon_1(q_B/2)$, where $E_b(a, Q)$ is the binding energy as a function of scattering length and quasimomentum (see Fig. 3). Furthermore, the bandwidth for molecules is always *smaller* than the one for single atoms because $2\epsilon_1(q_B/2) < \epsilon_1(q_B) = w_{\rm at}$. For instance, for $s = 2.5$ the width of the lowest band for atoms is $w_{\rm at} = 0.52E_R$.
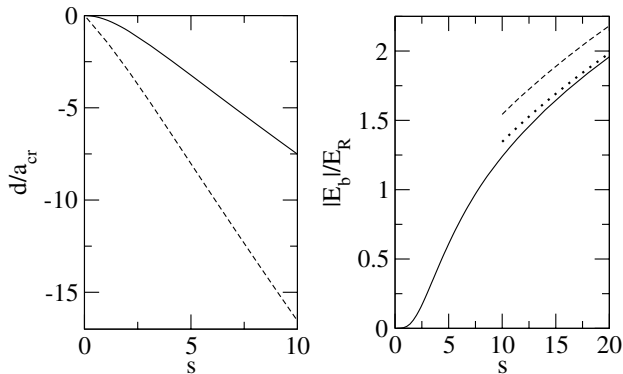

FIG. 2. Left panel: Critical value of the inverse scattering length as a function of the laser intensity for different values of quasimomentum: $Q = 0$ (solid line) and $Q = q_B$ (dashed line). Right panel: Binding energy at unitarity ($d/a = 0$) as a function of the laser intensity (solid line). Also shown are the harmonic approximation (dashed line) and the inclusion of anharmonic corrections (dots).
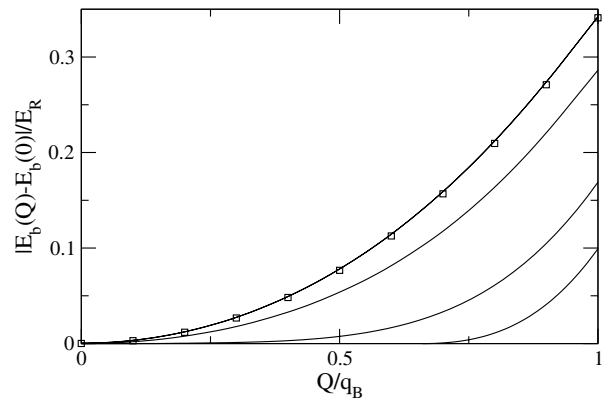

FIG. 3. Binding energy dispersion as a function of quasimomentum Q for fixed $s = 2.5$ and for different values of the inverse scattering length: from top to bottom, $d/a = 2, 0, -1.17 (= d/a_{\rm cr}), -1.66$. The open squares give the dispersion at $d/a = 2$ evaluated from Eqs. (8) and (9).

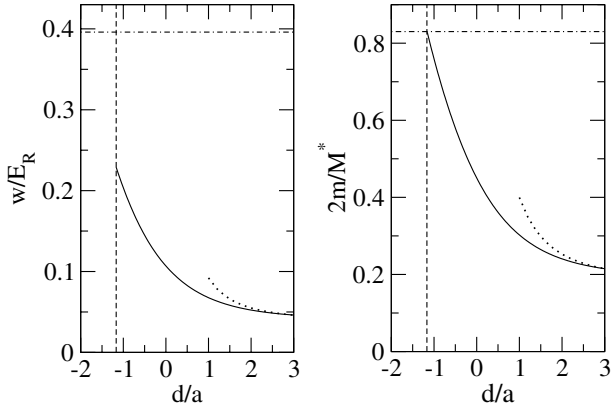P H Y S I C A L   R E V I E W   L E T T E R S

FIG. 4. Bandwidth (left panel) and effective mass ratio $2m/M^*$ (right panel) of the molecule as a function of the inverse scattering length for $s = 2.5$ (solid line). The asymptotic behavior for large positive d/a is also shown (dotted line). In the left panel the dot-dashed line indicates $2\epsilon_1(q_B/2) = 0.395E_R$, while in the right panel it indicates the effective atomic mass ratio $m/m^* = 0.83$.

In the right panel of Fig. 4 we show the result for the effective mass of molecules, defined via $1/M^* = (\partial^2 E(Q)/\partial Q^2)_{|Q=0}$, for the same value of the laser intensity. We see that, in complete analogy with the bandwidth, the ratio $2m/M^*$ decreases as d/a increases. This can be understood from the fact that, for larger d/a, the motion of the two atoms is more correlated and the molecule becomes heavier. Notice that at the critical point where the two atoms are no longer bound one finds $M^* = 2m^*$.

In the last part of the Letter, we discuss the relevance of our results for current experiments with ultracold atomic gases. The binding energy of molecules can be directly measured by rf spectroscopy [12], whereas the tunneling properties and M^* can be investigated through the observation of Bloch oscillations [13]. The gas should be sufficiently dilute in order to neglect many-body effects. This occurs when the size of the molecules is smaller than their mean separation distance or, equivalently [14], when $|E_b| > \hbar^2(n/2)^{2/3}/m$, where n is the atomic density. Using a sample of ^{6}Li, a lattice spacing of $d = 500$ nm, corresponding to $E_R = 200$ kHz, and choosing $n \sim 10^{12}$ cm^{-3}, we find that the diluteness condition corresponds to requiring $|E_b|/E_R > 0.03$. This condition is not very severe and allows one to access to the different regimes discussed above (see Fig. 1) by tuning the laser intensity and the scattering length. It should be also noticed that the atomic

bandwidth decreases fast with the laser intensity, so the 3D regime can only be investigated working with relatively low values of the laser intensity $s \sim 2.5$–5.

In conclusion, we have investigated the properties of the bound state formed by two atoms interacting via a short range potential near a Feshbach resonance, in the presence of a 1D periodic potential, for *arbitrary* values of laser intensity, scattering length and quasimomentum of the molecule. We have shown that the nonseparability of center of mass and relative motion has important consequences on the tunneling properties of the molecule, which become strongly dependent on the value of the scattering length. Our results could have important consequences for the many-body properties of these systems near a Feshbach resonance.

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