# Two-body problem in periodic potentials

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We investigate the problem of two atoms interacting via a short range *s*-wave potential in the presence of a deep optical lattice of arbitrary dimension *D*. Using a tight-binding approach, we derive analytical results for the properties of the bound state and the scattering amplitude. We show that the tunneling through the barriers induces a dimensional crossover from a confined regime at high energy to an anisotropic three-dimensional regime at low energy. The critical value of the scattering length needed to form a two-body bound state shows a logaritmic dependence on the tunneling rate for $D=1$ and a power law for $D>1$. For the special case $D=1$, we also compare our analytical predictions with exact numerics, finding remarkably good agreement.

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## I. INTRODUCTION

Recent progress in controlling and manipulating the interatomic forces via Feshbach resonances [1] and the availability of tunable periodic potentials generated by laser beams [2] are opening new fronts in the research on ultracold atomic gases. An important field of activities concerns the study of two-body physics in the presence of an external potential. This two-body problem is directly related to current experiments, and moreover, it forms a basic step toward understanding many-body states where strong correlations can play a significant role.

From the experimental point of view, a major achievement has been the formation of weakly bound diatomic molecules in experiments with two-component clouds of fermionic atoms [3–6]. Recently, also the binding energy of confinement induced molecules has been measured by the group of Esslinger [7] working with samples of potassium $^{40}$K in a deep two-dimensional optical lattice.

From the theoretical front, the two-body problem in the presence of harmonic trapping, has been solved analytically both for *s*-wave [8–12] and higher partial wave short range interactions [13–15]. The case of a periodic external potential is even more interesting as the center of mass and the relative motion no longer decouple [16,17]. This gives rise to an interesting interplay between tunneling and confinement effects.

The properties of the bound state of two interacting atoms in the presence of a one-dimensional optical lattice have been investigated *numerically* in Ref. [15]. For sufficiently deep lattices and binding energy $E_b$, which is small compared to the interband gap, two different regimes were identified: (i) a quasi-*two*-dimensional regime for $|E_b| \gg t$, $t$ being the interwell tunneling rate, where the molecular wave function is localized in one well and (ii) an anisotropic *three*-dimensional regime for $|E_b| \ll t$, where the wave function spreads over many lattice sites [18]. An analogous dimensional crossover occurs for the scattering amplitude as the total energy of the two incident states becomes large compared to the tunneling rate [19].

In this work, we apply the tight-binding approach introduced in Ref. [19] to study analytically the properties of the bound state and the scattering amplitude of two interacting atoms in the presence of a *D*-dimensional tight optical lattice. We derive simple, yet accurate predictions for many quantities that can be directly measured in current experiments with dilute ultracold gases.

The paper is organized as follows. In Sec. II, we present the general theory to solve the two-body problem in the presence of a periodic potential. In Sec. III, we apply the tight binding approach to the case $D=1$ and we extensively compare our analytical results with the exact numerics of Ref. [15]. In Sec. IV, we extend our analysis to the case of optical lattices of higher $(D=2,3)$ dimensions.

## II. GENERAL THEORY

We consider two atoms in ordinary space interacting in the presence of a *D*-dimensional periodic potential

$$V_{opt}(\mathbf{x}) = sE_R \sum_{i=1}^{D} \sin^2\left(\frac{\pi x_i}{d}\right), \tag{1}$$

where $D=1,2,3$. Here $s$ is the intensity of the laser beams generating the optical lattice, $E_R=\hbar^2\pi^2/2md^2$ is the recoil energy, $d$ is the lattice period, and $m$ the atom mass. There is no confinement in the remaining 3-*D* directions.

Modeling the interatomic interaction by a *s*-wave pseudopotential with coupling constant $g=4\pi\hbar^2 a/m$, with $a$ as the three-dimensional (3D) scattering length, the Schrödinger equation takes the form

$$\left(-\frac{\hbar^2}{m}\nabla_{\mathbf{r}}^2 - \frac{\hbar^2}{4m}\nabla_{\mathbf{R}}^2 + V(\mathbf{R},\mathbf{r}_\parallel) + g\,\delta(\mathbf{r})\frac{\partial}{\partial r}r\right)\Psi = E\Psi, \tag{2}$$

where $\mathbf{r}=\mathbf{x}_1-\mathbf{x}_2$ is the relative distance between the two atoms, $\mathbf{R}$ and $\mathbf{r}_\parallel$ are the components of the center of mass and the relative coordinates in the confined directions and $V(\mathbf{R},\mathbf{r}_\parallel)=V_{opt}(\mathbf{x}_1)+V_{opt}(\mathbf{x}_2)$ is the total external field.

With respect to the case of harmonic trapping, the periodic field introduces a conceptually new difficulty related to the fact that the center of mass and the relative motion no longer separate. Nevertheless, the quasimomentum $\mathbf{Q}$, asso-

 

ciated to the center of mass variable $\mathbf{R}$, remains a conserved quantity even in the presence of interaction and can be used to classify the solutions of Eq. (2). This can be seen by noticing that Eq. (2) is invariant under the transformation

$$\mathbf{R} \to \mathbf{R} + \mathbf{G}, \tag{3}$$

$$\mathbf{r} \to \mathbf{r}, \tag{4}$$

which shifts the center of mass of the two atoms by a lattice vector $\mathbf{G}$ leaving unchanged their relative distance.

### A. Bound state

Bound states are solutions of Eq. (2) whose energy $E$ does not belong to the energy spectrum in the absence of interaction. In this case, Eq. (2) can be written in the integral form

$$\Psi(\mathbf{r},\mathbf{R}) = \int d\mathbf{R}' G_E(\mathbf{r},\mathbf{R};\mathbf{0},\mathbf{R}') g \frac{\partial}{\partial r'}[r'\Psi(\mathbf{r}',\mathbf{R}')]_{\mathbf{r}'=0}, \tag{5}$$

where $G_E$ is the Green's function associated to Eq. (2) with $g=0$. The behavior of the Green's function at a short distance is dominated by the kinetic term in Eq. (2). Taking into account that for small $r$

$$\int \frac{e^{i\mathbf{Q}(\mathbf{R}-\mathbf{R}')} e^{i\mathbf{k}\cdot\mathbf{r}}}{\hbar^2 k^2/m + \hbar^2 Q^2/4m} \frac{d^3\mathbf{k}}{(2\pi)^3} \frac{d^D\mathbf{Q}}{(2\pi)^D} = \frac{m}{4\pi\hbar^2 r} \int e^{i\mathbf{Q}(\mathbf{R}-\mathbf{R}')} \frac{d^D\mathbf{Q}}{(2\pi)^D}, \tag{6}$$

the Green's function admits the following expansion

$$G_E(\mathbf{r},\mathbf{R};\mathbf{0},\mathbf{R}') = -\frac{m}{4\pi\hbar^2 r}\delta^D(\mathbf{R}-\mathbf{R}') + K_E(\mathbf{R},\mathbf{R}') + O(r), \tag{7}$$

where $K_E(\mathbf{R},\mathbf{R}')$ is a regular kernel which depends on the energy and the external potential.

When inserted into Eq. (5), Eq. (7) yields the Bethe-Peierls boundary condition $\Psi(\mathbf{r},\mathbf{R}) \sim (a/r-1)f(\mathbf{R})$ for $r \to 0$, where $f(\mathbf{R})$ is a function of the center of mass position satisfying the integral equation

$$\frac{1}{g} f(\mathbf{R}) = \int d\mathbf{R}' K_E(\mathbf{R},\mathbf{R}') f(\mathbf{R}'). \tag{8}$$

The solution of Eq. (8) yields the energy $E$ as a function of the 3D scattering length $a$.

Two comments are in order here. First, the integral equation (8) is completely general and is valid for any external potential. In the special case of harmonic trapping, $f(\mathbf{R})$ is also an eigenstate of the center of mass Hamiltonian and Eq. (7) reduces to a simpler *algebraic* equation. Second, the conservation of quasimomentum in periodic potentials is ensured by the symmetry property $K_E(\mathbf{R},\mathbf{R}') = K_E(\mathbf{R}+\mathbf{G},\mathbf{R}'+\mathbf{G})$ of the kernel, holding for any lattice vector $\mathbf{G}$.

In the following, we are mainly interested in the weakly bound state whose energy $E$ is below the minimum $E_{ref}$ of the noninteracting energy spectrum [20]. For a given quasimomentum $\mathbf{Q}$, the lowest energy solution of Eq. (2) for $g=0$ corresponds to the case where both atoms occupy the state of quasimomentum $\mathbf{Q}/2$ in the lowest Bloch band, that is $E_{ref}(\mathbf{Q}) = 2\epsilon_1(\mathbf{Q}/2)$. We define the binding energy of the molecule as $E_b \equiv E - E_{ref} < 0$.

A direct consequence of the nonseparability of the center of mass and the relative motion in the lattice is that the binding energy becomes a function of the quasimomentum of the molecule, or, the other way around, the tunneling properties of the molecule (strongly) depend on the value of the scattering length. A second important difference from the case of harmonic trapping is that, in the lattice, Eq. (8) predicts a *finite* critical value of the scattering length $a = a_{cr} < 0$, such that no bound state exists for $a_{cr} < a < 0$. Notice that in free space ($s=0$), a bound state exists only for positive value of the scattering length, i.e., $a_{cr} = -\infty$.

### B. Scattering amplitude

Let us consider a noninteracting two-particle state $\Psi_0(\mathbf{r},\mathbf{R}) = \phi_{\mathbf{n}_1,\mathbf{q}_1}(\mathbf{r}_1)\phi_{\mathbf{n}_2,\mathbf{q}_2}(\mathbf{r}_2)e^{i\mathbf{k}_\perp\cdot\mathbf{r}_\perp}$, where $\phi_{\mathbf{n},\mathbf{q}}(\mathbf{x}) = \Pi_{j=1}^D u_{n_j,q_j}(\mathbf{x})$. Here $u_{n,q}(z)$ are the solutions of the one-dimensional Hamiltonian $H = -(\hbar^2/2m)d^2/dz^2 + V_{opt}(z)$ with energy $\varepsilon_n(q)$, with $n$ the band index and $q$ the quasimomentum. A quantity of great physical interest is the scattering amplitude associated to $\Psi_0$, the incident state. In the presence of the lattice, we *define* it as

$$f_{sc}[\Psi_0] = a \int \Psi_0^*(0,\mathbf{R}) \partial_r [r\Psi(\mathbf{r},\mathbf{R})]_{r=0} d\mathbf{R}, \tag{9}$$

where $a$ is the 3D scattering length and $\Psi(\mathbf{r},\mathbf{R})$ is the solution of Eq. (2), which can be written as

$$\Psi(\mathbf{r},\mathbf{R}) = \Psi_0(\mathbf{r},\mathbf{R}) + \int d\mathbf{R}' G_{E+i0}(\mathbf{r},\mathbf{R};\mathbf{0},\mathbf{R}') g \frac{\partial}{\partial r'}[r'\Psi(\mathbf{r}',\mathbf{R}')]_{\mathbf{r}'=0}. \tag{10}$$

Here $G_{E+i0}$ is the *retarded* Green's function evaluated at the energy $E = \epsilon_{\mathbf{n}_1}(\mathbf{q}_1) + \epsilon_{\mathbf{n}_2}(\mathbf{q}_2) + \hbar^2 k_\perp^2/m$ of the incident state and $\epsilon_{\mathbf{n}}(\mathbf{q}) = \Sigma_{j=1}^D \epsilon_{n_j}(q_j)$. Introducing $f(\mathbf{R}) = \partial_r[r\Psi(\mathbf{r},\mathbf{R})]_{r=0}$ and making use of the expansion (7) in Eq. (10), we find the *inhomogeneous* integral equation

$$f(\mathbf{R}) = \Psi_0(\mathbf{R},\mathbf{0}) + g \int d\mathbf{R}' K_{E+i0}(\mathbf{R},\mathbf{R}') f(\mathbf{R}'), \tag{11}$$

which has to be solved to find the scattering amplitude (9). The comments below Eq. (8) apply here as well.

### C. Numerical and tight-binding solution

Equations (8) and (11) can be solved numerically following the method developed in Ref. [15] for the case of a one-dimensional (1D) optical lattice. In order to extract the regular kernel $K_E$ from the Green's function, the latter is expanded in the basis of the noninteracting states

$$G_E(\mathbf{r},\mathbf{R};\mathbf{0},\mathbf{R}') = \sum_{\mathbf{n}_1,\mathbf{n}_2} \int \frac{d^{3-D}\mathbf{k}_\perp}{(2\pi)^{3-D}} \int_{-q_B}^{q_B} \frac{d^D\mathbf{q}_1}{(2\pi)^D} \frac{d^D\mathbf{q}_2}{(2\pi)^D} e^{i\mathbf{k}_\perp\cdot\mathbf{r}_\perp} \times \frac{\phi_{\mathbf{n}_1,\mathbf{q}_1}\left(\mathbf{R}+\frac{\mathbf{r}_\parallel}{2}\right)\phi_{\mathbf{n}_2,\mathbf{q}_2}\left(\mathbf{R}-\frac{\mathbf{r}_\parallel}{2}\right)\phi^*_{\mathbf{n}_1,\mathbf{q}_1}(\mathbf{R}')\phi^*_{\mathbf{n}_2,\mathbf{q}_2}(\mathbf{R}')}{E-\epsilon_{\mathbf{n}_1}(\mathbf{q}_1)-\epsilon_{\mathbf{n}_2}(\mathbf{q}_2)-\hbar^2k_\perp^2/m}. \tag{12}$$

Since the singular term in the right-hand side (rhs) of Eq. (7) does not depend on the external potential, we add and substract from $G_E$, the Green's function (12) evaluated for $s=0$. This permits us to write the kernel as $K_E(\mathbf{R},\mathbf{R}') = \lim_{r\to 0}[G_E(\mathbf{r},\mathbf{R};\mathbf{0},\mathbf{R}') - G_E^{s=0}(\mathbf{r},\mathbf{R};\mathbf{0},\mathbf{R}')] + K_E^{s=0}(\mathbf{R},\mathbf{R}')$, where the latter is given by

$$K_E^{s=0}(\mathbf{R},\mathbf{R}') = \frac{m}{4\pi\hbar^2}\int \frac{d\mathbf{P}}{(2\pi)^D} e^{i\mathbf{P}(\mathbf{R}-\mathbf{R}')}\sqrt{|E|+\hbar^2P^2/4m}. \tag{13}$$

The term in square brackets is evaluated numerically from Eq. (12). Once the kernel $K_E$ is known, Eqs. (8) and (11) can be solved using standard diagonalization routines. This numerical method has been applied in Ref. [15] for the case $D=1$. It should be noticed that for $D>1$ the numerical effort needed to solve Eqs. (8) and (11), using the above method, grows considerably.

In this paper, we restrict ourselves to the case of sufficiently deep lattices and energy $E$ small compared to the interband gap $\epsilon_g$. In this limit, the energy dependence of the Green's function in Eq. (12) comes *entirely* from the lowest Bloch band and the two-body problem can be solved perturbatively using a tight-binding approach pioneered in Ref. [19].

## III. ONE-DIMENSIONAL LATTICE

Below, we discuss in detail the case of a one-dimensional optical lattice ($D=1$) by comparing our analytical predictions with the exact numerics of Ref. [15].

### A. Bound State

We start our analysis by noticing that for $D=1$ the integration over $\mathbf{k}_\perp$ in Eq. (12) is ultraviolet divergent for $\mathbf{r}_\perp \to 0$. Taking into account that the singular term in the rhs of Eq. (7) does not depend on energy, we can write identically

$$K_E(Z,Z') = [G_E(\mathbf{r},Z;\mathbf{0},Z') - G_{E=E_{ref}}(\mathbf{r},Z;\mathbf{0},Z')]_{r=0} + K_{E=E_{ref}}(Z,Z'). \tag{14}$$

We consider first the term between square brackets which contains the energy dependent part of the kernel. The integration over $\mathbf{k}_\perp$ in Eq. (12) converges even for $\mathbf{r}_\perp=0$. Moreover, for energy $E$ small compared to the interband gap, only the lowest band $n_1=n_2=1$ contributes significantly. For sufficiently large values of the laser intensity, the states of the lowest Bloch band can be written in terms of Wannier functions as $\phi_{1q_z}(z) \sim \Sigma_\ell e^{i\ell q_z d} w(z-\ell d)$, where

$$w(z) = \frac{1}{\pi^{1/4}\sigma^{1/2}} \exp\left(-\frac{z^2}{2\sigma^2}\right) \tag{15}$$

is a variational Gaussian ansatz. By minimizing the energy $\int dz w(z)[-(\hbar^2/2m)d^2/dz^2 + V_{opt}(z)]w(z)$ with respect to $\sigma$, one finds $d/\sigma \simeq \pi s^{1/4}\exp(-1/4\sqrt{s})$.

Substituting the tight-binding expression for the Bloch states in Eq. (12), we immediately see that the term in square brackets is diagonalized by the ansatz

$$f_Q(Z) \sim \sum_\ell w^2(Z-\ell d)e^{iQZ}, \tag{16}$$

where $Q$ is the quasimomentum of the molecule. Motivated by this fact, we have verified numerically that the ansatz (16) is a solution of Eq. (8) with $E=E_{ref}$, that is

$$\int dZ' K_{E=E_{ref}}(Z,Z')f_Q(Z')dZ' = f_Q(Z)m/4\pi\hbar^2 a_{cr}, \tag{17}$$

where $a_{cr}=a_{cr}(Q)$ is the critical value of the scattering length needed to form a two-body bound state with quasimomentum $Q$. The ratio $d/a_{cr}$ as a function of the laser intensity has been evaluated numerically in Ref. [15], and in Ref. [19], an analytical estimate was derived for the special case $Q=0$.

By inserting the ansatz (16) into Eq. (8) and integrating over $Z'$, we obtain

$$\left(\frac{1}{a}-\frac{1}{a_{cr}}\right)\sqrt{2\pi}\sigma = -\alpha_{1D}(E_b,Q), \tag{18}$$

where

$$\alpha_{1D}(E_b,Q) = -\int_{-\pi}^{\pi}\frac{dq}{2\pi} \times \ln\left[\frac{-E_b-2\epsilon_1(Q/2)+\epsilon_1(q)+\epsilon_1(Q-q)}{\epsilon_1(q)+\epsilon_1(Q-q)}\right], \tag{19}$$

and we have used the definition of binding energy $E_b \equiv E - 2\epsilon_1(Q/2)$. Equations (18) and (19) give $E_b$ as a function of the quasimomentum $Q$, the scattering length $a$, and the lattice parameters.

Let us first discuss the case of zero quasimomentum. By substituting the tight-binding dispersion $\epsilon_1(q)=2t[1-\cos(qd)]$ in Eq. (19) and integrating over $q$, we obtain

$$\alpha_{1D}(E_b,0) = \ln\left(1+\frac{|E_b|}{4t}+\sqrt{\frac{|E_b|}{2t}+\left(\frac{E_b}{4t}\right)^2}\right). \tag{20}$$

Equation (20) describes the dimensional crossover in the binding energy as the ratio $|E_b|/4t$ is varied. The three-dimensional regime $|E_b| \ll 4t$ is characterized by a molecular wave function extended over many lattice sites. Expanding Eq. (20) around $E_b=0$ and inserting it into Eq. (18), we find

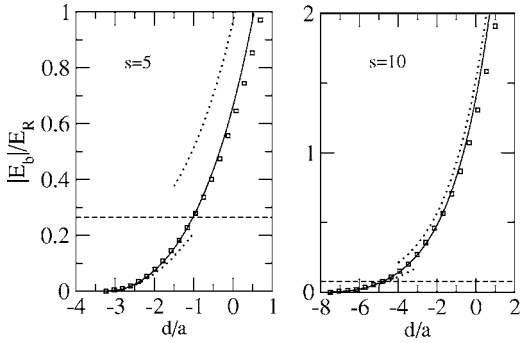


FIG. 1. Binding energy as a function of the inverse scattering length for different values of the laser intensity: the analytical prediction (solid line) is compared with the exact numerical data (squares). Also shown are the position of the bandwidth (dashed line) and the asymptotic behaviors for the binding energy (dotted lines) in the two regimes [see Eqs. (21) and (22)].

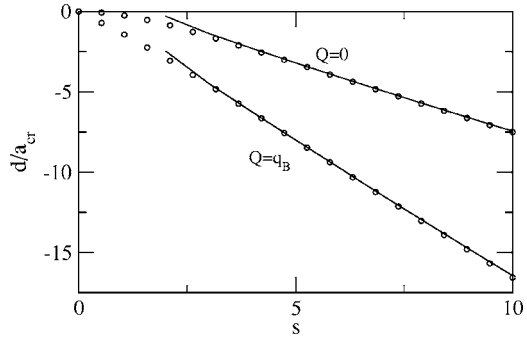


FIG. 2. Critical value of the inverse scattering length as a function of the laser intensity for quasimomentum $Q=0$ and $Q=q_B$. The analytical prediction (solid line) is shown with the exact numerical data (circles).

$$1/a - 1/a_{cr} = C\sqrt{|E_b|m^*}/\hbar, \tag{21}$$

where $m^* = \hbar^2/2td^2$ is the atomic effective mass evaluated at the bottom of the band and $C = d/\sqrt{2\pi}\sigma$. The above result shows that the optical lattice gives rise to an effective shift of the resonance from $1/a=0$ to $1/a=1/a_{cr}<0$. In the quasi-two-dimensional (2D) regime $4t \ll |E_b| \ll \epsilon_g$, the two interacting atoms are localized at the bottom of the same optical well, where, to a first approximation, the potential (1) is harmonic with frequency $\omega_0 = \hbar/m\sigma^2$. In this case, the center of mass and the relative motion decouple and the problem can been solved analytically. In the relevant limit $|E_b| \ll \omega_0 \sim \epsilon_g$, the binding energy is given by

$$E_b^{ho} = -\lambda\hbar\omega_0 \exp(-\sqrt{2\pi}\sigma/|a|) \tag{22}$$

with $\lambda = 0.915/\pi$ [10]. In Fig. 1, we plot the binding energy versus inverse scattering length derived from Eqs. (18) and (20) for different values of the laser intensity (the value of the parameter $d/a_{cr}$ has been taken from Ref. [15]). We find that the analytical predictions (solid line) are in perfect agreement with the numerical data (squares) provided the binding energy is small compared to the interband gap. This condition is no longer satisfied approaching the resonance from the negative side, so our method is accurate only for scattering length $a<0$.

Interestingly enough, the fact that $E_b \simeq E_b^{ho}$ for $E_b \gg 4t$ can be used to derive an analytical expression for the critical scattering length [21]. By substituting the expansion $\alpha_{1D}(E_b,0) \simeq -\ln(|E_b|/2t)$ in Eq. (18) with $E_b$ given by Eq. (22), we find [19]

$$\frac{d}{a_{cr}}(Q=0) = -\frac{d}{\sqrt{2\pi}\sigma}\ln\left(\frac{\lambda\hbar\omega_0}{2t}\right). \tag{23}$$

This is plotted in Fig. 2 as a function of the laser intensity (solid line) together with the numerical results of Ref. [15] (circles). We see that the agreement is excellent already at relatively low values of the laser intensity. The approximate linear behavior as a function of $s$ shown in Fig. 2 is due to the logarithmic dependence of the ratio (23) on the tunneling rate $t$ and is a specific feature of the case $D=1$. It is worth pointing out that a good estimate of $a_{cr}$ can be obtained by the following physical argument. In the presence of a deep lattice, the binding energy is basically given by Eq. (22) provided $|E_b| \gg 4t$. The tunneling effects that cause the molecule to break become important when the binding energy (in modulus) is of the order of the bandwidth $4t$ or smaller. This suggests that the critical scattering length $a=a_{cr}$ can be estimated from Eq. (22) by setting $-E_b^{ho} \simeq 4t$. This reproduces the result (23) in the limit $t \ll \hbar\omega_0$.

The effective mass $M^*$ of the molecule is defined as $\hbar^2/M^* = \partial^2 E(Q)/\partial Q^2$ evaluated at $Q=0$. From Eqs. (18) and (19), after some algebra, we obtain

$$\frac{2m^*}{M^*} = 1 + \frac{|E_b|}{4t} - \sqrt{\left(\frac{E_b}{4t}\right)^2 + \frac{|E_b|}{2t}}. \tag{24}$$

where $E_b = E_b(0)$ and $m^*$ is the effective mass for single atoms. We see that in the anisotropic three-dimensional regime, the mass ratio $2m^*/M^* = 1$ for $E_b = 0$ and decreases as $-E_b$ increases. In the quasi-two-dimensional regime, $-E_b \gg 4t$, Eq. (24) yields $2m^*/M^* = 2t/|E_b| \ll 1$, showing that the correlation between the two atoms results in an increased inertia of the molecule. The mass ratio (24) is plotted in Fig. 3 against the inverse scattering length for $s=5$ together with the exact numerical result (dots). We emphasize that the de-

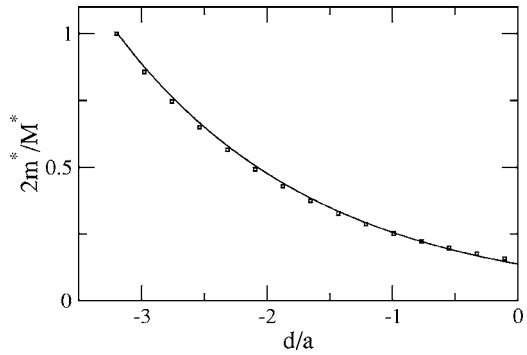


FIG. 3. The inverse effective mass of the molecule as a function of the inverse scattering length for $s=5$: analytical prediction (solid line) and exact numerical data (squares).

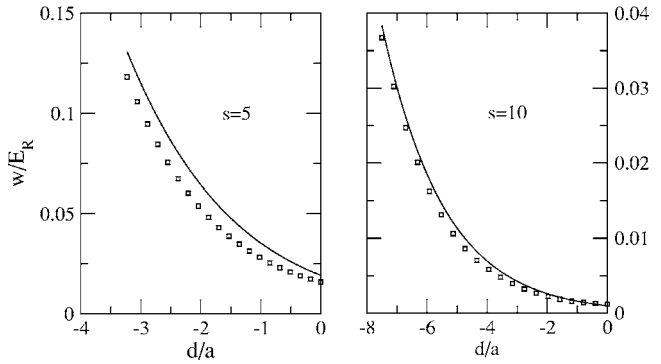


FIG. 4. Molecular bandwidth as a function of the inverse scattering length for different values of the laser intensity: analytical prediction (solid line) and exact numerical data (squares). The atomic bandwidth is $w_{at}=0.264E_R$ for $s=5$ and $w_{at}=0.077E_R$ for $s=10$.

pendence of the effective mass of the molecule on the value of the scattering length is a clear consequence of the nonseparability of the center of mass and the relative motion in the lattice.

Let us now discuss the solution of Eq. (8) corresponding to finite value of the quasimomentum $Q$. The binding energy $E_b(Q)$ can be obtained from Eqs. (18) and (19) provided the critical scattering length $a_{cr}(Q)$ is known. This quantity can be easily calculated by noticing that in the quasi-two-dimensional limit, $|E_b(Q)| \gg 4t$, to lowest order in tunneling, the binding energy does not depend on the center of mass motion and, therefore, $E_b(Q)=E_b(0)=E_b^{ho}$. We have found that for $Q \simeq q_B$ the use of the tight-binding dispersion $\epsilon_1(q)=2t[1-\cos(qd)]$ in Eq. (19) gives inaccurate results. This dispersion relation predicts indeed a continuous degeneracy for the lowest energy state with quasimomentum $Q=q_B$ of the two atoms in the absence of interaction. As a result, the integration over quasimomentum in Eq. (19) is divergent at this point. This artifact can be easily eliminated by using the numerically exact dispersion or by including higher harmonics. With this important remark, the calculated critical value of the scattering length for $Q=q_B$ agrees fairly well with numerics, see Fig. 2.

Another quantity of physical interest is the molecular bandwidth $w=E(Q=q_B)-E(0)$. Within our notation, the latter can be written as $w=E_{ref}(q_B)+E_b(q_B)-E_b(0)$. This is plotted in Fig. 4 as a function of the inverse scattering length. Similar to the effective mass, the bandwith decreases as $d/a$ increases. However, for $s=5$ (left panel) there is a discrepancy between the analytical prediction and the numerical result which was not found in Fig. 3. This is due to the fact that the interband gap is smaller at the edge of the Brillouin zone and there is a residual contribution to $E_b(q_B)$ coming from higher bands. This effect disappears when $s$ is increased so that for $s=10$, good agreement with the numerical results is obtained (right pannel). Notice that the molecular bandwidth is always smaller than the atomic bandwidth $w_{at}$. This can be seen from the fact that $E_b(q_B)-E_b(0)<0$ and $E_{ref}(q_B)=2\epsilon_1(q_B/2) \leqslant \epsilon_1(q_B)=w_{at}$.

### B. Scattering amplitude

We assume that the two scattering atoms belong to the lowest Bloch band, so the incident state in Eq. (11) is given by $\Psi_0(\mathbf{r},Z)=\phi_{1q_1}(z_1)\phi_{1q_2}(z_2)e^{i\mathbf{k}_\perp\cdot\mathbf{r}_\perp}$. The energy is $E=\hbar^2k_\perp^2/m+\epsilon_1(q_1)+\epsilon_1(q_2)$ and the quasimomentum $Q$ is given by

$$\begin{aligned} Q &= q_1+q_2, \quad \text{if } q_1+q_2 \leqslant q_B \\ &= q_1+q_2 \pm 2q_B, \quad \text{if } |q_1+q_2| > q_B. \end{aligned} \tag{25}$$

Notice that we only require $E \ll \epsilon_g$, but there is no restriction on the value of the scattering length $a$. We insert the ansatz $f_Q(Z)=A\Sigma_\ell w^2(Z-\ell d)e^{iQZ}$ in Eq. (11), where $A$ is a numerical coefficient which is related to the scattering amplitude (9) by $f_{sc}=aCA$, where $C=d/\sqrt{2\pi\sigma}$. Repeating the same steps as in Sec. III A, after integration over $Z'$, we find

$$f_{sc}=\frac{aC}{1-a/a_{cr}+(a/\sqrt{2\pi\sigma})\beta_{1D}(E,Q)}, \tag{26}$$

where

$$\begin{aligned} \beta_{1D}(E,Q) = &-\int_{-\pi}^{\pi}\frac{dq}{2\pi}\ln\left|\frac{-E+\epsilon_1(q)+\epsilon_1(Q-q)}{\epsilon_1(q)+\epsilon_1(Q-q)}\right| \\ &+i\pi\int_{-\pi}^{\pi}\frac{dq}{2\pi}\Theta[E-\epsilon_1(q)-\epsilon_1(Q-q)]. \end{aligned} \tag{27}$$

This function is related to the analytical continuation of $\alpha_{1D}$, defined in Eq. (19). Here $\Theta(x)$ is the unit-step function and we have used the formula $(x-E-i0)^{-1}=P(x-E)^{-1}+i\pi\delta(x-E)$, where the symbol $P$ stands for principal value. In the special case $Q=0$, the integration over quasimomentum in Eq. (27) can be done analytically using the dispersion relation $\epsilon_1(q_z)=2t[1-\cos(q_zd)]$ and one finds [19]

$$\begin{aligned} \beta_{1D}(E,0) &= i\arccos(1-E/4t), \quad \text{if } E<8t, \\ &-\ln[E(1+\sqrt{1-8t/E})^2/8t]+i\pi, \quad \text{if } E>8t. \end{aligned} \tag{28}$$

Equations (27) and (28) show that the scattering amplitude undergoes a dimensional crossover as the ratio $E/8t$ is changed. In the anisotropic, three-dimensional regime $E \ll 8t$, one has $f_{sc}=aC/(1-a/a_{cr}+iaC\sqrt{Em^*}/\hbar)$. Taking into account Eq. (23), in the quasi-two-dimensional regime $E \gg 8t$, we obtain $f_{sc}=d(a/\sqrt{2\pi\sigma})/\{1+(a/\sqrt{2\pi\sigma})[\ln(\lambda\hbar\omega_0/E)+i\pi]\}$ and $\lambda=0.915/\pi$ in agreement with Ref. [10].

It is interesting to notice that the scattering amplitude for $Q=0$ is related to the effective coupling constant $g_{eff}$ for Fermi atoms undergoing Cooper pairing in the case of weak attractive interaction ($a<0$). This result was used in Ref. [19] to calculate the superfluid transition temperature of a two-component Fermi gas in the presence of a one-dimensional optical lattice.

## IV. TWO-DIMENSIONAL AND THREE-DIMENSIONAL LATTICES

In this section, we extend our analysis to higher dimensional lattices. Different from the case $D=1$, the integration

over $k_\perp$ in Eq. (12) for $D=2,3$ is convergent for $r_\perp=0$, which considerably simplifies our analysis. Moreover, in the limit $E \ll \hbar\omega_0$, the energy dependence of the kernel comes entirely from the contribution of the lowest band ($\mathbf{n}_1=\mathbf{n}_2=\mathbf{1}$). The inclusion of higher bands gives small correction to the binding energy but is crucial to reproduce the correct behavior of the scattering amplitude close to Feshbach resonance, as discussed below.

### A. Bound state

For a $D$-dimensional optical lattice, the tight binding ansatz (16) for the function $f(\mathbf{R})$ in Eq. (8) generalizes to

$$f(\mathbf{R}) = \Pi_{i=1}^{D} f_{Q_i}(R_i), \tag{29}$$

where $Q_i$ and $R_i$ are the $i$th components of the quasimomentum $\mathbf{Q}$ and the center of mass position $\mathbf{R}$, respectively. By inserting the ansatz (29) in Eq. (8) and integrating over $\mathbf{R}'$, we find

$$1/g = \Lambda_D(E_b, \mathbf{Q}) + B_D(\mathbf{Q}), \tag{30}$$

where $\Lambda_D$ gives the contribution of the lowest Bloch band

$$\Lambda_2(E_b,\mathbf{Q}) = \frac{-C^2\sqrt{m}}{2\hbar}\int_{-q_B}^{q_B}\frac{d^2\mathbf{q}}{(2\pi)^2} \times \frac{1}{\sqrt{-E_b - 2\epsilon_1(\mathbf{Q}/2) + \epsilon_1(\mathbf{q}) + \epsilon_1(\mathbf{Q}-\mathbf{q})}}, \tag{31}$$

$$\Lambda_3(E_b,\mathbf{Q}) = -C^3\int_{-q_B}^{q_B}\frac{d^3\mathbf{q}}{(2\pi)^3} \times \frac{1}{-E_b - 2\epsilon_1(\mathbf{Q}/2) + \epsilon_1(\mathbf{q}) + \epsilon_1(\mathbf{Q}-\mathbf{q})}, \tag{32}$$

and $C$ has been defined previously. The quantity $B_D(Q)$ in Eq. (30) takes into account the small correction coming from the contribution of all higher bands and can be evaluated either numerically or analytically, as explained below. Equations (30)–(32) permit us to calculate the binding energy as a function of the scattering length for a given quasimomentum $\mathbf{Q}$.

For simplicity, we restrict our discussion to the case $\mathbf{Q}=0$. In analogy with the case $D=1$, there are two regimes: (i) an anisotropic, three-dimensional regime for $E_b \ll t$ and (ii) a confined regime of reduced dimensionality for $t \ll |E_b| \ll \hbar\omega_0 \sim \epsilon_g$. The constant $B_D$ can be fixed by matching the binding energy in the limit $|E_b| \gg t$ with the corresponding result valid for the harmonic oscillator potential [8,9] in the limit $|E_b| \ll \omega_0$

$$|E_b| = \frac{\hbar^2}{m}\frac{a^2}{\sigma^4\left(1-\eta_2\frac{a}{\sigma}\right)^2}, \quad (D=2), \tag{33}$$

$$|E_b| = \frac{\hbar^2}{m}\sqrt{\frac{2}{\pi}}\frac{a}{\sigma^3\left(1-\eta_3\frac{a}{\sigma}\right)}, \quad (D=3), \tag{34}$$

where $\eta_2=1.0326$ and $\eta_3=0.2448$. This gives $B_D=\eta_D m/4\pi\hbar^2\sigma$. Taking into account that the range of applicability of our method is $|E_B| \ll \hbar\omega_0$ or, equivalently, $|a| \ll \sigma$, we see that the contribution from higher bands to the binding energy is typically small.

The critical value of the scattering length $a=a_{cr}$ can be obtained by setting $E_b=0$ in Eqs. (31) and (32) and integrating over the quasimomenta using the tight-binding dispersion $\epsilon_n(\mathbf{q})=\Sigma_{j=1}^{D} 2t[1-\cos(q_j d)]$. This gives

$$\frac{1}{a_{cr}} = -\frac{1}{\sigma}\left(I_2\sqrt{\frac{\hbar\omega_0}{t}} - \eta_2\right), \quad (D=2), \tag{35}$$

$$\frac{1}{a_{cr}} = -\frac{1}{\sigma}\left(I_3\frac{\hbar\omega_0}{t} - \eta_3\right), \quad (D=3), \tag{36}$$

where $I_2=0.454$ and $I_3=0.101$. Similar results for $D=3$ have been obtained by Fedichev *et al.* [18] using a different method. Similar to the 1D case, the functional dependence of the critical scattering length on the ratio $\hbar\omega_0/t$ simply follows from Eqs. (33) ($D=2$) and (34) ($D=3$) by substituting the binding energy with the tunneling rate ($|E_b| \to t$). We see from Eqs. (35) and (36) that the ratio $d/a_{cr}$ has a power law dependence on the tunneling rate $t$ and, therefore, it increases exponentially fast as a function of the laser intensity, in contrast with the case $D=1$ shown in Fig. 2.

From Eqs. (31) and (32), we recover the behavior of the binding energy close to the critical point

$$\frac{1}{a} - \frac{1}{a_{cr}} = \frac{1}{\hbar}\frac{m^{*D/2}}{m^{(D-1)/2}}C^D\sqrt{|E_b|}, \tag{37}$$

which characterizes the three-dimensional regime.

The effective mass $M^*$ for the molecule (at $Q=0$) can be calculated from Eqs. (35) and (36). For zero binding energy, the mass ratio $2m^*/M^*=1$ and decreases rapidly by increasing $|E_b|$ as an effect of the correlated motion of the two atoms. In the confined regime $|E_b| \gg t$, we find $2m^*/M^* = (D+1)t/|E_b|$.

### B. Scattering amplitude

We assume again that the two scattering atoms belong to the lowest Bloch band, so the incident state in Eq. (11) is given by $\Psi_0(\mathbf{r},\mathbf{R}) = \phi_{\mathbf{1q}_1}(\mathbf{x}_1)\phi_{\mathbf{1q}_2}(\mathbf{x}_2)e^{i\mathbf{k}_\perp\cdot\mathbf{r}_\perp}$ and its energy is $E=\hbar^2k_\perp^2/m+\epsilon_{\mathbf{1}}(\mathbf{q}_1)+\epsilon_{\mathbf{1}}(\mathbf{q}_2)$. By inserting the ansazt $f_{\mathbf{Q}}(\mathbf{R}) = A\Pi_{i=1}^{D} f_{Q_i}(R_i)$, in Eq. (11) and taking into account that $f_{sc} = aC^D A$, we find

$$f_{sc} = \frac{aC^D}{1 - g[\beta_D(E,\mathbf{Q}) + B_D]}, \tag{38}$$

where $B_D$ has been defined above and

$$\beta_2(E,\mathbf{Q}) = \frac{-C^2\sqrt{m}}{2\hbar}\int_{-q_B}^{q_B}\frac{d^2\mathbf{q}}{(2\pi)^2} \times\left[\frac{\Theta[\epsilon_1(\mathbf{q})+ymp_1(\mathbf{Q}-\mathbf{q})-E]}{\sqrt{\epsilon_1(\mathbf{q})+\epsilon_1(\mathbf{Q}-\mathbf{q})-E}} + i\frac{\Theta[E-\epsilon_1(\mathbf{q})-\epsilon_1(\mathbf{Q}-\mathbf{q})]}{\sqrt{E-\epsilon_1(\mathbf{q})-\epsilon_1(\mathbf{Q}-\mathbf{q})}}\right], \tag{39}$$

$$\beta_3(E,\mathbf{Q}) = -C^3\int_{-q_B}^{q_B}\frac{d^3\mathbf{q}}{(2\pi)^3} \times\frac{1}{-E-i0+(\mathbf{Q}/2)+\epsilon_1(\mathbf{q})+\epsilon_1(\mathbf{Q}-\mathbf{q})}. \tag{40}$$

Equations (38) and (40) permit us to calculate the low energy scattering amplitude $f_{sc}=aC^2A$ in the presence of the lattice. Notice that $f_{sc}$ has a pole at the critical value of the scattering length $a=a_{cr}(\mathbf{Q})$ for $E=E_{ref}(\mathbf{Q})$, corresponding to the bound state with vanishing binding energy.

For simplicity, we confine ourselves to the case $Q=0$ where $E_{ref}=0$. In the three-dimensional regime, from Eqs. (39) and (40), we find the typical result

$$f_{sc} = \frac{aC^D}{1-a/a_{cr}+iaC^Dm^{*D/2}\sqrt{E}/m^{(D-1)/2}\hbar}, \tag{41}$$

which is valid in the limit $E \ll t$. This result was also found in Ref. [18] for the case of a 3D lattice. In the case $D=2$, the system undergoes for $E>8t$ a crossover to a quasi-one-dimensional regime. The dispersion of the lowest band can be neglected in Eq. (39) and the scattering amplitude (9) reduces to the asymptotic value [21]

$$f_{sc} \approx \frac{aC^2\sqrt{E}}{\left(1-\eta_2\frac{a}{\sigma}\right)\sqrt{E}+i\frac{\hbar a}{\sqrt{m}\sigma^2}}. \tag{42}$$

The inclusion of higher bands ($\eta_2 \neq 0$) becomes crucial when the scattering length is large, and only when they are taken into account, does one recover the confinement induced resonance for $a=\sigma/\eta_2$. Notice that our definition of the scattering amplitude [see Eq. (9)] is related to the amplitude $f(E)$ used in Ref. [21] by a scaling factor $f(E)=-i(\sqrt{2\pi}/d^2\sqrt{Em})f_{sc}(E)$.

Finally, we have verified that for $D \geqslant 2$, Eqs. (30) and (38) also follow from a Hubbard-like model with hopping along the the optical lattice, free motion in the perpendicular direction and the contact interaction strength equal to $U=g/[(1-\eta_D a/\sigma)(\sqrt{2\pi}\sigma)^D]$ [22].

## V. CONCLUSIONS

In this paper, we have generalized the two-body scattering theory to include the effect of periodic fields, where the center of mass and the relative motion do not separate. The interplay between confinement and tunneling effects gives rise to an interesting crossover between a low dimensional regime, where the interwell hopping can be treated perturbatively, and an anisotropic, three-dimensional regime, where the wave function for the relative motion spreads over many lattice sites. By using a tight-binding approach, we have investigated the low energy properties of the bound state and the scattering amplitude across the two regimes. The precision of our analytical predictions has been tested for the case of a one-dimensional lattice where exact numerics are available, finding very good agreement. Our results are relevant for current experiments on ultracold gases in optical lattices.

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