Two-dimensional scattering and bound states of polar molecules in bilayers

Michael Klawunn,[1,2] Alexander Pikovski,[1] and Luis Santos[1]
[1]*Institut für Theoretische Physik, Leibniz Universität Hannover, Appelstrasse 2, D-30167 Hannover, Germany*
[2]*INO-CNR BEC Center and Dipartimento di Fisica, Università di Trento, I-38123 Povo, Italy*
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Low-energy two-dimensional scattering is particularly sensitive to the existence and the properties of weakly bound states. We show that interaction potentials $V(r)$ with the vanishing zero-momentum Born approximation $\int dr\, rV(r) = 0$ leads to an anomalously weak bound state that crucially modifies the two-dimensional scattering properties. This anomalous case is especially relevant in the context of polar molecules in bilayer arrangements.

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I. INTRODUCTION

Ultracold atomic gases are many-body systems, but most of their fundamental properties originate from the underlying two-body problem, given by an interaction potential which is typically considered as short range. The situation is completely different in dipolar gases due to the long-range character of the dipole-dipole interaction [1,2]. Polar molecules with a potentially large electric-dipole moment constitute a particularly exciting dipolar gas. However, achieving quantum degeneracy is handicapped by exothermic chemical reactions [3]. The latter may be avoided by confining the gas in two-dimensional geometries if the dipoles are polarized perpendicular to the trap plane, due to the repulsive character of the dipole-dipole interaction [4].

Bilayer (and in general multilayer) arrangements of polar molecules offer the possibility of stability against inelastic reactions and give rise to interlayer pairing due the dipole-dipole force [5–7]. A dipole in layer 1 interacts with a dipole in layer 2, where both dipoles are oriented perpendicularly to the layers, by the potential

$$V_{\rm dd}(r) = U_0\,(r^2-2)/(r^2+1)^{5/2}. \tag{1}$$

Here r is the relative in-plane distance between the two dipoles, the interlayer distance λ is set to 1, and U_0 is a positive dimensionless coupling constant. We have $U_0 = md^2/\hbar^2\lambda$ and the unit of energy is $E_0 = \hbar^2/m\lambda^2$, with m the mass and d the dipole moment of the molecule. This potential is attractive at short distances and repulsive at large distances, fulfilling the peculiar condition $\int dr\, rV_{\rm dd}(r) = 0$ (i.e., its zero-momentum Born approximation vanishes [7–9]). Interlayer interactions of a different type may be attained in binary mixtures, where one of the species is confined in a bilayer while the other moves freely. The free species mediates a two-dimensional (2D) interaction with a Ruderman-Kittel–Kasuya-Yosida (RKKY)–type potential [10], which may as well have a vanishing zero-momentum Born approximation.

Low-energy 2D scattering, which determines the properties of 2D quantum gases [11–13], is particularly sensitive to the existence and properties of weakly bound states. Although 2D scattering [14–18] and weakly bound states [19–21] have been intensively studied, little is known for the case when $\int dr\, rV(r) = 0$. The binding energy for weakly coupled bound states in this case was calculated in Ref. [19]. However, a detailed investigation of the binding energy at larger coupling and of the low-energy scattering properties is still lacking.

In this Brief Report we discuss the low-energy scattering and weakly bound states for radial potentials $V(r)$ satisfying $\int dr\, rV(r) = 0$. We extend (using an alternative method) the expression derived in Ref. [19] for the binding energy of the weakly bound state. We show that the presence of this anomalously weak bound state modifies significantly the scattering amplitude compared to the usual case of potentials with a nonvanishing zero-momentum Born approximation. As an example, we specialize for the potential $V_{\rm dd}$ appearing in bilayer gases of polar molecules and check the validity of the obtained analytical expressions using exact numerical calculations.

This paper is organized as follows. In Sec. II we introduce the Jost function formalism to study the binding energy of weakly bound states and evaluate the general expressions for $V_{\rm dd}$. In Sec. III we discuss the modifications introduced in the two-dimensional scattering properties if $\int dr\, rV(r) = 0$ and study this for $V_{\rm dd}$ in detail. Our conclusions are summarized in Sec. IV.

II. WEAKLY BOUND STATES

Reference [19] studied the bound states of the Schrödinger equation $[-\nabla^2 + V(\mathbf{r})]\psi = \epsilon\psi$ for potentials of the form $V(\mathbf{r}) = U_0 v(\mathbf{r})$, where as above U_0 denotes a positive dimensionless coupling constant characterizing the potential strength.[1] For the case of weak coupling ($U_0 \to 0$) it was shown that a shallow bound state always exists if $\int d^2r\, v(\mathbf{r}) \leqslant 0$, but there is no bound state if $\int d^2r\, v(\mathbf{r}) > 0$. Furthermore, it was shown that for $\int d^2r\, v(\mathbf{r}) < 0$ the binding energy of the shallow bound state is of the form $\epsilon_b \sim -\exp[4\pi/\int d^2r\, V(\mathbf{r})]$, as expected from, e.g., Ref. [22]. However, for our case of interest $\int d^2r\, v(\mathbf{r}) = 0$, the binding energy acquires the anomalous form $\epsilon_b \sim -\exp(1/cU_0^2)$, with

$$c = \frac{1}{8\pi}\int d^2r \int d^2r' v(\mathbf{r}) \ln|\mathbf{r}-\mathbf{r}'| v(\mathbf{r}'). \tag{2}$$

It can be shown that $c < 0$ for any $v(\mathbf{r})$. For the potential $V_{\rm dd}(r)$ appearing in a bilayer system of polar molecules, one obtains

[1]In Ref. [19] it was assumed that $\int d^2r(1+|\mathbf{r}|^\delta)|v(\mathbf{r})| < \infty$, with $\delta > 0$.

$c = -1/8$, and hence the binding energy becomes

$$\epsilon_b^{\rm dd} \sim -\exp\left(-8/U_0^2\right). \tag{3}$$

However, a numerical calculation of the binding energy (see below) shows that this result is not very accurate even for very small U_0. This motivates us to derive a more accurate analytic expression for the binding energy which remains valid for larger U_0.

The two-body scattering problem for a radially symmetric potential $V(r)$ in two dimensions is described by the Schrödinger equation

$$\left[-\left(\frac{d^2}{dr^2}+\frac{1}{r}\frac{d}{dr}\right)+V(r)\right]\phi(r)=k^2\phi(r), \tag{4}$$

where all quantities are dimensionless and $\phi(r)$ is the radial wave function. Only s waves are considered since we are only interested in low-energy properties. Following Ref. [23], we employ the Jost function formalism to study the scattering problem and the shallow bound states. The definition of the Jost function $\mathcal{F}(k)$ in the 2D case may be found in Ref. [23]. The properties of $\mathcal{F}(k)$ are similar to those of the Jost function for the three-dimensional (3D) case [24].

The scattering phase shift $\delta(k)$ is related to $\mathcal{F}(k)$ by

$$\tan\delta(k) = -\frac{\text{Im } F(k)}{\text{Re } \mathcal{F}(k)}, \tag{5}$$

the scattering amplitude is

$$f(k) = \frac{\tan\delta(k)}{1 - i\tan\delta(k)}, \tag{6}$$

and $\sigma = (4/k)|f(k)|^2 = (4/k)\sin^2\delta(k)$ is the total 2D s-wave cross section. For complex k, the zeros of the Jost function on the positive imaginary axis, $\mathcal{F}(i\alpha) = 0$ with $\alpha > 0$, are the bound states of the potential with binding energy $\epsilon_b = -\alpha^2$.

The following integral representation of the Jost function $\mathcal{F}(k)$ will be employed:

$$\mathcal{F}(k) = 1 + e^{i\pi/4}\sqrt{\frac{\pi}{2k}}\int_0^\infty dr\sqrt{r}\,V(r)J_0(kr)f_0(kr), \tag{7}$$

where $f_0(k,r)$ satisfies the integral equation

$$f_0(k,r) = \sqrt{\frac{i\pi kr}{2}}H_0(kr) + \int_r^\infty ds\, g(k,r,s)V(s)f_0(k,s), \tag{8}$$

with

$$g(k,r,r') = \frac{\pi}{2}\sqrt{rr'}[J_0(kr)Y_0(kr') - J_0(kr')Y_0(kr)].$$

In the previous expressions J_0, Y_0 are Bessel functions, and H_0 is the Hankel function of the first kind.

In the following we are interested in determining the weakly bound states. To this aim we expand the Jost function for small k:

$$\mathcal{F}(k) = A\ln k + B - i\frac{\pi}{2}A, \tag{9}$$

where A, B are real constants independent of k. These constants can be represented by infinite series of the form $A = \sum A_j$, $B = 1 - \sum B_j$.[2] The first terms of the A_j series are of the form

$$A_1 = -\int_0^\infty dr\, rV(r), \tag{10}$$

$$A_2 = -\int_0^\infty dr\, rV(r)\int_r^\infty ds\, sV(s)\ln\left(\frac{s}{r}\right), \tag{11}$$

whereas those of the B_j series are

$$B_1 = \int_0^\infty dr\, rV(r)\ln(r) - C_1 \tag{12}$$

$$B_2 = \int_0^\infty dr\, rV(r)\int_r^\infty ds\, sV(s)\ln\left(\frac{s}{r}\right)\ln(s) - C_2, \tag{13}$$

with $C_i = A_i\ln(e^\gamma/2)$ and $\gamma \approx 0.577$ the Euler constant.

As mentioned above, the bound states are given by the zeros of $\mathcal{F}(k)$ on the positive imaginary axis. Using (9) with $k = i\alpha$ we hence obtain the expression of the binding energy:

$$\epsilon_b = -\exp\left(-2\frac{B}{A}\right). \tag{14}$$

Note that Eq. (14) is valid as long as the binding energy is small enough such that the logarithmic term dominates the Jost function. For potentials with $\int dr\, rV(r) < 0$, it is sufficient to take $A \approx A_1$ and $B \approx 1$, recovering the expression $\epsilon_b \sim \exp[4\pi/\int d^2r\,V(r)]$ for small U_0.

However, for the case of potentials such that $\int dr\, rV(r) = 0$, we have $A_1 = 0$, and the first nonvanishing term is $A \approx A_2$, $B \approx 1$, providing an alternative derivation of Eq. (3). A more precise formula is obtained by including higher-order terms,

$$\epsilon_b = -\exp\left(-2\,\frac{1 - B_1 - B_2 - \cdots}{A_1 + A_2 + \cdots}\right). \tag{15}$$

For the case of the interlayer dipole-dipole potential $V_{\rm dd}$, the integrals can be carried out analytically to find a corrected expression for the binding energy

$$\epsilon_b^{\rm dd} \simeq -\exp\left\{-\frac{8}{U_0^2}\left[1 - U_0 + \frac{U_0^2}{4}\left(\frac{5}{2} + \ln\tfrac{e^\gamma}{2}\right)\right]\right\}. \tag{16}$$

Figure 1 compares the numerical result for the binding energy for $V_{\rm dd}$ (obtained directly from the 2D Schrödinger equation) with the analytical expressions of Eqs. (3) and (16). Note that whereas Eq. (3) provides a relative inaccurate approximation even at rather low U_0, the newly derived expression (16) is in excellent agreement with the numerics, all the way to $U_0 \lesssim 1.2$.

Finally, we note that for large U_0 the binding energy for $V_{\rm dd}$ can be determined by a variational calculation, giving [25] $\epsilon_b^{\rm dd} \approx -2U_0 + 4\sqrt{3U_0/2} - 15/4$, which coincides with the numerics only for $U_0 \gtrsim 5$.

III. SCATTERING PHASE SHIFT

We have shown above that the Jost function formalism is particularly useful for the analysis of weakly bound states. In

[2]We always assume $A \neq 0$. The exceptional case $A = 0$ (cf. [23]) is the two-dimensional analog of zero-energy resonance in three dimensions.

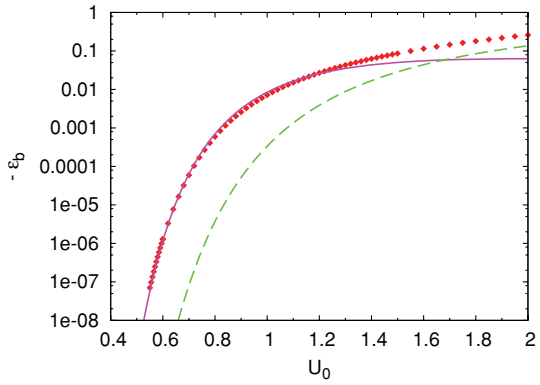

FIG. 1. (Color online) Binding energy for $V_{\rm dd}$ as a function of the dipole strength U_0 calculated numerically (dots), from Eqs. (16) (solid) and (3) (dashed).

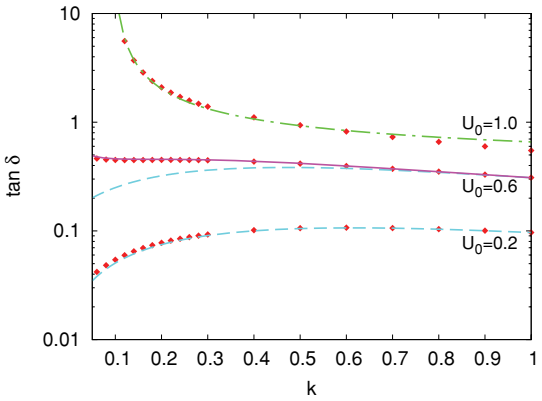

FIG. 2. (Color online) Scattering phase shift for $V_{\rm dd}$ as a function of k for different U_0 calculated numerically (dots) compared to the logarithmic behavior (20) for $U_0 = 1.0$ (dash-dotted, green), to formula (17) for $U_0 = 0.6$ (solid, orange), and to the second Born approximation (21) for $U_0 = 0.6$ and $U_0 = 0.2$ (dashed, cyan).

this section we employ this formalism for the study of 2D scattering and in particular for the calculation of the s-wave scattering phase shift $\delta(k)$.

An approximate expression of the Jost function $\mathcal{F}(k)$ for small U_0 is obtained by iterating twice the integral equation (8). Note that we keep all orders in k. The resulting scattering phase shift follows from the relation (5):

$$\tan\delta(k) = \frac{-\frac{\pi}{2} I_{JJ}(k) - \frac{\pi^2}{4}[I_{JJ,JY}(k) - I_{JY,JJ}(k)]}{1 - \frac{\pi}{2} I_{JY}(k) - \frac{\pi^2}{4}\left[I_{JJ,YY}(k) - \frac{1}{2} I_{JY}^2(k)\right]}, \tag{17}$$

where we have introduced the notation

$$I_{FG} = \int_0^\infty dr\, r V(r) F(r) G(r), \tag{18}$$

$$I_{FG,PQ} = \int_0^\infty dr\, r V(r) F(r) G(r) \int_r^\infty ds\, s V(s) P(s) Q(s), \tag{19}$$

and J, Y stand for $J_0(kr)$ and $Y_0(kr)$.

For small k it is possible to simplify Eq. (17). Employing the logarithmic expression (9), the relation (5), and the expression for the binding energy (14), we recover the well known logarithmic expression (see, e.g., [12])

$$\tan\delta(k) = \left(\frac{1}{\pi} \ln \frac{k^2}{|\epsilon_b|}\right)^{-1}, \tag{20}$$

characteristic of 2D scattering, which relates the scattering shift and the binding energy of the weakly bound state. However, for the case $\int dr\, r V(r) = 0$ the binding energy $|\epsilon_b|$ can become anomalously small, and hence the expression at the right-hand side of Eq. (20) can become very small for reasonable k. In this case, it is not any more the leading term for the low-energy scattering.

On the other hand, for large enough k and small U_0, the first integral $I_{JJ}(k)$ in Eq. (17) dominates, and we recover, as expected for sufficiently large k, the Born approximation. Therefore, formula (17) interpolates smoothly between the correct low-energy and the correct high-energy behavior. This suggests that it may be valid, at least qualitatively, even for large U_0. By expanding Eq. (17) in powers of U_0, one recovers the Born series, which reads to second order:

$$\tan\delta(k) = -\frac{\pi}{2} I_{JJ} - \frac{\pi^2}{2} I_{JJ,JY}. \tag{21}$$

It is interesting to discuss these results for the case of the interlayer dipole-dipole potential $V_{\rm dd}$. We have computed the scattering phase shift numerically from the Schrödinger equation and compared it to the results of Eq. (17), obtaining that Eq. (17) provides the correct scattering phase shift with excellent accuracy, at least in the range $0.03 \leqslant k \leqslant 5$ and $0.05 \leqslant U_0 \leqslant 2.0$. Hence Eq. (17) is a good approximation not only for $U_0 \ll 1$, but also for $U_0 \sim 1$. Of course, if the interactions are too large ($U_0 \gg 1$), the contributions from higher iterations of the integral equation (8) become more important and Eq. (17) loses its accuracy.

Figure 2 compares the numerical results for the scattering phase shift for $V_{\rm dd}$ with the limiting cases provided by expressions (20) and (21) for small k and different values of U_0. It is seen that for $U_0 \sim 1$, the scattering phase shift is best approximated by the logarithmic expression (20), and for $U_0 \ll 1$ by the second Born approximation (21). For intermediate values of U_0 none of the limiting cases is accurate and the full expression (17) must be used. We sketch in Fig. 3 qualitatively the regimes of k and U_0, where the logarithm (20), the first Born approximation (22), and the second Born approximation (21) are good approximations, as obtained by comparison with the numerical solution. Note that, excluding unreasonably small k, the logarithmic form (20) is just valid for $k < 1$ and the window $0.7 \lesssim U_0 \lesssim 2.0$.

Finally, we note that the first Born approximation for $V_{\rm dd}$ can be evaluated exactly analytically,

$$\tan\delta^{\rm dd}(k) \simeq -\frac{\pi}{2} U_0 \left(-\frac{4k}{\pi} - 2k\,[\mathbf{L}_1(2k) - I_1(2k)]\right), \tag{22}$$

where $\mathbf{L}_1$ is the modified Struve function. The second Born approximation (21) can be expanded for small k

$$\tan\delta^{\rm dd}(k) \approx 2U_0 k - \pi U_0 k^2 + \tfrac{1}{8} U_0^2 \pm \cdots, \tag{23}$$

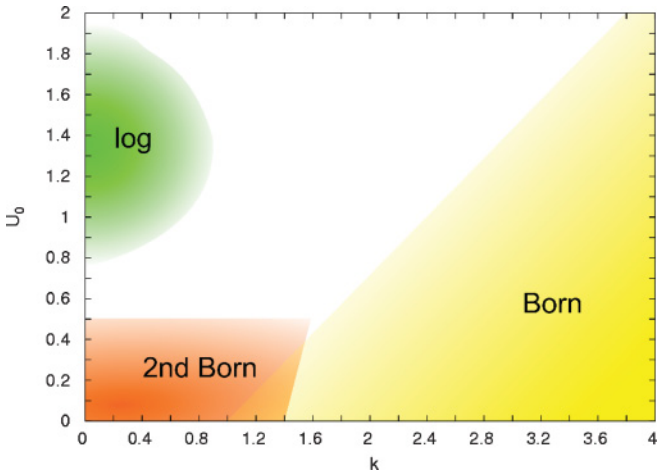

FIG. 3. (Color online) Qualitative sketch of the regimes of k and U_0 where the scattering phase shift for V_{dd} can be approximated by the logarithm Eq. (20) (green), the Born approximation Eq. (22) (yellow), and the second Born approximation Eq. (21) (orange).

which gives a maximum in the scattering phase shift at $k \approx 1/\pi$ as observed in the numerical results.

IV. CONCLUSIONS

In conclusion, two-dimensional radial interaction potentials $V(r)$ with a vanishing zero-momentum Born approximation, $\int dr\, r V(r) = 0$, result in interesting physics crucially different from purely attractive or purely repulsive potentials. Using the Jost function formalism, we have derived an expression for the binding energy as a function of the potential strength U_0, which remains accurate for a wide regime of U_0 values. Moreover, we have investigated the scattering amplitude in different parameter regimes. In particular, we have shown a significant deviation of the scattering behavior in comparison with potentials with $\int dr\, r V(r) \neq 0$ due to the anomalously low binding energy of the weakly bound state.

These results are of particular importance in the physics of two-dimensional systems, and more specifically on two-dimensional ultracold gases. Standard theories, in particular the theory of BCS-BEC crossover [12,13], are based on the fact that the scattering amplitude possesses the logarithmic dependence (20). These results are therefore modified if the potential has a vanishing zero-momentum Born approximation. This has particularly important consequences for the properties of a gas of polar Fermi molecules confined in a bilayer geometry, including interlayer pairing [7].

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