Atom-Atom Scattering under Cylindrical Harmonic Confinement: Numerical and Analytic Studies of the Confinement Induced Resonance

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It was recently predicted [Phys. Rev. Lett. **81**, 938 (1998)] that atom-atom scattering under transverse harmonic confinement is subject to a "confinement-induced resonance" where the effective one-dimensional coupling strength diverges at a particular ratio of the confinement and scattering lengths. As the initial prediction made use of the zero-range pseudopotential approximation, we now report numerical results for finite-range interaction potentials that corroborate this resonance. In addition, we now present a physical interpretation of this effect as a novel type of Feshbach resonance in which the transverse modes of the confining potential assume the roles of "open" and "closed" scattering channels.

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There have been a number of recent experiments in which ultracold atoms have been loaded into magnetic or optical "atom waveguides" [1–8]. One goal of such experiments is to reach the single-mode or quasi-1D regime, where only the ground state of transverse motion is significantly populated. This regime is important for the design of ultrasensitive rotation and gravitational gradient detectors based on guided-atom interferometers. In addition, the 1D delta-interacting boson gas is of significant theoretical interest as one of the few known fully integrable quantum field theories; e.g., in a finite system with infinitely strong delta-function interactions, boson N-body states have been shown to correspond via a one-to-one mapping with the highly correlated states of the corresponding noninteracting Fermi gas [9–15]. The homogeneous 1D Bose with arbitrary-strength delta-function interactions is also a fully integrable system [16].

To connect experiments in tightly confining waveguides with theoretical 1D models, it is necessary to relate the effective 1D coupling constant, g_{1D}, and the 3D scattering length, a. This problem was first addressed rigorously in [17], resulting in the prediction of a "confinement induced resonance" (CIR). At the CIR, the g_{1D} can be tuned from $-\infty$ to $+\infty$ by varying the transverse width of the waveguide, $a_\perp$, over a small range in the vicinity of the resonance at $a_\perp = Ca$, where $C = 1.4603\ldots$. Until now, however, there has been no convincing physical explanation for the effect, thus raising questions concerning its appearance in systems with finite-range interactions.

The primary goal of this Letter is to present numerical results for atom-atom scattering in a harmonic waveguide via finite-range interaction potentials, to confirm the existence of the CIR. In addition, we provide a much-needed physical interpretation of the effect as a Feshbach-type resonance involving bound states of the energetically closed transverse modes ("channels"). Analogous numerical scattering studies in spherically symmetric traps have been reported [18,19], while scattering under harmonic confinement in one dimension is discussed in [20,21].

We begin by considering a collision between two atoms, each initially in the ground state of transverse motion. In a harmonic potential, the center-of-mass motion and relative motions are separable, with the wave function of the relative coordinate satisfying an effective single-particle model with a stationary scatterer at the origin. If the longitudinal kinetic energy in the center-of-mass frame is less than the transverse level spacing, then the atoms remain asymptotically frozen in the ground state. Low-energy scattering in this regime can then be modeled in the pseudopotential approximation [22] by the 1D Hamiltonian

$$H_{1D} = -\frac{\hbar^2}{2\mu}\frac{\partial^2}{\partial z^2} + g_{1D}\delta(z), \tag{1}$$

where z is the longitudinal atomic separation and μ is the reduced mass. In the pseudopotential approximation, g_{1D} is typically obtained as in [15] by assuming that the wave function of the relative coordinate $\mathbf{r} = z\hat{\mathbf{z}} + \rho\hat{\boldsymbol{\rho}}$ factorizes as $\Psi(\mathbf{r}) = \phi_0(\rho)\psi(z)$, where $\phi_0(\rho) = (a_\perp\sqrt{\pi})^{-1}e^{-\rho^2/2a_\perp^2}$ is the transverse ground state. Here $a_\perp = \sqrt{\hbar/\mu\omega_\perp}$ is the transverse oscillator length for the relative atomic motion, $\omega_\perp$ being the transverse trap frequency. The effective 1D potential is then defined via $g_{1D}\delta(z) = \int 2\pi\rho d\rho|\phi_0(\rho)|^2 \frac{2\pi\hbar^2 a}{\mu}\delta^3(\mathbf{r})$, which gives

$$g_{1D} \approx \frac{2\hbar^2 a}{\mu a_\perp^2}. \tag{2}$$

By matching the low-energy ($ka_\perp \ll 1$) scattering amplitude of the exact solution in 3D to that of Eq. (1), however, it was determined [17] that

$$g_{1\mathrm{D}} = \frac{2\hbar^2 a}{\mu a_\perp^2} \frac{1}{(1 - Ca/a_\perp)}, \tag{3}$$

where $C = -\zeta(1/2) = 1.4603\ldots$ The appearance of a resonance term in the denominator implies that the hard-core Tonks-Girardeau regime can be accessed via the CIR condition $a_\perp \approx Ca$. The naive formulation (2), on the other hand, implies that accessing this regime would require the more extreme condition $a \gg na_\perp^2$, where n is the linear density.

Before addressing the physical interpretation of this resonance, we first describe our numerical calculations of 1D scattering amplitudes for finite-range interactions. The relation between $g_{1\mathrm{D}}$ and the 1D scattering amplitude may be found by assuming that the scattering eigenstates $\Psi(z)$ of Hamiltonian (1) take the form given in [17]:

$$\Psi(z) = e^{ikz} + f_e e^{ik|z|}; \qquad E = \hbar^2 k^2/2\mu. \tag{4}$$

Substituting this form into Schrödinger's equation with (1) then gives

$$g_{1\mathrm{D}} = \lim_{k \to 0} \frac{\hbar^2 k f_{eR}(k)}{\mu f_{eI}(k)}, \tag{5}$$

where f_{eR} and f_{eI} are the real and imaginary parts of f_e. To extract analogous values for $g_{1\mathrm{D}}$ from numerical scattering calculations, we obtain eigenfunctions of the Hamiltonian $\hat{H} = \hat{H}_z + \hat{H}_\perp + \hat{V}$, where

$$\begin{aligned} \hat{H}_z &= -\frac{\hbar^2}{2\mu}\frac{\partial^2}{\partial z^2}; \\ \hat{H}_\perp &= -\frac{\hbar^2}{2\mu}\left[\frac{\partial^2}{\partial \rho^2} + \frac{1}{\rho}\frac{\partial}{\partial \rho}\right] + \frac{\mu}{2}\omega_\perp^2 \rho^2. \end{aligned} \tag{6}$$

In the present work, we restrict ourselves to the case of zero azimuthal angular momentum $m = 0$, as there is negligible s-wave scattering for $m \neq 0$. For the interaction potential, we study two cases: $V(r) = C_{12}/r^{12} - C_6/r^6 r^2 = z^2 + \rho^2$ and the spherical square well, $V(r) = -\bar{V}S(b - r)$, $S(r)$ being the unit step function.

With application to the case of Cs atoms in a 1D optical well [8] in mind, we consider atoms with the mass of ^{133}Cs, and with the C_6 coefficients as determined recently [23] to be $C_6(\mathrm{Cs}) = 6890$ a.u. For Cs atoms in the $(F, M) = (3, 3)$ state, the scattering length is determined only as an upper bound, $a < -140$ nm, as compared with $a_\perp = 29.5$ nm reported in [8]. In order to study the general situation, we allow C_{12} to vary, and focus on the regime of 1 to 3 $J = 0$ bound states, rather than the 47 bound states in the actual $\mathrm{Cs}^2\ {}^3\Sigma_u^+$ state, and we neglect other terms in the dispersion potential. The 6–12 potential may be characterized by R_e, the minimum of the potential well, where $R_e = (2C_{12}/C_6)^{1/6}$. For $C_6 = C_6(\mathrm{Cs})$ and for a series of values of C_{12} we obtain the free-space s-wave scattering length, a, by Numerov integration of the Schrödinger equation. When a resonance state passes through threshold a exhibits a simple pole, thus the 6–12 potential provides the full range of 3D scattering lengths. For the case of a spherical well potential, the scattering length for a well of depth $\bar{V}$ and range b is given by $a = b - \tan(b\eta)/\eta$, where $\eta^2 = 2\mu\bar{V}/\hbar^2$.

To solve the scattering problem for such central potentials plus a transverse harmonic potential, we employ a numerical mesh in ρ and z, and find eigenfunctions in a cylindrical box of finite length. The box is sufficiently long in z that the asymptotic form of the wave function as $|z| \to \infty$ is readily determined. The eigenfunctions are of odd or even parity, with the odd-parity functions exhibiting negligible scattering effects. For even functions of energy $E = \hbar\omega_\perp + \hbar^2 k^2/2\mu$, the asymptotic form is

$$\Psi(\rho, z) \xrightarrow{|z| \to \infty} \mathcal{N}[(1 + f_{eR})\cos(kz) - f_{eI}\sin(k|z|)]\phi_0(\rho). \tag{7}$$

Values for f_{eR}, f_{eI}, and $\mathcal{N}$ are thus extracted from a fit to Eq. (7), determined over a range of z values for which $V(r)$ is negligible, and from conservation of probability current. From f_{eR} and f_{eI}, $g_{1\mathrm{D}}$ is then obtained from Eq. (5) via extrapolation of finite k data to $k = 0$. The numerical mesh was provided by the discrete variable representation (DVR). In order to increase the density of points near $z = 0$, the z coordinate was scaled by $z = U(y)$, where $U(y) = a\cosh(z/b)$, analogous to scaling used in [24]. A uniform mesh in y was then used [25] along with a Laguerre DVR in ρ [26].

Numerical results for $g_{1\mathrm{D}}$ with model potentials are shown in Fig. 1, along with the analytic result (3). The numerical calculations clearly exhibit a singularity in $g_{1\mathrm{D}}$ at $a/a_\perp \approx 1/C$. For a less than this value, the calculated $g_{1\mathrm{D}}$ values agree well with the analytic expression. There do appear to be systematic deviations between the exact numerical results and the pseudopotential theory that are greater for the 6–12 potential than for the spherical well for $a/a_\perp > 1/C$. As we will see, this effect can be explained via a Feshbach-resonance interpretation.

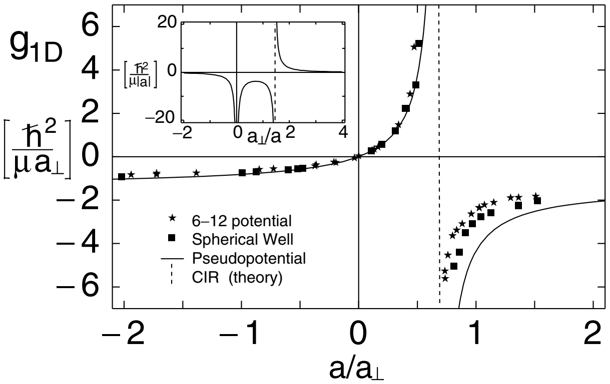

FIG. 1. The 1D coupling constant, $g_{1\mathrm{D}}$, in units of $\hbar^2/(\mu a_\perp)$, as a function of $a/a_\perp$ for the 6–12 potential (stars) and the spherical well potential (triangles), as compared to the pseudopotential theory (solid line). The inset shows $g_{1\mathrm{D}}$ in units of $\hbar^2/(\mu|a|)$ versus $a_\perp/a$, to illustrate the behavior in the tight-confinement regime ($a_\perp/a \to 0$).

These numerical results validate the pseudopotential analytic result [17], demonstrating that the CIR is indeed a physical phenomena rather than an artifact of the pseudopotential approximation. It is therefore important to establish the physical origin of the CIR. In what follows, we show that the CIR is in fact a zero-energy Feshbach resonance, occurring when the energy of a bound state of the asymptotically closed channels (i.e., the excited transverse modes) coincides with the continuum threshold of the open channel (lowest transverse mode).

This explanation is best verified by artificially severing the coupling between the ground transverse mode and the manifold of excited modes. If a bound state of the decoupled excited manifold exists, then a zero-energy Feshbach resonance will occur when this bound-state energy coincides with the continuum threshold of the ground transverse mode. To determine the relevant bound-state energies, we consider the total Hamiltonian $\hat{H} = \hat{H}_z + \hat{H}_\perp + \hat{V}_{\text{pseudo}}$, where the V_{pseudo} is the standard Huang-Fermi pseudopotential. Because our interpretation of the CIR relies heavily on the behavior of two-atom bound states, it might be useful to recall that the Huang-Fermi pseudopotential, $\hat{V}_{\text{pseudo}}$, supports a single bound state in free space at $E = \hbar^2/(\mu a^2)$ for the case $a > 0$. To determine the location of the CIR, we need to ask what happens to the energy of this bound state if a single transverse mode is projected out of the Hilbert space. We therefore proceed by formally splitting the Hamiltonian onto "ground," "excited," and "ground-excited coupling" parts according to

$$\begin{aligned}\hat{H} &= \hat{H}_g + \hat{H}_e + \hat{H}_{g-e}\\ &= \hat{P}_g\hat{H}\hat{P}_g + \hat{P}_e\hat{H}\hat{P}_e + (\hat{P}_e\hat{H}\hat{P}_g + \text{H.c.}),\end{aligned} \tag{8}$$

where $\hat{P}_g = |0\rangle\langle 0|$, $\hat{P}_e = \sum_{n=1}^{\infty} |n\rangle\langle n|$, are the corresponding projection operators, $|n\rangle$ being the eigenstate of the transverse two-dimensional harmonic oscillator with *radial* quantum number n and zero axial angular momentum. The corresponding eigenvalues of the transverse Hamiltonian are given by $\hat{H}_\perp|n\rangle = \hbar\omega_\perp(2n+1)|n\rangle$.

The ground Hamiltonian has a 1D coordinate representation of the form of Eq. (1), corresponding to the motion of a one-dimensional particle in the presence of a δ barrier with the "bare" coupling constant given by Eq. (2). The spectrum of $\hat{H}_g$ is continuous for energies above the threshold energy $E_{C,g} = \hbar\omega_\perp$. Likewise, the spectrum of the excited Hamiltonian is clearly continuous for energies $E_{C,e} = 3\hbar\omega_\perp$ but, as we will see below, $\hat{H}_e$ supports one bound state of an energy $E_{B,e} < E_{C,e}$ for *all* values of the 3D scattering length, a.

According to the Feshbach scheme, one would predict a resonance in the renormalized $g_{1\text{D}}$ for a set of parameters, such that the energy of the bound state of $\hat{H}_e$ coincides with the continuum threshold of $\hat{H}_g$. Thus, the CIR condition can be expressed as $E_{B,e} = E_{C,g}$. As we will see below, this scheme indeed predicts a position of the CIR *exactly.*

The energy $E_{B,e}$ of the bound state of $\hat{H}_e$ can be found using the following two step procedure. First, we identify the bound-state energy of the full Hamiltonian $\hat{H}$ as a pole of the scattering amplitude on the physical Riemann sheet. Second, we make use of the peculiar property of the two-dimensional harmonic oscillator that the excited Hamiltonian $\hat{H}_e$ and the full Hamiltonian $\hat{H}$ can be transformed to each other via a simple unitary transformation. This leads to a simple relation between their bound-state energies.

The even-wave one-dimensional scattering amplitude f_e at an energy E ($E_{c,g} \le E < E_{c,e}$), as defined in (4), has been derived in [17]. We have now obtained a closed-form analytic expression for the previously derived result, so that the scattering amplitude can be expressed as

$$f_e(k) = -\frac{2i}{ka_\perp[\frac{a_\perp}{a} + \zeta(1/2,\ -(ka_\perp/2)^2)]}, \tag{9}$$

where

$$\begin{gathered}\zeta(s,\ \alpha) = \lim_{N\to\infty}\left[\sum_{n=0}^{N}\frac{1}{(n+\alpha)^s} - \frac{(N+\alpha)^{-s+1}}{-s+1}\right],\\ \text{Re}(s) > 0, \qquad \text{Im}(s) = 0, \qquad z^s = |z|^s e^{is[\text{Arg}(z) - 2\pi]},\\ 0 < \text{Arg}(z) \le 2\pi\end{gathered} \tag{10}$$

is the Hurwitz zeta function [27], and the wave vector k is given by $E = E_{C,g} + \hbar^2k^2/2\mu$. The bound-state energies of the full Hamiltonian $\hat{H}$ will be given by the poles, $\bar{k}$, on the *positive imaginary* axis of the analytic continuation of $f_e(k)$: $E_B = -\hbar^2\,\text{Im}^2(\bar{k})/2\mu$. One can see that, in order to avoid crossing the branch cuts of the zeta function, the continuation should be performed inside the $0 \le \text{Arg}(k) \le \pi/2$ quadrant of the complex plane. In the end, we find a single pole corresponding to the following implicit equation for the bound-state energy: $\zeta[1/2,\ -E_B/(2\hbar\omega_\perp) + 1/2] = -a_\perp/a$.

Now the full Hamiltonian $\hat{H}$ and the excited Hamiltonian $\hat{H}_e$ are connected via a simple transformation: $\hat{H}_e = \hat{A}^\dagger\hat{H}\hat{A}$, where $\hat{A}^\dagger = \sum_{n=0}^{\infty}|n+1\rangle\langle n|$. Note that both $\hat{H}_e$ and $\hat{H}$ include interactions; thus the above property is highly nontrivial and stems from the fact that the $m = 0$ eigenfunctions of the two-dimensional harmonic oscillator all have the same value at the origin. The 3D δ interaction thus has *the same* matrix elements between all the harmonic oscillator states; hence, the interaction matrix is unaffected by the shift operator.

From the above, we conclude that the bound-state energy $E_{B,e}$ of the excited Hamiltonian is related to the bound-state energy E_B of the full Hamiltonian via $E_{B,e} = E_B + 2\hbar\omega_\perp$, and thus satisfies the equation $\zeta[1/2, -E_{B,e}/(2\hbar\omega_\perp) + 3/2] = -a_\perp/a$. The CIR condition can now be explicitly formulated as $\zeta[1/2, -E_{C,g}/(2\hbar\omega_\perp) + 3/2] = -a_\perp/a$. Using $E_{C,g} = \hbar\omega_\perp$, we finally arrive at the exact CIR condition $a_\perp/a = \zeta(1/2, 1) = \zeta(1/2, 0) = -C$. A similar effect is associated with resonance behavior in harmonically confined 2D scattering for $a < 0$ [20]. This

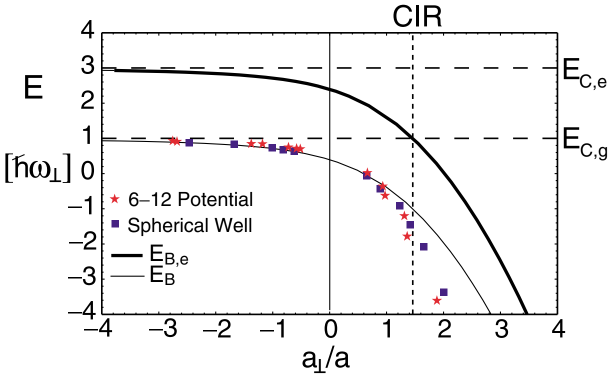

FIG. 2 (color online). Numerical bound-state energies and schematic of the Feshbach resonance scheme. The solid lines correspond to the analytic pseudopotential results.

resonance would most likely be observed via changes in the macroscopic properties of the ground state of a many-atom system, e.g., the density distribution, as described in detail in [12].

This Feshbach scheme is illustrated in Fig. 2, where we plot the bound-state energies $E_{B,e}$ (dark solid line) and E_B (thin solid line) as a function of the ratio $a_\perp/a$. The continuum thresholds $E_{C,e}$ and $E_{C,g}$ are also indicated, illustrating that the CIR occurs when the bound state of the manifold of closed channels, $E_{B,e}$, crosses the continuum threshold of the open channel, $E_{C,g}$. In addition, we have plotted the bound-state energies of the full Hamiltonian as determined numerically for the 6–12 and spherical well potentials, showing good agreement with the pseudopotential result. As the bound-state energy deepens, we start to see quantitative disagreement between the bound-state energies of the finite-range potentials and the pseudopotential. This disagreement is consistent with the discrepancy in the position of the CIR shown in Fig. 1, showing that it is the bound-state energy, and not the scattering length which determines the location of the CIR.

Last, we note that, while in free space a weakly bound state exists only for $a > 0$, we see that in the waveguide such a state exists for all a. These bound states may be of significant interest, allowing the formation of dimers via a modulation of the waveguide potential at the frequency $(E_{C,g} - E_B)/\hbar$. This may lead to an atom-waveguide based scheme for forming ultracold molecules, as well as the possibility to use molecular spectroscopy as a sensitive probe of the atomic field inside the waveguide.

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