Tuning the Interactions of Spin-Polarized Fermions Using Quasi-One-Dimensional Confinement

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We develop a multichannel scattering theory for atom-atom collisions in quasi-1D geometries. We apply our general framework to the low energy scattering of two spin-polarized fermions and show that tightly confined fermions have infinitely strong interactions at a particular value of the 3D, free-space p-wave scattering volume. Moreover, we describe a mapping of this strongly interacting system of two quasi-1D fermions to a weakly interacting system of two 1D bosons.

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Two particle scattering is ubiquitous in physics. With the achievement of quantum degeneracy in ultracold atomic gases [1,2], renewed interest in the scattering of two atoms at low temperatures has arisen. This is because, to first order, the many-body physics of an ultracold atomic gas depends on a single atom-atom scattering parameter [3]. For spin-polarized bosons, this parameter is the s-wave scattering length $a_s = -\lim_{k\to 0} \tan\delta_s/k$, where δ_s is the s-wave scattering phase shift at collision momentum k. For spin-polarized fermions, in contrast, the antisymmetric character of the wave function forbids s-wave scattering, and, instead, p-wave scattering becomes dominant. The interaction is then characterized by the p-wave scattering volume $V_p = -\lim_{k\to 0} \tan\delta_p/k^3$ [4].

An exciting feature of ultracold atomic gases is that the effective two-body scattering properties can be manipulated by external magnetic fields [5,6], or by strong confinement [7,8]. Of particular interest are quasi-1D geometries created by atomic waveguides or optical lattices, which may, if loaded with ultracold bosons or fermions [9,10], provide an opportunity to study novel 1D many-body states [11], and to perform high precision measurements [12]. Because the many-body physics of such quasi-1D systems depends predominantly on the atom-atom scattering properties *in the waveguide,* it is imperative to understand how the waveguide modifies the free-space scattering properties.

For a waveguide with harmonic confinement, the 3D Hamiltonian for the relative coordinate $\vec{r} = (\rho, \phi, z)$ of two atoms reads

$$H = -\frac{\hbar^2}{2\mu}\nabla^2 + \frac{1}{2}\mu\omega_\perp^2\rho^2 + V_{3D}(r), \tag{1}$$

where μ denotes the reduced mass, $V_{3D}(r)$ the full atom-atom interaction potential, and $\omega_\perp$ the trapping frequency in the ρ direction. Using a zero-range potential, Olshanii [13] derives an effective 1D Hamiltonian,

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

and coupling constant g_{1D},

$$\frac{g_{1D}}{a_\perp\hbar\omega_\perp} = 2\frac{a_s}{a_\perp}\left(1 - \frac{a_s}{a_\perp}|\zeta(1/2)|\right)^{-1} \tag{3}$$

for *two bosons,* which reproduce the low energy scattering solutions of Eq. (1). This elegant result [13,14] shows that the strong confinement of the waveguide gives rise to an effective 1D interaction, parametrized by g_{1D}, which can be tuned to any strength by changing the ratio of a_s to the transverse oscillator length $a_\perp = \sqrt{\hbar/\mu\omega_\perp}$. Notably, the effective 1D interaction for two bosons becomes infinitely strong (g_{1D} diverges) when a_s takes on the particular *finite* value $a_s/a_\perp = 1/|\zeta(1/2)| \approx 0.6848$, where $\zeta(\cdot)$ is the Riemann zeta function [15].

The results obtained for quasi-1D bosons lead us to the following question: How do two spin-polarized *fermions* under quasi-1D confinement behave? To answer this question, we develop a general framework to obtain scattering solutions of the waveguide Hamiltonian, Eq. (1), that are applicable to bosons *and* fermions at any energy, as well as to a large class of quasi-1D scattering processes, single- *or* multichannel in nature. Application to identical fermions shows that confinement modifies the free-space scattering properties of two fermions significantly; i.e., spin-polarized fermions can have infinitely strong effective interactions for a finite 3D scattering volume V_p when confined to a quasi-1D geometry.

A key quantity in our formalism is the familiar K matrix $\underline{K}^{3D}(E)$ [16], which encapsulates the free-space (no confinement) scattering physics of a given atom-atom potential V_{3D} at all energies. One advantage of using K matrices is that the complications of using zero-range potentials are avoided. Below, we derive an effective 1D K matrix, $\underline{K}^{1D}$, that (i) is written in terms of the known 3D K matrix, $\underline{K}^{3D}$, and (ii) characterizes the effective interaction of two tightly confined atoms.

In the presence of a magnetic field, the 3D K matrix depends in general on the angular momentum quantum number l as well as on the quantum number m, which denotes the projection of l onto the field axis. Our framework assumes a spherically symmetric atom-atom interaction potential, which implies an m-independent 3D K matrix. For s-wave scattering, this treatment describes s-wave Feshbach resonances exactly. For higher partial waves, however, we neglect, e.g., anisotropic dipole-dipole interactions. In the absence of channel coupling, the 3D K matrix reduces to a diagonal matrix of scattering phase shifts $\tan\delta_l$. The extension to m-dependent interactions will be the subject of future studies.

The 3D K matrix reaches its asymptotic limit at a distance r_c, which we assume to be much smaller than the transverse oscillator length $a_\perp$. Configuration space can then be partitioned into two regions: (i) $r < r_c$. The two-body potential dominates, while the confining potential is negligible. (ii) $r > r_c$. The confinement is felt, while the atom-atom potential is negligible. For realistic trapping geometries, i.e., for $a_\perp \approx 1000$ a.u., the condition $r_c \ll a_\perp$ implies usage of short-range model potentials that closely mimic the behaviors of realistic two-body potentials. Note the scattering length or volume, for example, can take on any value including $\pm\infty$. For $r \approx r_c$, the full wave function can then be written in spherical coordinates [16]:

$$\Psi_\beta(\mathbf{r}) = \sum_l F_l(\mathbf{r})\delta_{l\beta} - G_l(\mathbf{r})K^{3D}_{l\beta}, \quad (4)$$

where the 3D K matrix, $\underline{K}^{3D}$, contains all the "scattering information" about the atom-atom potential $V_{3D}(r)$ and β labels the linearly independent solutions. As usual, the energy normalized regular $F_l(\mathbf{r})$ and irregular $G_l(\mathbf{r})$ spherical solutions at energy $E/\hbar\omega_\perp = (ka_\perp)^2/2$ are given in terms of the spherical harmonics $Y_{lm}(\theta, \phi)$ and the spherical Bessel functions $j_l(kr)$ and $n_l(kr)$, respectively. Since the quantum number m is conserved, F and G depend only parametrically on m. For notational simplicity, in Eq. (4) and below, the m dependence is not indicated explicitly.

To obtain the 1D scattering properties, the spherical solution, Eq. (4), must be propagated outward to large $|z|$ where the cylindrical symmetry of the harmonic confinement dominates. For $|z| \gg a_\perp \gg r_c$, the wave function is a product of 2D harmonic oscillator wave functions $\Phi_n(\rho, \phi)$ and free particle solutions in z. We choose the energy normalized regular $\psi_n(\mathbf{r})$ and irregular $\chi_n(\mathbf{r})$ cylindrical solutions to be eigenstates of the parity $\pi_{\text{tot}} = \pi_z(-1)^m$:

$$\begin{Bmatrix} \psi_n(\mathbf{r}) \\ \chi_n(\mathbf{r}) \end{Bmatrix} = \Phi_n(\rho, \phi) \times \begin{Bmatrix} f_n(z) \\ g_n(z) \end{Bmatrix}. \quad (5)$$

Here, the cylindrical channels are labeled by the harmonic oscillator quantum number n, so that the z-direction momentum q_n in each channel is defined by the relationship,

$$\frac{E}{\hbar\omega_\perp} = \frac{(ka_\perp)^2}{2} = (2n + 1 + |m|) + \frac{(q_n a_\perp)^2}{2}. \quad (6)$$

The parity π_z is determined by the forms of the regular $f_n(z)$ and irregular $g_n(z)$ free particle wave functions. The full asymptotic wave function at large $|z|$ can then be written in terms of the solutions $\psi_n(\mathbf{r})$ and $\chi_n(\mathbf{r})$, and a 1D K matrix $\underline{K}^{1D}$ (α labels the linearly independent solutions):

$$\Psi_\alpha(\mathbf{r}) = \sum_n \psi_n(\mathbf{r})\delta_{n\alpha} - \chi_n(\mathbf{r})K^{1D}_{n\alpha}. \quad (7)$$

To express the 1D K matrix in terms of the 3D K matrix we use a frame transformation [17–19], which transforms one set of solutions of the Schrödinger equation (labeled by a set of quantum numbers) to another set of solutions (labeled by a different set of quantum numbers). Such a transformation is exact and orthogonal when the two sets of solutions satisfy the same Schrödinger equation everywhere. A local, nonorthogonal frame transformation, on the other hand, is useful for transforming between two sets of solutions that satisfy the same Schrödinger equation only in a limited region of space. Following Greene [20], we use the local frame transformation to relate our spherical free particle solutions, Eq. (4), to our harmonically confined cylindrical solutions, Eq. (7), through a nonorthogonal matrix $\underline{U}$:

$$\psi_n(\mathbf{r}) = \sum_l F_l(\mathbf{r})U_{ln} \quad \text{and} \quad \chi_n(\mathbf{r}) = \sum_l G_l(\mathbf{r})(U^T)^{-1}_{ln}. \quad (8)$$

The sum over l in these expressions is understood to be over $l = 0, 2, 4, \ldots$ for $\pi_z = 1$ and over $l = 1, 3, 5, \ldots$ for $\pi_z = -1$. The elements of the frame transformation matrix U_{ln} are calculated by projecting the expressions given in Eq. (8) onto the spherical harmonics [20]. Using the transformation expressions, Eq. (8), in Eq. (7), the 1D K matrix $\underline{K}^{1D}$ can be expressed in terms of $\underline{K}^{3D}$ *at all energies:*

$$\underline{K}^{1D} = \underline{U}^T \underline{K}^{3D} \underline{U}. \quad (9)$$

This relationship is essentially exact for any $\underline{K}^{3D}$, including multichannel cases, as long as $r_c \ll a_\perp$.

Up to now, the cylindrical asymptotic wave function $\Psi_\alpha(\mathbf{r})$, Eq. (7), is written in terms of the regular and irregular cylindrical functions $\psi_n(\mathbf{r})$ and $\chi_n(\mathbf{r})$, which contain exponentially diverging pieces in channels n that are energetically closed ($E/\hbar\omega_\perp < 2n + 1 + |m|$). To obtain asymptotic solutions with the correct, exponentially decaying boundary conditions in the closed channels, these divergencies must be eliminated. To do this, we use the approach of multichannel quantum defect theory and partition $\underline{K}^{1D}$ into a closed ("c") and an open ("o") subspace [16]:

$$\underline{K}^{1D} = \begin{pmatrix} \underline{K}^{1D}_{oo} & \underline{K}^{1D}_{oc} \\ \underline{K}^{1D}_{co} & \underline{K}^{1D}_{cc} \end{pmatrix}. \quad (10)$$

Eliminating the closed channels results in a "physical" K matrix in the open channels, $\underline{K}_{oo}^{1D,phys}$,

$$\underline{K}_{oo}^{1D,phys} = \underline{K}_{oo}^{1D} + i\underline{K}_{oc}^{1D}(\underline{1} - i\underline{K}_{cc}^{1D})^{-1}\underline{K}_{co}^{1D}. \tag{11}$$

The corresponding asymptotic wave function Ψ_{α}^{phys}—α now denotes an open channel—having the correct physical boundary conditions in all channels involves a sum over only the open channels:

$$\Psi_{\alpha}^{phys}(\mathbf{r}) = \sum_{n\in \text{open}} \Phi_n(\rho,\phi)[f_n(z)\delta_{n\alpha} - g_n(z)K_{n\alpha}^{1D,phys}]. \tag{12}$$

Equations (9), (11), and (12) provide a rigorous path from the full 3D scattering properties encapsulated in $\underline{K}^{3D}(E)$, to an effective 1D system, Eq. (12), whose scattering properties are given by $\underline{K}_{oo}^{1D,phys}(E)$. Our framework shows that the closed channels contribute significantly to the effective 1D scattering properties at energies E near closed channel resonances, where $\det[\underline{1} - i\underline{K}_{cc}^{1D}(E)] \approx 0$ (see also [14]).

We now introduce an important simplification. When the 3D scattering properties are dominated by the phase shift $\tan\delta_l$ in a single partial wave l ($K_{l''l'}^{3D} = \delta_{l''l}\delta_{ll'}\tan\delta_l$), the 1D K matrix, Eq. (9), becomes a rank one matrix, $K_{nn'}^{1D} = (U^T)_{nl}\tan\delta_l U_{ln'}$. Thus, the closed channel part of $\underline{K}^{1D}$ also has rank one with a single eigenvalue λ_c:

$$\lambda_c = \text{Tr}\underline{K}_{cc}^{1D} = \tan\delta_l \sum_{n\in\text{closed}} (U_{nl})^2. \tag{13}$$

This fact allows $\underline{K}_{oo}^{1D,phys}$, Eq. (11), to be simplified by diagonalizing and inverting the matrix $[\underline{1} - i\underline{K}_{cc}^{1D}]$ analytically:

$$\underline{K}_{oo}^{1D,phys}(E) = \underline{K}_{oo}^{1D}[1 - i\lambda_c(E)]^{-1}. \tag{14}$$

Equation (14) shows that the "bare" 1D K matrix $\underline{K}_{oo}^{1D}$ is renormalized by the closed channels physics encapsulated in the eigenvalue $\lambda_c(E)$, which can be strongly energy dependent. As the relative energy E increases, new channels become open and the dimension of $\underline{K}_{oo}^{1D,phys}$ increases to reflect the multichannel nature of the scattering.

Application of our framework to the scattering of two identical bosons under strong transverse confinement predicts the following general result: when $a_s(E) = -\tan\delta_s(E)/k = 0.6848a_\perp$, a divergence of the effective 1D interaction occurs at *all* threshold energies, $E = \hbar\omega_\perp(2n+1)$ for $m=0$, where a new transverse mode becomes open. This extension of Olshanii's zero energy result [13] to all energies suggests that a Tonks-Girardeau regime [13,21] can be realized experimentally not only when the transverse motion of the Bose gas is in its ground state, that is, when the transverse motion is completely cooled, but also when the transverse motion is in an excited state.

We now present an application of our framework to the low energy scattering ($m=0$, $1 \le E/\hbar\omega_\perp < 3$) of two spin-polarized fermions, whose 3D scattering properties are parametrized by the energy dependent scattering volume $V_p(E) = -\tan\delta_p(E)/k^3$. In this case, the resulting effective fermionic 1D K matrix, Eq. (14), becomes

$$K^{1D,-} \equiv K^{1D,phys} = -\frac{6V_p}{a_\perp^3}q_0 a_\perp \times \left[1 - 12\frac{V_p}{a_\perp^3}\zeta\left(-\frac{1}{2}, \frac{3}{2} - \frac{E}{2\hbar\omega_\perp}\right)\right]^{-1}. \tag{15}$$

Here, the Hurwitz zeta function $\zeta(\cdot,\cdot)$ [15] arises from the eigenvalue λ_c of $\underline{K}_{cc}^{1D}$. The K matrix given in Eq. (15) along with the odd-parity wave function,

$$\psi^-(z) \sim \frac{z}{|z|}[\sin(q_0|z|) + \cos(q_0|z|)K_{00}^{1D,-}], \tag{16}$$

provides a complete scattering solution to the waveguide Hamiltonian, Eq. (1), when a single cylindrical channel is energetically open. The 1D K matrix, Eq. (15), diverges when the scattering volume V_p has the particular value

$$\frac{V_p^{crit}}{a_\perp^3} = \left[12\zeta\left(-\frac{1}{2}, \frac{3}{2} - \frac{E}{2\hbar\omega_\perp}\right)\right]^{-1}. \tag{17}$$

This implies that two spin-polarized quasi-1D fermions have infinitely strong interactions for a finite 3D scattering volume $V_p = V_p^{crit}$.

Next, we derive an effective 1D Hamiltonian that describes many of the low energy properties of two spin-polarized fermions in a waveguide [see Eq. (1)]. Importantly, the 1D zero-range potential $g_{1D}\delta(z)$ [see Eq. (2)], which has been very successful in treating bosons [11,13], cannot be used *directly* since it results in an unphysical scattering amplitude for fermions. One way around this difficulty would be to use a zero-range potential that gives a meaningful scattering amplitude for fermions [22]. Alternatively, we propose to map the fermionic $K^{1D,-}$, Eq. (15), to a bosonic 1D K matrix (along with the corresponding wave functions). Mappings between fermions and bosons are important in theoretical treatments of 1D *many body* systems, as they allow one to understand systems of strongly interacting 1D bosons (fermions) by mapping them to weakly interacting systems of 1D fermions (bosons) [11,21].

At low energies, the 1D scattering wave function $\psi^-(z)$ for two fermions is given by Eq. (16) while that for two bosons reads

$$\psi^+(z) \sim [\cos(q_0|z|) - \sin(q_0|z|)K^{1D,+}], \tag{18}$$

where $K^{1D,+}$ denotes the even parity 1D K matrix. With the choice $K_{00}^{1D,+} = -1/K_{00}^{1D,-}$, the bosonic wave function can be written in terms of the fermionic one (and vice versa): $\psi^+(z) = \frac{|z|}{z}\psi^-(z)/K_{00}^{1D,-}$. Application of the proposed mapping to our effective 1D K matrix for two fermions, Eq. (15), results in an equivalent system of two 1D bosons interacting through the potential $g_{1D}^{map}\delta(z)$, with the "mapped coupling constant":

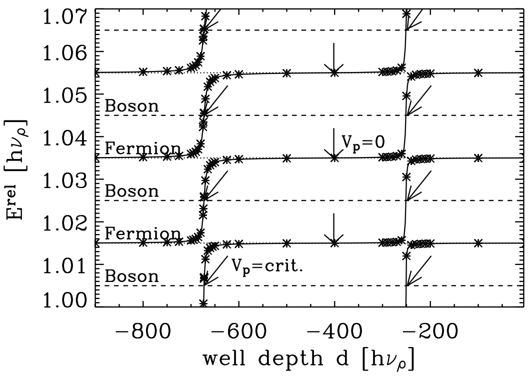

FIG. 1. Relative 3D and 1D energies (solid lines and asterisks, respectively) as a function of the well depth d (b is fixed at $b = 0.13a_\perp$) for two spin-polarized fermions under quasi-1D confinement. Straight dotted (dashed) lines indicate the relative eigenenergies of two noninteracting spin-polarized fermions (noninteracting bosons). Vertical and tilted arrows indicate values of d for which the scattering volumes $V_p(E)$ are $V_p = 0$ and $V_p = V_p^{\rm crit}$, respectively, ($\nu_\rho = \omega_\perp/2\pi$).

$$\frac{g_{\rm 1D}^{\rm map}}{a_\perp \hbar\omega_\perp} = \frac{-a_\perp^3}{6V_p}\left[1 - 12\frac{V_p}{a_\perp^3}\zeta\left(-\frac{1}{2}, \frac{3}{2} - \frac{E}{2\hbar\omega_\perp}\right)\right]. \quad (19)$$

This remarkable result implies that two spin-polarized quasi-1D fermions with *infinitely strong* interactions [see Eq. (17)] can be mapped to a system of *noninteracting* bosons; the converse of the Bose-Fermi mapping [21]. Importantly, our mapped $g_{\rm 1D}^{\rm map}$, Eq. (19), applies to any interaction strength V_p.

To confirm our analytical results we perform numerical calculations for two spin-polarized fermions (odd parity about $z = 0$) in a highly elongated trap interacting through a two-body model potential, $V_{\rm 3D}(r) = d/\cosh^2(r/b)$. We use a B-spline basis set to solve the 3D Schrödinger equation for the relative Hamiltonian given in Eq. (1) with the confining potential replaced by $\frac{1}{2}\mu\omega_\perp^2(\rho^2 + \lambda^2 z^2)$, where $\lambda = 0.01$. Solid lines in Fig. 1 show the resulting relative energies, $E^{\rm rel} > \hbar\omega_\perp$, as a function of the two-body well depth d. Straight dotted lines indicate the relative energies of two noninteracting spin-polarized fermions, while straight dashed lines indicate those for two noninteracting bosons. As predicted analytically (and indicated by tilted arrows in Fig. 1), the relative 3D eigenenergies coincide with those of two noninteracting bosons for well depths d corresponding to $V_p = V_p^{\rm crit}$.

Figure 1 additionally shows the spectrum of the 1D bosonic Hamiltonian, Eq. (2), with the additional potential $\frac{1}{2}\mu\lambda^2\omega_\perp^2 z^2$, using the mapped coupling constant $g_{\rm 1D}^{\rm map}$ [Eq. (19)] (asterisks). To account for the energy dependence of $g_{\rm 1D}^{\rm map}$ we self-consistently solve for V_p and the 1D energy levels for each well depth d [23]. Figure 1 shows that the 1D energies agree very well with the 3D energies. Two interacting spin-polarized fermions under quasi-1D confinement can hence be mapped to a system of two 1D bosons interacting through a δ-function potential with a mapped coupling strength $g_{\rm 1D}^{\rm map}$. Present-day experiments [6] can access regimes where our theory applies; the question of how to experimentally verify our predictions, however, is beyond the scope of this Letter.

This Letter develops a framework for atom-atom scattering under quasi-1D confinement, which includes multichannel collisions and is limited only in the assumption that the characteristic length of the two-body potential is small compared to $a_\perp$. Its application to two spin-polarized fermions shows that scattering resonances associated with quasi-1D confinement can lead to infinitely strong effective 1D interactions for finite V_p and that the resulting system of quasi-1D fermions can be mapped to a system of two 1D bosons.

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