

Analytical treatment of bosonic d -wave scattering in isotropic harmonic waveguides

P. Giannakeas,^{1,*} V. S. Melezhik,^{2,†} and P. Schmelcher^{1,‡}

¹Zentrum für Optische Quantentechnologien, Universität Hamburg, Luruper Chaussee 149, 22761 Hamburg, Germany

²Bogoliubov Laboratory of Theoretical Physics, Joint Institute for Nuclear Research, Dubna, Moscow Region 141980, Russian Federation

(Received 10 February 2012; published 3 April 2012)

We analyze d -wave resonances in atom-atom scattering in the presence of harmonic confinement by employing a higher-partial-wave pseudopotential. Analytical results for the scattering amplitude and transmission are obtained and compared to corresponding numerical ones, which employ the Lennard-Jones potential. Qualitative agreement is observed for weak confinement. For strong confinement the pseudopotential does not capture the s - and d -wave interference phenomena, yielding an asymmetric Fano profile for the transmission resonance.

DOI: [10.1103/PhysRevA.85.042703](https://doi.org/10.1103/PhysRevA.85.042703)

PACS number(s): 34.50.Cx, 03.75.Be, 34.10.+x

I. INTRODUCTION

The characteristics of ultracold bosonic two-body scattering processes provide a key ingredient for the modeling and understanding of the properties of degenerate atomic gases. The dominant s -wave interactions of the two-body collisions can be conveniently modeled by the Huang-Fermi pseudopotential [1–3]. Over the last decade, this pseudopotential has become an essential theoretical tool in particular for analytical studies of ultracold systems; e.g., see Busch *et al.* [4] for two atoms in harmonic traps, Olshanii [5] for atomic collisions in cylindrical waveguides, where the so-called confinement-induced resonances (CIRs) were predicted and experimentally observed in Refs. [6–8], or Refs. [9–11] which employed approaches based on the energy-dependent scattering lengths $a_s(E)$.

The theory of pseudopotentials has been developed further in order to describe scattering processes involving higher partial waves, i.e., with relative angular momentum $\ell > 0$ [2,3,12–20]. Higher-partial-wave interactions represent an intriguing perspective in research on ultracold gases and are expected to provide novel many-body phenomena, such as unconventional superfluidity and superconductivity [21–23]. So far, theoretical studies with pseudopotentials for $\ell > 0$ have mainly been used to describe fermionic systems, e.g., in quasi-one-dimensional [13,15,24] or quasi-two-dimensional [14,17] geometries, which have been studied experimentally in Ref. [25]. For the case of bosons an analytical description of collisions in a planar waveguide has been derived, where the cross section possesses s - and d -wave resonances [17]. In harmonic waveguides higher-partial-wave interactions were shown to have important impact on bosonic scattering [26] through the interference of d -wave resonances (DWRs) with the underlying continuum. A theoretical treatment of d -wave scattering of bosons in the case of quasi-one-dimensional geometries is, however, still needed.

In this work we derive an approximate analytical solution for bosonic collisions in a harmonic waveguide, which goes beyond mere s -wave scattering. Our starting point is to assume that the transverse confinement frequency is weak enough in order to avoid a strong interference between the

free-space d -wave shape resonance and the s -wave scattering. The latter permits modeling the interatomic potential through a zero-range regularized d -wave pseudopotential suggested in Refs. [14,15], which is parametrized by a single parameter, the energy-dependent d -wave scattering length $[a_d(k)]$. The associated regularization operator contains exclusively derivatives. Taking into account the virtual excitations occurring during the scattering process, we analytically describe the appearance of the DWR. An important aspect of our approximate formula for the d -wave scattering amplitude is that one can map the total Hamiltonian onto an effective one-dimensional Hamiltonian, where the interaction is modeled by a one-dimensional contact potential. The strength of the contact potential depends on the above-mentioned d -wave scattering amplitude, similar to the case of the s -wave CIR [5].

In order to verify the validity of the approximate analytical results, we compare them with corresponding numerical calculations, where the interatomic interaction is modeled by a Lennard-Jones potential. A good agreement is obtained only for a sufficiently weak confinement. For strong confinement the pseudopotential does not capture the s - and d -wave interference and therefore lacks the description of the numerically obtained Fano asymmetric line shape of the transmission coefficient [27].

The sectioning of this paper is as follows. In Sec. II we review the recent developments of pseudopotential theory for higher-partial-wave interactions. In Sec. III we describe and discuss the d -wave scattering process. Section IV contains a comparison of the analytical results and the numerical calculations and Sec. V provides a brief summary and conclusions.

II. PSEUDOPOTENTIALS FOR HIGHER-PARTIAL-WAVE INTERACTIONS

The pseudopotential approximation to the interatomic interaction is a ubiquitous tool for the theoretical description of ultracold gases: the atomic interactions are modeled in terms of a contact potential. Huang and Yang [2,3] derived a generalized pseudopotential for all partial waves, which represents a multipolar expansion over δ -function contributions. The Huang-Yang approach (HY) was revised by Derevianko [12], who corrected an algebraic error for $\ell > 0$. However, other derivations have been developed for higher-partial-wave pseudopotentials, which differ from the HY approach, by using

*pgiannak@physnet.uni-hamburg.de

†melezhik@theor.jinr.ru

‡pschmelc@physnet.uni-hamburg.de

a more rigorous treatment of the derivatives of the δ functions in the framework of distribution theory [14,15] yielding the following representation:

$$V_{ps}(\mathbf{r})\Psi(\mathbf{r}) = \sum_{\ell=0}^{\infty} \frac{(-1)^\ell [(2\ell+1)!!]^2}{4\pi(2\ell)!!} g_\ell \frac{\delta^{(\ell)}(r)}{r^2} \times \left[\frac{\partial^{2\ell+1}}{\partial r'^{2\ell+1}} r'^{\ell+1} \int d\Omega' P_\ell(\hat{\mathbf{r}} \cdot \hat{\mathbf{r}}') \Psi(\mathbf{r}') \right]_{r'=0}, \quad (1)$$

where $g_\ell = \hbar^2 a_\ell^{2\ell+1}(k)/(2\mu)$, with $a_\ell^{2\ell+1}(k) = -\tan\delta_\ell(k)/k^{2\ell+1}$ defined as the ℓ th energy-dependent scattering length [10,11]. Here, $\delta^{(\ell)}(r)$ is the ℓ th derivative of the δ function, and the integral over the solid angle Ω' acts as a projection operator of the total wave function on each ℓ state. For $\ell = 0$ one obtains from Eq. (1) the Huang-Fermi pseudopotential. However, Eq. (1) for $\ell > 0$ differs by a factor $(2\ell+1)/(\ell+1)$ from Huang and Yang's result [3], whereas if we substitute in Eq. (1) the relations $\delta(\mathbf{r}) = \delta(r)/(4\pi r^2)$ and $\delta^{(\ell)}(r) = (-1)^\ell \ell! \delta(r)/r^\ell$ we obtain the pseudopotential of Derevianko [12].

Additionally, Stampfer and Wagner [16] introduce the following pseudopotential for higher partial waves:

$$\tilde{V}_{ps}(\mathbf{r})\Psi(\mathbf{r}) = \sum_{\ell=0}^{\infty} \sum_{m=-\ell}^{\ell} \frac{4\pi(-1)^\ell}{(2\ell)!!} g_\ell Y_{\ell m}(\partial) \delta(\mathbf{r}) \times \left[\frac{\partial^{2\ell+1}}{\partial r'^{2\ell+1}} r'^{\ell+1} \int d\Omega' Y_{\ell m}^*(\hat{\mathbf{r}}') \Psi(\mathbf{r}') \right]_{r'=0}, \quad (2)$$

where the operator $Y_{\ell m}(\partial)$, introduced by Maxwell [28], is obtained from the spherical harmonic polynomial $r^\ell Y_{\ell m}(\hat{\mathbf{r}})$, by replacing the Cartesian coordinates x_k with the partial derivatives ∂_{x_k} . Note that Eq. (2) is equal to Eq. (1) as was proven in Ref. [15] by using the relation

$$\frac{\delta^{(\ell)}(r)}{r^2} Y_{\ell m}(\hat{\mathbf{r}}) = \frac{4\pi \ell!}{(2\ell+1)!!} Y_{\ell m}(\partial) \delta(\mathbf{r}). \quad (3)$$

The above-mentioned pseudopotentials can be simplified [15] in order to describe interactions of a single-partial-wave character. This simplification is based on the fact that in general the atomic interaction is dominated by the ℓ -partial-wave scattering in the vicinity of the corresponding ℓ -partial-wave resonance. Thus, one can focus on a single partial wave, which yields the following pseudopotential:

$$V_{ps,\ell}(\mathbf{r})\Psi(\mathbf{r}) = \sum_{m=-\ell}^{\ell} \frac{16\pi^2(-1)^\ell}{(2\ell+1)!} g_\ell Y_{\ell m}(\partial) \delta(\mathbf{r}) \times \left[\frac{\partial^{2\ell+1}}{\partial r'^{2\ell+1}} r'^{\ell+1} Y_{\ell m}^*(\partial') \Psi(\mathbf{r}') \right]_{r'=0}. \quad (4)$$

Furthermore, the sum with respect to m can be simplified with the help of the following summation formula:

$$\frac{4\pi}{2\ell+1} \sum_{m=-\ell}^{\ell} Y_{\ell m}(\partial) Y_{\ell m}^*(\partial') = \sum_{k=0}^{[\ell/2]} c_k (\nabla \cdot \nabla')^{\ell-2k} \nabla^{2k} (\nabla')^{2k}, \quad (5)$$

where $[\ell/2]$ is the largest, smaller or equal integer of $\ell/2$ and $c_k = [(-1)^\ell (2\ell+1)! / (2^\ell k! (\ell-k)! (\ell-2k)!)]$ are the coefficients of the Legendre polynomials $P_\ell(x) = \sum_{k=0}^{[\ell/2]} c_k x^{\ell-2k}$.

Equations (4) and (5) constitute pseudopotentials for any ℓ partial wave. These pseudopotentials are expressed in terms of differential operators which are more convenient in analytical derivations than the pseudopotential with the projection operator [see Eqs. (1) and (2)].

III. QUASI-1D SCATTERING WITH s - AND d -WAVE INTERACTIONS

A. s - and d -wave pseudopotentials

In the following we consider ultracold collisions of identical bosons in the presence of an external harmonic confinement. The scattering process is taking place in the low-energy regime, $ka_\perp \ll 1$, where k is the relative momentum in the unconfined degree of freedom and $a_\perp = \sqrt{\frac{\mu\omega_\perp}{\hbar}}$ is the oscillator length defined via the trap frequency ω_\perp and the reduced mass μ of the colliding bosonic pair. Furthermore, in order to go beyond s -wave physics we assume that the momentum k is very small but not equal to zero. Consequently, as was shown in Ref. [26], except for the well-known s -wave CIR [5], an additional resonance emerges in this system, the so-called DWR, which is based on the interference of a free-space d -wave shape resonance with s -wave scattering. The coexistence of s - and d -wave resonances implies interactions between the bosons of s - and d -wave symmetries [see Fig. 1(c) in Ref. [26]].

The main goal of this paper is to present an analytical model for the DWR effect in a harmonic waveguide. However, the modeling of s - and d -wave interactions with pseudopotentials in systems of nonspherical symmetry, like the one mentioned above, is not a trivial task. As the symmetry of the system is cylindrical the angular momentum is not conserved, and consequently the application of pseudopotentials Eqs. (1) and (2) leads to an explicit integration over all ℓ partial waves.

However, as proposed in Ref. [15], one can avoid such difficulties by considering a single ℓ partial wave in the vicinity of the ℓ -wave resonance, where contributions from other partial waves are sufficiently suppressed. The latter means that in the vicinity of the s -wave resonance, we assume that the interaction can be modeled by the following pseudopotential with the help of Eqs. (4) and (5):

$$V_{ps,s}(\mathbf{r}) = \frac{2\pi\hbar^2 a_s(k)}{\mu} \delta(\mathbf{r}) \frac{\partial}{\partial r} [r \cdot], \quad (6)$$

which is the Huang-Fermi pseudopotential, with the s -wave scattering length $a_s(k)$ being energy dependent. Note that Eq. (6) coincides with the pseudopotential proposed in Ref. [11].

Equivalently, in the vicinity of the d -wave resonance, we assume that the interaction can be modeled by the following pseudopotential [14,15]:

$$V_{ps,d}(\mathbf{r}) = \frac{\pi\hbar^2 a_d^5(k)}{8\mu} \sum_{i,j,k,l} D_{ijkl}^{\leftarrow} (\partial_{x_i x_j}^2) \delta(\mathbf{r}) \frac{\partial^5}{\partial r^5} r^5 (\partial_{x_k x_l}^2)^{\rightarrow}, \quad (7)$$

where $D_{ijkl} = \delta_{ik}\delta_{jl} - \frac{1}{3}\delta_{ij}\delta_{kl}$ with the indices $i, j, k, l = 1, \dots, 3$, and $a_d^5(k) = -\tan\delta_{\ell=2}(k)/k^5$ is the energy-dependent

d -wave scattering length. The bidirectional operator $\overleftarrow{(\partial_{x_i}^2)}$ $[(\partial_{x_i}^2)\overrightarrow{(\cdot)}]$ denotes the differential operator in Cartesian coordinates, which acts to the left (right) of the pseudopotential $V_{ps,d}(\mathbf{r})$.

We emphasize that application of the expressions (6) and (7) simultaneously is inconsistent and incompatible since the pseudopotentials $V_{ps,s}(\mathbf{r})$ and $V_{ps,d}(\mathbf{r})$ are valid for the cases where the wave function exhibits only $1/r$ or $1/r^3$ singularities for small r , respectively.

B. Hamiltonian, scattering states, and virtual excitations

We assume two-body collisions of identical bosons in a waveguide with their transverse degrees of freedom being confined by a harmonic oscillator potential. The harmonic confinement permits the separation of the center-of-mass and relative motions, yielding a single-particle Hamiltonian with a scatterer fixed at the origin for the relative degree of freedom.

$$H(z, \rho, \phi) = -\frac{\hbar^2}{2\mu} \left(\frac{\partial^2}{\partial z^2} + \frac{\partial^2}{\partial \rho^2} + \frac{1}{\rho} \frac{\partial}{\partial \rho} + \frac{1}{\rho^2} \frac{\partial^2}{\partial \phi^2} \right) + \frac{1}{2} \mu \omega_{\perp}^2 \rho^2 + V_{ps,\ell}(\mathbf{r}), \quad (8)$$

where $\mathbf{r} = \mathbf{r}_1 - \mathbf{r}_2$ is the relative coordinate of the two bosons, and $V_{ps,\ell}(\mathbf{r})$ is the pseudopotential which models the arbitrary ℓ -wave interatomic interaction.

The symmetry of the transverse potential $\frac{1}{2} \mu \omega_{\perp}^2 \rho^2$ implies that the scattering solutions should be expanded in an axially symmetric basis. Such a basis set is given by the eigenstates of the two-dimensional (2D) harmonic oscillator, which satisfy the Schrödinger equation

$$\left[-\frac{\hbar^2}{2\mu} \left(\frac{\partial^2}{\partial \rho^2} + \frac{1}{\rho} \frac{\partial}{\partial \rho} + \frac{1}{\rho^2} \frac{\partial^2}{\partial \phi^2} \right) + \frac{1}{2} \mu \omega_{\perp}^2 \rho^2 \right] \tilde{\Phi}_{n,m_z}(\rho, \phi) = E_{n,m_z} \tilde{\Phi}_{n,m_z}(\rho, \phi), \quad (9)$$

where $\tilde{\Phi}_{n,m_z}(\rho, \phi)$ are the eigenfunctions of the 2D harmonic oscillator, m_z is the azimuthal quantum number, and $E_{n,m_z} = \hbar \omega_{\perp} (n + |m_z| + 1)$ is the transverse energy spectrum of the 2D harmonic oscillator, with $n = 0, 2, 4, \dots$ being the principal quantum number.

The spherical symmetry imprinted by the pseudopotential $V_{ps,\ell}(\mathbf{r})$ leads to a separation of the azimuthal ϕ angle from the z, ρ coordinates in Eq. (9). The latter means that during the collision no virtual excitations will occur with respect to the m_z quantum number. However, virtual excitations will emerge with respect to the principal quantum number n , which will be taken into account in the calculation given below.

We focus on the single-mode regime, where the collision takes place in the ground state of the transverse confinement with angular momentum $m_z = 0$ and represents the only ‘‘open channel.’’ The latter means that the total energy of the pair collision is limited between the ground and the first axially symmetric transversal states

$$E_{n=0, m_z=0} \leq E < E_{n=2, m_z=0}. \quad (10)$$

Furthermore, the above-mentioned lack of dependence on the angle ϕ results in the following simplified Schrödinger

equation:

$$\left[-\frac{\hbar^2}{2\mu} \left(\frac{\partial^2}{\partial z^2} + \frac{\partial^2}{\partial \rho^2} + \frac{1}{\rho} \frac{\partial}{\partial \rho} \right) + \frac{1}{2} \mu \omega_{\perp}^2 \rho^2 + V_{ps,\ell}(\mathbf{r}) \right] \Psi(z, \rho) = E \Psi(z, \rho), \quad (11)$$

where $E = E_{\parallel} + E_{n=0, m_z=0}$ is the total colliding energy, which is defined as the sum of the longitudinal kinetic energy $E_{\parallel} = \frac{\hbar^2}{2\mu} k^2$ and the energy of the transverse ground state $E_{n=0, m_z=0} = \hbar \omega_{\perp}$. Due to the constraint of Eq. (10), the momentum k is limited according to the relation $k < \sqrt{\frac{2\mu}{\hbar^2} (E_{n=2, m_z=0} - E_{n=0, m_z=0})}$. Here, $\Psi(z, \rho)$ denotes the full 2D axially symmetric solution, which can be expanded in the $\tilde{\Phi}_{n,0}(\rho, \phi) \equiv \Phi_n(\rho)$ basis:

$$\Psi(z, \rho) = \sum_{n=0}^{\infty} C_n(z) \Phi_n(\rho), \quad (12)$$

where we sum over all even n due to the bosonic symmetry.

Substituting Eq. (12) into Eq. (11), multiplying by $2\pi\rho\Phi_n^*(\rho)$, integrating, and using Eq. (9) yields the following equation for the functions $C_n(z)$:

$$\left[-\frac{\hbar^2}{2\mu} \frac{\partial^2}{\partial z^2} + E_{n, m_z=0} - E \right] C_n(z) = - \int_0^{\infty} \Phi_n^*(\rho) V_{ps,\ell}(\mathbf{r}) \Psi(z, \rho) 2\pi\rho d\rho. \quad (13)$$

By solving Eq. (13) for $n = 0$ we obtain the scattering wave function $C_0(z)$ in the open channel, which has the following asymptotic form:

$$C_0(z) = \cos(kz) + f_{e,\ell} e^{ik|z|} \quad \text{for } |z| \rightarrow \infty, \quad (14)$$

where $f_{e,\ell}$ is the one-dimensional scattering amplitude of the ℓ -wave interaction which describe the even scattered waves.

For $n > 0$, Eq. (13) provides us with the solution for the virtual excitations associated with the closed channels, which decay exponentially according to the relation

$$C_n(z) = A_{n,\ell} e^{-\sqrt{n/2 - (ka_{\perp}/2)^2} 2|z|/a_{\perp}}, \quad (15)$$

where the coefficients $A_{n,\ell}$ refer to the ℓ -wave interaction and denote the transition amplitudes from the transverse ground state to the n th excited state.

In the case of the d -wave pseudopotential we substitute Eq. (14) into Eq. (13) for $n = 0$ and Eq. (15) into Eq. (13) for $n > 0$ and integrate over the z variable, in the interval $[-\epsilon, \epsilon]$ with $\epsilon \rightarrow 0$. Finally, we obtain the following relations for the d -wave scattering and transition amplitudes:

$$f_{e,d} = i \frac{a_d^5(k) \sqrt{\pi}}{24ka_{\perp}^3} \eta_d, \quad A_{n,d} = \frac{a_d^5(k) \sqrt{\pi}}{48a_{\perp}^3} \eta_d \frac{2n+1}{\sqrt{\frac{n}{2} - \left(\frac{ka_{\perp}}{2}\right)^2}}, \quad (16)$$

where η_d is the regularized part of the wave function Ψ in the limit $\mathbf{r} \rightarrow \mathbf{0}$,

$$\eta_d = \frac{\partial^5}{\partial z^5} \left\{ z^5 \left[\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} \right) \Psi(z, \rho) \right]_{\substack{x \rightarrow 0 \\ y \rightarrow 0}} - 2 \frac{\partial^2}{\partial z^2} \Psi(z, \rho) \right]_{\substack{x \rightarrow 0 \\ y \rightarrow 0}} \Bigg|_{z \rightarrow 0^+}, \quad (17)$$

with ρ given by the relation $\rho = \sqrt{x^2 + y^2}$.

Then the expression for the wave function reads

$$\Psi(z, \rho) = \left[\cos(kz) + i \frac{a_d^5(k) \sqrt{\pi}}{24ka_\perp^3} \eta_d e^{ik|z|} \right] \Phi_0(\rho) + \frac{a_d^5(k) \sqrt{\pi}}{48a_\perp^2} \eta_d \Lambda_1(z, \rho), \quad (18)$$

where $\Lambda_1(z, \rho)$ is defined as follows:

$$\Lambda_1(z, \rho) = \sum_{n=2}^{\infty} \frac{2n+1}{\sqrt{\frac{n}{2} - \left(\frac{ka_\perp}{2}\right)^2}} e^{-\sqrt{n/2 - (ka_\perp/2)^2} 2|z|/a_\perp} \Phi_n(\rho). \quad (19)$$

Let us now to proceed with the explicit definition of the regular part η_d of the wave function, which is a solution of Eq. (17). The action of the operator $(\partial_x^2 + \partial_y^2)$ on $\Psi(\mathbf{r})$ for $x, y \rightarrow 0$ results in the following relation:

$$\begin{aligned} & (\partial_x^2 + \partial_y^2) \Psi(z, \rho) \Big|_{\substack{x \rightarrow 0 \\ y \rightarrow 0}} \\ &= -\frac{2}{a_\perp^3 \sqrt{\pi}} \left[\cos(kz) + i \frac{a_d^5(k) \sqrt{\pi}}{24ka_\perp^3} \eta_d e^{ik|z|} \right] \\ & \quad - \frac{a_d^5(k)}{24a_\perp^5} \eta_d \Lambda_2(z, \rho = 0), \end{aligned} \quad (20)$$

where $\Lambda_2(z, \rho = 0)$ reads

$$\Lambda_2(z, \rho = 0) = \sum_{n=2}^{\infty} \frac{(2n+1)^2}{\sqrt{\frac{n}{2} - \left(\frac{ka_\perp}{2}\right)^2}} e^{-\sqrt{n/2 - (ka_\perp/2)^2} 2|z|/a_\perp}. \quad (21)$$

Here, we should note that the Λ series at $\rho = 0$ are not converging uniformly as $z \rightarrow 0$. This means that the partial derivative with respect to the z coordinate cannot be interchanged with the sum over all even n . Thus, first one has to perform the summation and then differentiate with respect to the z coordinate. However, with the help of Euler's summation formula [29] one can express the Λ series as an expansion with respect to the z variable, where the singular part of the Λ series will be written in closed form, yielding the following expressions:

$$\begin{aligned} \Lambda_1(z, \rho = 0) &= \frac{2a_\perp^3}{|z|^3} + \frac{a_\perp}{|z|} + q_1 + q_2 \frac{2|z|}{a_\perp} \\ & \quad + q_3 \left(\frac{2|z|}{a_\perp} \right)^2 + \dots, \end{aligned} \quad (22)$$

$$\Lambda_2(z, \rho = 0) = \frac{24a_\perp^5}{|z|^5} + \frac{4a_\perp^3}{|z|^3} + \frac{a_\perp}{|z|} + b_1 + \dots, \quad (23)$$

where $q_1 \approx -2.29225$, $q_2 = 0.83333$, $q_3 \approx -0.154912$, and $b_1 \approx -3.5336$ are constants calculated via Euler's summation formula.

Consequently, by substituting Eqs. (18)–(23) into Eq. (17) we obtain η_d , which is now free of divergences. This in turn yields the following expression for the one-dimensional

scattering amplitude:

$$f_{e,d} = -\frac{1}{1 + ika_\perp \left(-\frac{a_\perp^5}{10a_d^5(k)} + b_2 \right)}, \quad (24)$$

where the constant $b_2 \approx 2.386445$ is defined by the relation $b_2 = -\frac{b_1}{2} - 4q_3$. The resonance condition for $f_{e,d}$ then reads

$$\frac{a_\perp}{a_d(k)} = \sqrt[5]{10b_2}. \quad (25)$$

Equation (24) shows that the d -wave scattering in the presence of the waveguide becomes resonant at an off-resonant value of the free-space $a_d(k)$ scattering length, due to the significant contributions of the virtual excitations. The latter holds equally for the case of s -wave CIRs. Therefore, one can conclude that in general the appearance of resonances in systems with transverse confinement is caused by the virtual excitations in the transverse modes.

By applying the s -wave pseudopotential, given in Eq. (6), and performing the derivation as mentioned above, we will obtain the same relation for the one-dimensional scattering amplitude as in Ref. [5] with the difference that in this case the s -wave scattering length is energy dependent [9]:

$$f_{e,s} = -\frac{1}{1 + ika_\perp \left(-\frac{a_\perp}{2a_s(k)} + \frac{c_1}{2} \right)}. \quad (26)$$

The constant c_1 in Eq. (26) is equal to 1.4603.

IV. RESULTS AND DISCUSSION

In this section we compare the analytical results of the previous section for the s - and d -wave pseudopotentials with the corresponding numerical simulations. First we evaluate the d - and s -wave energy-dependent scattering lengths by solving numerically a model of Cs atoms in free space interacting via a Lennard-Jones potential $V(r) = \frac{C_{12}}{r^{12}} - \frac{C_6}{r^6}$. Note that Cs atoms are ideal candidates for studying scattering phenomena, since they provide a rich spectrum of resonances [30,31].

The dispersion coefficient C_6 has been taken from [32,33] and C_{12} is a free parameter, which controls the values for the s - and d -wave scattering lengths. This yields a parametrization of the one-dimensional s - and d -wave scattering amplitudes, Eqs. (26) and (24), respectively, in terms of C_{12} .

In order to numerically solve the Cs-Cs collisions in the harmonic waveguide we employ the units $m_{\text{Cs}}/2 = \hbar = \omega_0 = 1$, where m_{Cs} is the mass of the Cs atom and $\omega_0 = 2\pi \times 10$ MHz. The longitudinal energy is set to $\varepsilon_{\parallel} = 2 \times 10^{-6}$ and the transverse energy is varied within the interval $10^{-5} \leq \varepsilon_{\perp} \leq 8 \times 10^{-4}$, corresponding to a range $0.2\pi \leq \omega_{\perp} \leq 16\pi$ kHz for the waveguide confinement frequency. We thereby focus on the low-energy regime, characterized by $ka_{\perp} \ll 1$. In the following we calculate the transmission coefficient given by

$$T_{\ell} = |1 + f_{e,\ell}|^2, \quad (27)$$

where $f_{e,\ell}$ is the one-dimensional scattering amplitude for the ℓ wave.

In Fig. 1 we show the transmission coefficient as a function of C_{12} with the transverse frequency $\omega_{\perp} = 10^{-5}$. T_n in Fig. 1(a) denotes the numerically calculated transmission coefficient, as was shown in Refs. [26,34,35]. We observe the appearance of

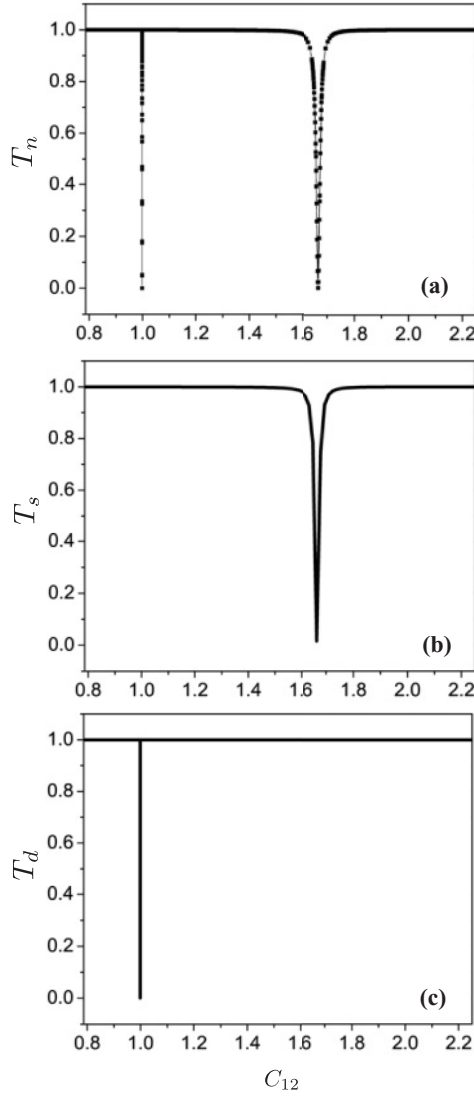


FIG. 1. (a) Numerically calculated transmission coefficient T_n , which shows the DWR on the LHS and the s -wave CIR on the RHS. The analytically calculated (b) s -wave transmission coefficient T_s and (c) d -wave transmission coefficient T_d . The transverse confinement is $\omega_{\perp} = 10^{-5}$.

two minima ($T_n = 0$) due to resonances. The minimum on the right-hand side (RHS) of Fig. 1(a) refers to the s -wave CIR and the minimum on the LHS to the DWR. Due to the centrifugal barrier, the width of the DWR is much smaller than that of the s -wave CIR. Additionally, we observe that both resonances yield a Lorentzian-like line shape in the transmission spectrum. This occurs due to the fact that the weak confinement suppresses the interference effects between the s -wave and d -wave interactions.

In Fig. 1(b) the analytically calculated transmission coefficient T_s , as given by Eqs. (26) and (27), is shown, which refers to s -wave interactions only. T_s describes very accurately the s -wave CIR [see Figs. 1(a) and 1(b)], whereas there is no trace of the DWR, since contributions from higher partial waves are not included in Eq. (26). In Fig. 1(c) the analytic expression of the transmission coefficient T_d is depicted according to Eqs. (24) and (27). We observe that the DWR is described qualitatively accurately enough [see also the insets of Figs. 2(a)

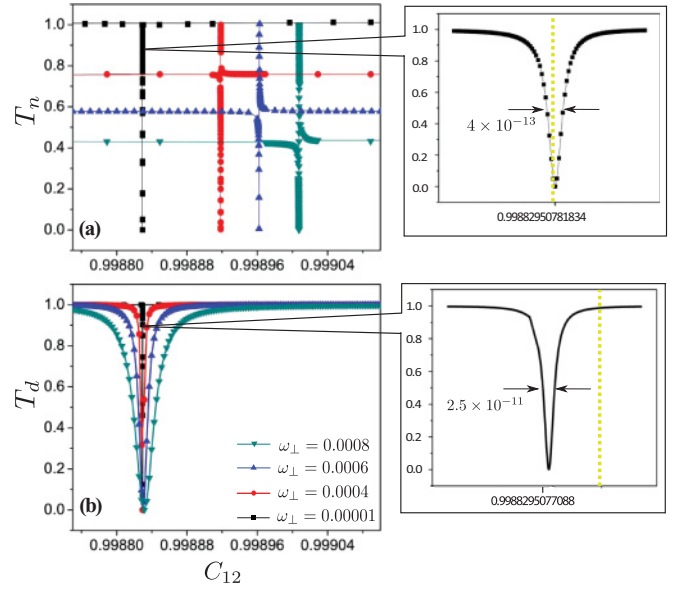


FIG. 2. (Color online) (a) Left panel: The numerically calculated transmission coefficient T_n versus C_{12} parameter for several confinement frequencies ω_{\perp} ; right panel: high-resolution graph of the DWR for $\omega_{\perp} = 10^{-5}$ where the inward-pointing arrows denote the width of the resonance. (b) Left panel: The analytically calculated transmission coefficient T_d as a function of the C_{12} parameter calculated with the d -wave pseudopotential for the corresponding values of ω_{\perp} ; right panel: high-resolution graph of the DWR for $\omega_{\perp} = 10^{-5}$. The yellow dashed line in the right panels indicates the minimum of the numerical calculated transmission coefficient ($T_n = 0$) in comparison with the corresponding analytical result.

and 2(b)], despite the fact that in the analytical calculations we have neglected the contributions of s -wave scattering, since the transverse confinement is very weak. We note that the results shown in Figs. 1(b) and 1(c), being obtained analytically for the pure s - and d -wave scattering cases, lead to an accurate description of the scattering processes in the presence of a weak external harmonic potential.

Let us now determine the regime of validity of the approximate analytical results for the d -wave pseudopotential scattering by comparing it with the corresponding numerical simulations. In Fig. 2 we show the transmission coefficient T calculated numerically [Fig. 2(a)] and analytically [Fig. 2(b)] for several transversal confinement frequencies ω_{\perp} . In Fig. 2(a) for a strong confinement, e.g., $\omega_{\perp} = 8 \times 10^{-4}$, we first observe that the numerically calculated position of the resonance deviates substantially from the analytical one. However, as ω_{\perp} decreases, the numerical results for the position of the DWR converge to the corresponding analytical one. The origin of this behavior is the fact that we considered only d -wave interactions in the analytical calculations and neglected contributions from the s -wave interactions. This approximation is eligible in the regime of a weak confinement, e.g., $\omega_{\perp} \leq 4 \times 10^{-5}$, where the s - and d -wave free-space resonances are weakly coupled, and in the vicinity of the DWR the d -wave interactions are dominant over those of the s waves. In the regime of strong confinement the transmission spectrum T , in the vicinity of the DWR, exhibits a strong asymmetric Fano line shape,

with T_n changing abruptly from zero to 1. The latter is an interference effect of the strong s - and d -wave interactions in the confinement and cannot be described by this analytical pure- d -wave model. However, this asymmetric profile gets suppressed with decreasing ω_{\perp} , yielding a Lorentzian-like line shape.

The right panels of Fig. 2 show a high-resolution graph of the DWR calculated analytically and numerically for $\omega_{\perp} = 10^{-5}$, where the dashed vertical line in both plots indicates the position of the minimum of the numerically calculated transmission coefficient T_n . We observe that the d -wave pseudopotential approximation qualitatively describes the numerical simulations in the regime of weak confinement. However, in this small scale of the C_{12} values the analytical results show that the DWR is two orders of magnitude wider than the numerical predictions, and also there is a slight difference in the position of the DWR. These quantitative deviations again occur due to s -wave interactions, which act as corrections in the transmission coefficient T_n despite the weak coupling of the s -wave and d -wave interactions.

V. BRIEF SUMMARY

We have derived and analyzed analytical expressions for resonant d -wave scattering in a harmonic waveguide, in the framework of pseudopotential theory. The interatomic interaction has been modeled by a pure d -wave pseudopotential introduced in Refs. [14,15]. We observe that the analytical

pseudopotential approach provides results which are in qualitative agreement with the corresponding numerical results in the regime of weak confinement due to the very small interference effects of s - and d -wave interactions. The appearance of the DWR in a waveguide is strongly affected by the virtual excitations over all the closed excited modes of the transverse confinement. For a strong transverse confinement the analytically and numerically calculated line shapes and the positions of the DWR deviate from each other. The interference effect of the s - and d -wave free-space resonances in the confinement yields an asymmetric Fano profile which cannot be derived by a single-partial-wave model. Our analytical result Eq. (24) for weak confinement can be used for the analysis of resonant scattering processes in confined geometries beyond s -wave physics. Finally, we remark that our work clearly demonstrates the necessity of an extended pseudopotential theory capable of describing systems which possess a nonspherical symmetry that yields interference phenomena between different partial-wave scattering amplitudes.

ACKNOWLEDGMENTS

P.G. thanks C. Morfonios and F. K. Diakonov for valuable comments and discussions. V.S.M. acknowledges financial support by the Deutsche Forschungsgemeinschaft and the Heisenberg-Landau Program. P.S. acknowledges the Deutsche Forschungsgemeinschaft for financial support.

-
- [1] E. Fermi, *Nuovo Cimento* **11**, 157 (1934).
 - [2] K. Huang and C. N. Yang, *Phys. Rev.* **105**, 767 (1957).
 - [3] K. Huang, *Statistical Mechanics* (John Wiley & Sons, New York, 1963).
 - [4] T. Busch, B.-G. Englert, K. Rzazewski, and M. Wilkens, *Found. Phys.* **28**, 549 (1998).
 - [5] M. Olshanii, *Phys. Rev. Lett.* **81**, 938 (1998).
 - [6] T. Kinoshita, T. Wegner, and D. S. Weiss, *Science* **305**, 1125 (2004).
 - [7] B. Paredes *et al.*, *Nature (London)* **429**, 277 (2004).
 - [8] E. Haller, M. Gustavsson, M. J. Mark, J. G. Danzl, R. Hart, G. Pupillo, and H. C. Nägerl, *Science* **325**, 1224 (2009).
 - [9] E. Tiesinga, C. J. Williams, F. H. Mies, and P. S. Julienne, *Phys. Rev. A* **61**, 063416 (2000).
 - [10] D. Blume and C. H. Greene, *Phys. Rev. A* **65**, 043613 (2002).
 - [11] E. L. Bolda, E. Tiesinga, and P. S. Julienne, *Phys. Rev. A* **66**, 013403 (2002).
 - [12] A. Derevianko, *Phys. Rev. A* **72**, 044701 (2005).
 - [13] R. Stock, A. Silberfarb, E. L. Bolda, and I. H. Deutsch, *Phys. Rev. Lett.* **94**, 023202 (2005).
 - [14] Z. Idziaszek and T. Calarco, *Phys. Rev. Lett.* **96**, 013201 (2006).
 - [15] Z. Idziaszek, *Phys. Rev. A* **79**, 062701 (2009).
 - [16] F. Stampfer and P. Wagner, *J. Math. Anal. Appl.* **342**, 202 (2008).
 - [17] L. Pricoupenko, *Phys. Rev. Lett.* **96**, 050401 (2006).
 - [18] K. Huang, *Int. J. Mod. Phys. A* **4**, 1037 (1989).
 - [19] Y. N. Demkov and G. F. Drukarev, *Sov. Phys. JETP* **54**, 650 (1981).
 - [20] M. V. Frolov, N. L. Manakov, E. A. Pronin, and A. F. Starace, *Phys. Rev. Lett.* **91**, 053003 (2003).
 - [21] A. M. Rey, R. Sensarma, S. Fölling, M. Greiner, E. Demler, and M. D. Lukin, *Europhys. Lett.* **87**, 60001 (2009).
 - [22] B. Deb and J. Hazra, *Phys. Rev. Lett.* **103**, 023201 (2009).
 - [23] W. Hofstetter, J. I. Cirac, P. Zoller, E. Demler, and M. D. Lukin, *Phys. Rev. Lett.* **89**, 220407 (2002).
 - [24] K. Kanjilal and D. Blume, *Phys. Rev. A* **70**, 042709 (2004).
 - [25] K. Günter, T. Stöferle, H. Moritz, M. Köhl, and T. Esslinger, *Phys. Rev. Lett.* **95**, 230401 (2005).
 - [26] P. Giannakeas, V. S. Melezhik, and P. Schmelcher, *Phys. Rev. A* **84**, 023618 (2011).
 - [27] U. Fano, *Phys. Rev.* **124**, 1866 (1961).
 - [28] T. M. MacRobert, *Spherical Harmonics* (Dover, New York, 1948).
 - [29] T. M. Apostol, *Am. Math. Mon.* **106**, 409 (1999).
 - [30] C. Chin, V. Vuletic, A. J. Kerman, S. Chu, E. Tiesinga, P. J. Leo, and C. J. Williams, *Phys. Rev. A* **70**, 032701 (2004).
 - [31] M. Mark, F. Ferlaino, S. Knoop, J. G. Danzl, T. Kraemer, C. Chin, H. C. Nägerl, and R. Grimm, *Phys. Rev. A* **76**, 042514 (2007).
 - [32] A. Derevianko, J. F. Babb, and A. Dalgarno, *Phys. Rev. A* **63**, 052704 (2001).
 - [33] S. G. Porsev and A. Derevianko, *Phys. Rev. A* **65**, 020701(R) (2002).
 - [34] V. S. Melezhik, *J. Comput. Phys.* **92**, 67 (1991).
 - [35] S. Saedian, V. S. Melezhik, and P. Schmelcher, *Phys. Rev. A* **77**, 042721 (2008).