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

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M. Olshanii [Phys. Rev. Lett. 81, 938 (1998)] recently solved the atom-atom scattering problem with a pseudopotential interaction in the presence of transverse harmonic confinement, i.e. within an ‘atom waveguide’, deriving an effective one-dimensional coupling constant that diverged at a “confinement induced resonance” (CIR). Here, we report numerical results for finite range 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 waveguide assume the roles of ‘open’ and ‘closed’ scattering channels.

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Recently, there have been a number of experiments in which ultracold atoms and/or Bose-Einstein condensates have been loaded into magnetic or optical ‘atom waveguides’ [1, 2, 3, 4, 5, 6, 7, 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 at thermal equilibrium. This regime is of great practical interest due to the potential for ultra-sensitive rotation and gravitational gradient detection with guided single-mode atom interferometers. In addition to such applications, reaching the quasi-1D regime is of significant theoretical interest as a stationary scatterer at the origin. Furthermore, 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 one dimension using the highly-correlated states of the corresponding non-interacting Fermi gas [9]. The properties of this Tonks-Girardeau gas have been a topic of significant current theoretical interest [10, 11, 12, 13, 14, 15] in anticipation of future atom-waveguide experiments. Additionally, the homogeneous 1D Bose with arbitrary-strength delta-function interactions, known as the Lieb Liniger model, is also a fully integrable system [16].

To make the connection between experiments in tightly confining waveguides and theoretical models in 1D, it is necessary to know the relationship between the effective 1D coupling constant, \( g_{1D} \), and the 3D scattering length, \( a \). This problem was first addressed rigorously in [22], where it was predicted that a ‘confinement induced resonance’ (CIR) modifies the effective interaction, resulting in an effective 1D coupling strength which can be tuned 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 \( C = 1.4603\ldots \). Hence this resonance clearly has significant implications for atom-waveguide experiments. 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, therefore, is to present numerical calculations of scattering in the presence of a cylindrical harmonic potential using finite-range atom-atom potentials, confirming 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 [17, 18], while scattering in the presence of harmonic confinement in one dimension is discussed in [19, 20].

We begin our analysis by considering a collision between two atoms initially in the ground state of transverse motion. In the presence of harmonic transverse confinement the center-of-mass motion and relative motions are separable, with the wavefunction of the relative coordinate satisfying an effective single-particle model with a stationary scatterer at the origin. Furthermore, 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

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

where \( z \) is the longitudinal atomic separation and \( \mu \) is the reduced mass. In the pseudopotential approximation, \( g_{1D} \) is typically obtained as in [15] by assuming that the wavefunction of the relative coordinate \( \mathbf{r} = r_1 - r_2 = z \hat{z} + \rho \hat{\rho} \) factorizes as \( \Psi(\mathbf{r}) = \phi_0(\rho) \psi(z) \), where \( \phi_0(\rho) = \exp(-\rho^2/2a_\perp^2)/(a_\perp \sqrt{\pi}) \) is the transverse ground...
state, and \( a_\perp = \sqrt{\hbar/\mu \omega_\perp} \) is the transverse harmonic oscillator length for the relative atomic motion, \( \omega_\perp \) being the transverse trap frequency. The effective 1D potential is then defined via \( \int 2\pi \rho d\rho \phi_0(\rho)^2 \frac{2\pi \hbar^2 a}{\mu} \delta^3(r) = g_{1D} \delta(z), \) where \( a \) is the 3D scattering length, which leads to
\[
g_{1D} \approx \int_0^\infty 2\pi \rho dp = \frac{2\hbar^2 a}{\mu a_\perp^2}. \tag{2}
\]

From an exact solution of the three-dimensional scattering problem with a zero-range s-wave interaction, however, it was recently predicted \( \cite{22} \) that a “confined induced resonance” (CIR) modifies the effective interaction. By matching the low-energy scattering amplitude of the exact solution to that of Eq. \( \cite{11} \), it was found that:
\[
g_{1D} = \frac{2\hbar^2 a}{\mu a_\perp^2} \frac{1}{(1 - Ca/a_\perp)}, \tag{3}
\]
where \( C = -\zeta(1/2) = 1.4603... \) We note that the use of Eqs. \( \cite{11} \) and \( \cite{13} \) requires \( ka_\perp \ll 1 \), where \( \hbar k \) is the collision momentum. The appearance of the resonance term in the denominator implies that to obtain an infinite delta-function interaction (thereby accessing the Tonks-Girardeau regime), it is sufficient to satisfy the CIR condition \( a_\perp \approx Ca \). From the naive formulation \( \cite{2} \) one would conclude that accessing this regime requires the more extreme condition \( a \gg na_\perp^2 \), where \( n \) is the linear density.

Before addressing the physical interpretation of the CIR, we first describe our numerical results pertaining to low-energy scattering and the effective 1D coupling constant with finite-range interactions. The relation between \( g_{1D} \) and the 1D scattering amplitude may be found by assuming that the scattering eigenstates \( \Psi(z) \) of Hamiltonian \( \cite{11} \) take the form given in \( \cite{22} \)
\[
\Psi(z) = e^{ikz} + f_+ e^{i|z|}; \quad E = \hbar^2 k^2/2\mu, \tag{4}
\]
where \( f_+ \) is the coefficient for the even part of \( \Psi \), while the odd part can be shown to vanish by continuity arguments. From Eq. \( \cite{11} \), we find \( \Psi''(z) = -k^2 \Psi(z) + 2ikf_+(k)\delta(z) \), which must equal \( (2\mu/\hbar^2)g_{1D} \Psi(z) \) in the limit \( k \to 0 \). This gives
\[
g_{1D} = \lim_{k\to 0} \frac{\hbar^2 k f_R(k)}{\mu f_+(k)} \tag{5}
\]
where \( f_R \) and \( f_+ \) are the real and imaginary parts of \( f_+ \). To extract analogous values for \( g_{1D} \) from numerical scattering calculations, we obtain eigenfunctions of the Hamiltonian \( H = H_+ + H_\perp + V \), where
\[
\hat{H}_z = -\frac{\hbar^2}{2\mu} \frac{\partial^2}{\partial z^2}; \quad \hat{H}_\perp = -\frac{\hbar^2}{2\mu} \left[ \frac{\partial^2}{\partial \rho^2} + \frac{1}{\rho} \frac{\partial}{\partial \rho} \right] + \frac{\mu}{2} \omega_\perp^2 \rho^2. \tag{6}
\]
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 atom-atom potential, we will study two cases: \( V(r) = C_{12}/r^{12} - C_6/r^6 \) and the spherical square-well, \( V(r) = -\tilde{V} S(b-r), S(r) \) being the unit step function.

With application to the case of Cs atoms in a 1D optical well \( \cite{8} \), we consider atoms with the mass of \(^{133}\text{Cs} \), and with the \( C_6 \) coefficients as determined recently \( \cite{24} \) to be \( C_6(\text{Cs}) = 6800 \) a.u. For Cs atoms in the \( (F, M) = (3, 3) \) state, the scattering length is determined only as an upper bound, \( a(\text{Cs}) < -140 \) nm, as compared with \( a_{1S} = 29.5 \) nm reported in citeDWeiss. In order to study a more general situation, we allow \( C_{12} \) to vary. To simplify the numerics we consider the regime of just \( 1 \rightarrow 3 \) bound states, rather than the 47 bound states in the actual \( \text{Cs} \) \(^{3}\Sigma^+_u \) 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 \( C_5 = C_6(\text{Cs}) \) 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 \( \alpha \) exhibits a simple pole, thus the 6-12 potential provides the full range of 3D scattering lengths.

For the second case of a spherical well potential the scattering length for a well of depth \( \tilde{V} \) and range \( b \) is given by \( a = b - \tan(\theta)/\eta \), where \( \eta = 2\mu V/h^2 \).

To solve the scattering problem for such central potentials plus a transverse harmonic potential, we employed a numerical mesh in \( \rho \) and \( z \), and found eigenfunctions in a cylindrical box of finite length. The box was sufficiently long in \( z \) that the asymptotic form of the wavefunction as \( |z| \to \infty \) could be determined. The eigenfunctions were of odd or even parity, with the odd parity functions exhibiting negligible scattering effects. For even functions of energy \( E = \hbar^2 \omega_\perp + \hbar^2 k^2/2\mu \), the asymptotic form is
\[
\Psi(\rho, z) \frac{|z| \to \infty}{\sim} \frac{N}{(1 + f_{R})(kz) - f_{1s} \sin (k|z|)} \phi_0(\rho). \tag{7}
\]
Values for \( f_{R}, f_{1s} \) and \( N \) were extracted from the coefficients of \( \sin(kz) \) and \( \cos(kz) \) in Eq. \( \cite{9} \), determined over a range of \( z \) values for which \( V(r) \) is negligible, and from conservation of probability current. From \( f_{R} \) and \( f_{1s} \), \( g_{1D} \) is then obtained from Eq. \( \cite{10} \) 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 \( U(y) = \alpha \cosh(z/b) \), analogous to scaling used in \( \cite{21} \). A uniform mesh in \( y \) was then used along with a Laguerre DVR in \( \rho \) \( \cite{21} \). Eigenfunctions in first iteration were found by exact diagonalization over a relatively small mesh \( (<10,000 \text{ mesh points}) \). Additional mesh points were added, sparse matrix diagonalization techniques were used.

Numerical results for \( g_{1D} \) with the 6-12 potential and with the spherical well are shown in Fig. \( \cite{1} \) in comparison with the analytic result \( \cite{11} \). The numerical calculations clearly exhibit a singularity in \( g_{1D} \) at \( a/a_\perp = 1/C \). For a less than this value the calculated \( g_{1D} \) values agree well.
The pseudopotential operator is defined by the continuum threshold of the open channel (lowest transverse two-dimensional harmonic oscillator with non-zero axial angular momentum) coincides with the energy of a bound state of the asymptotically closed channels. This allows for simple relation between their energy spectra, in particular the energy of the bound state of $H_c$ coincides with the continuum threshold of $H_g$:

$$E_{B,c} = E_{C_g} \Rightarrow \text{CIR}$$

As we will see below this scheme indeed predicts a position of the CIR exactly. The energy $E_{B,c}$ of the bound state of $H_c$ can be found using the following two step procedure. First we identify the bound state energy of the full Hamiltonian $H$ 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 excited Hamiltonian $H_c$ and the full Hamiltonian $H$ can be transformed to each other via a simple unitary transformation. This allows for simple relation between their energy spectra, in particular the energy of the bound states.

The even-wave one-dimensional scattering amplitude $f_e$ at an energy $E$ ($E_{C_g} \leq E < E_{C,e}$), as defined in Eq. 4, has been derived in [22]. We have now obtained a closed-form analytic expression for the previously derived result, so that the scattering amplitude can be expressed as

$$f_e(k) = -\frac{2i}{ka_\perp} \left[ \frac{ka_\perp}{2} \right] \zeta(1/2, -(ka_\perp/2)^2)$$

where

$$\zeta(s, \alpha) = \lim_{N \to \infty} \sum_{n=0}^{N} \frac{1}{(n+\alpha)^s} - \frac{(N+\alpha)^{-s+1}}{-s+1};$$

$$Re(s) > 0, \; Im(s) = 0,$$

$$z^s = |z|^s e^{is(\text{Arg}(z) - 2\pi)}, \; 0 < \text{Arg}(z) \leq 2\pi$$

is the Hurwitz Zeta function [27], and the wave-vector $k$ is given by $E = E_{C_g} + \hbar^2 k^2/2\mu$. The bound state

![Diagram](image-url)
energies of the full Hamiltonian \( \hat{H} \) will be given by the poles, \( k \), on the positive imaginary axis of the analytic continuation of \( f_\varepsilon(k) \): \( E_{B,full} = -\hbar^2 m^2(k)/2\mu \). One can see that in order to avoid crossing the branch-cuts of the Zeta function, the continuation should be performed inside the \( 0 \leq \text{Arg}(k) \leq \pi/2 \) quadrant of the complex plane. We find a single pole corresponding to the following implicit equation for the bound state energy: 
\[
\zeta(1/2, -E_{B,full}/(2\hbar \omega_\perp) + 1/2) = -a_\perp/a.
\]

Notice now, that the full Hamiltonian \( \hat{H} \) and the excited Hamiltonian \( \hat{H}_c \) are connected via a simple transformation: \( \hat{H}_c = A^\dagger \hat{H} A \), where \( A = \sum_{n=0}^\infty |n + 1\rangle \langle n| \). Note that both \( \hat{H}_c \) 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, \( 1/\sqrt{\pi a_\perp} \), at the origin. Thus the three dimensional \( \delta \)-interaction has the same matrix elements between all the harmonic oscillator states so that interaction matrix is unaffected by the shift operator.

From the above we conclude that the bound state energy \( E_{B,c} \) of the ‘excited’ Hamiltonian is related to the bound state energy \( E_B \) of the full Hamiltonian via \( E_{B,c} = E_B + 2\hbar \omega_\perp \), and thus obeys an implicit equation 
\[
\zeta(1/2, -E_{B,c}/(2\hbar \omega_\perp) + 3/2) = -a_\perp/a.
\]

The CIR condition \([22]\) can be now 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 
\[
\frac{\omega_\perp}{\omega} = \zeta(1/2, 1) = \zeta(1/2, 0) = -C.
\]

A similar effect is associated with resonance behavior in harmonically confined 2D scattering for \( a < 0 \) \([13]\). We note that this resonance would most-likely be observed via changes in the macroscopic properties of the ground-state of a many-atom system, i.e. density distribution, as described in \([12]\).

This Feshbach scheme is illustrated in Figure 2, where we plot the bound-state energies \( E_{B,c} \) (dark solid line) and \( E_B \) (thin solid line) as a function of the ratio \( a_\perp/a \). The continuum thresholds \( E_{C,c} \) and \( E_{C,g} \) are also indicated, illustrating that the CIR occurs when the bound state of the manifold of closed channels, \( E_{B,c} \), 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. Lastly, 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 dimer 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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