Tuning the interactions of spin-polarized fermions using quasi-one-dimensional confinement

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The behavior of ultracold atomic gases depends crucially on the two-body scattering properties of these systems. We develop a multichannel scattering theory for atom-atom collisions in quasi-one-dimensional (quasi-1D) geometries such as atomic waveguides or highly elongated traps. 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.

PACS numbers: 03.75.-b,F34.50.-s,34.10.+x

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 interest in atom-atom scattering stems from the fact that, 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 \(a_s = -\lim_{k \to 0} \delta_s/k\), where \(\delta_s\) is the s-wave scattering phase shift at collision momentum \(k\). For two colliding 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 \(V_p = -\lim_{k \to 0} \delta_p/k^3\) [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 in one or more directions [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 [3]. 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.

The scattering of two bosons in a quasi-1D geometry has been studied by Olshanii [12]. For a waveguide with harmonic confinement the 3D Hamiltonian for the relative coordinate \(\mathbf{r} = (\rho, \phi, z)\) of two atoms of mass \(m\) reads:

\[ H = -\frac{\hbar^2}{2\mu} \nabla^2 + \frac{1}{2} \mu \omega_z^2 \rho^2 + V_{3D}(r), \]

where \(\mu = m/2\) denotes the reduced mass, and \(V_{3D}(r)\) the full atom-atom interaction potential. Using a regularized zero-range potential, \(V_{3D}(r) = 2\hbar^2 a_s \delta(r) \mu r\), Olshanii derives an effective 1D Hamiltonian,

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

and coupling constant \(g_{1D}\):

\[ \frac{g_{1D}}{a_{\perp} \hbar \omega_{\perp}} = 2 \frac{a_{s}}{a_{\perp}} \left( 1 - \frac{a_{s}}{a_{\perp}} |\zeta(1/2)| \right)^{-1}, \]

which reproduce the low energy scattering solutions of the full 3D Hamiltonian, Eq. (1). This elegant result [13, 14] shows that the strong confinement of the waveguide gives rise to an effective 1D interaction, parameterized by \(g_{1D}\), which can be tuned to virtually any strength by changing the ratio of the 3D s-wave scattering length \(a_s\) to the transverse oscillator length \(a_{\perp} = \sqrt{\hbar/\mu \omega_{\perp}}\) through, for example, application of an external magnetic field. Notably, the effective 1D interaction becomes infinitely strong \((g_{1D}\) diverges\) when the 3D scattering length 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 [13].

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, at any energy. When applied to identical fermions, this framework shows that the confinement modifies the free-space scattering properties of two spin-polarized fermions significantly. In particular, we show that two spin-polarized fermions — just as two spin-polarized bosons — 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 \(\mathbf{K}^{D}(E)\) [15], which encapsulates the free-space (no confinement) scattering physics of a given atom-atom potential \(V_{3D}(r)\) at all energies. One advantage of using \(K\)-matrices is that the complications of using zero-range potentials are avoided. For general multichannel collisions the 3D \(K\)-matrix, \(\mathbf{K}^{3D}\), can be determined accurately by a number of numerical techniques [16, 17]; for a single channel scattering process it reduces to a diagonal matrix of scattering phase shifts \(\tan \delta_s\). Below, we derive an effective 1D \(K\)-matrix, \(\mathbf{K}^{1D}\), that i) is written in terms of the known 3D \(K\)-matrix, \(\mathbf{K}^{3D}\), and
ii) fully characterizes the effective interaction of two tightly-confined atoms.

For now, we assume an interaction potential \( V_{3D}(r) \) such that the 3D K-matrix reaches its asymptotic limit at a distance \( r_c \) much smaller than the transverse confinement length \( a_\perp \) (\( r_c \ll a_\perp \)). While this condition may not necessarily be fulfilled for a realistic atom-atom potential, one can often construct a model potential that fulfills this requirement while mimicking the behavior of a realistic two-body potential as closely as possible. 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 \( r \approx r_c \), the full wavefunction can be conveniently written in spherical coordinates [16]:

\[
\Psi_\beta(r) = \sum_i F_{lm}(r) \delta_{\beta\alpha} - G_{lm}(r) K_{lm}^{3D},
\]

where the 3D K-matrix, \( K_{3D} \), contains all the “scattering information” about the atom-atom potential \( V_{3D}(r) \). The energy normalized regular solution \( F_{lm}(r) \) at energy \( E/\hbar \omega_{\perp} = (ka_\perp)^2/2 \) is given in terms of the spherical Bessel function \( j_l(kr) \):

\[
F_{lm}(r) = Y_{lm}(\theta, \phi) \frac{1}{\sqrt{\hbar \omega_d a_\perp}} \sqrt{\frac{2ka_\perp}{\pi}} j_l(kr).
\]

The irregular solution \( G_{lm}(r) \) is identical to \( F_{lm}(r) \), but with \( j_l(kr) \) replaced by \( n_l(kr) \). In the spherical representation, the parity of the relative wavefunction is simply \( \pi_{rel} = (-1)^l \).

To obtain the 1D scattering properties, the cylindrical 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 wavefunction is a product of 2D harmonic oscillator wavefunctions \( \Phi_{nm}(r, \phi) \) and free particle solutions in \( z \). We choose the energy normalized regular \( \psi_{nm}(r) \) and irregular \( \chi_{nm}(r) \) cylindrical solutions to be eigenstates of the parity \( \pi_{rot} = \pi_z(-1)^m \):

\[
\begin{align*}
\left\{ \psi_{nm}(r) \right\} &= \Phi_{nm}(r, \phi) \times \left\{ f_n(z) \right\}, \\
\left\{ \chi_{nm}(r) \right\} &= \Phi_{nm}(r, \phi) \times \left\{ g_n(z) \right\}.
\end{align*}
\]

Here, the cylindrical channels are labeled by the harmonic oscillator quantum number \( n \) and the angular momentum \( m \), so that the \( z \)-direction momentum \( q_n \) in each channel is defined by the relationship:

\[
\frac{E}{\hbar \omega_{\perp}} = \frac{(ka_\perp)^2}{2} = (2n + 1 + |m|) + \frac{(qa_\perp)^2}{2}.
\]

The parity \( \pi_z \) is determined by the forms of the regular \( f_n(z) \) and irregular \( g_n(z) \) free particle wavefunctions. To always work with eigenstates of \( \pi_z \) and to keep the regular and irregular functions \( 90^\circ \) out of phase at both positive and negative \( z \), we use the conventions [20],

\[
f_n(z) = \frac{1}{\sqrt{\hbar \omega_d a_\perp}} \frac{1}{\sqrt{\hbar \omega_{\perp} a_\perp}} \times \left\{ \begin{array}{ll}
\cos(q_n |z|) & \text{for } \pi_z = 1, \\
\frac{\pi}{|z|} \sin(q_n |z|) & \text{for } \pi_z = -1.
\end{array} \right.
\]

The full asymptotic wavefunction at large \( |z| \) can then be written in terms of the solutions \( \psi_{nm}(r) \) and \( \chi_{nm}(r) \), and a 1D K-matrix \( K_{1D} [28] 
\]

\[
\Psi_\alpha(r) = \sum_n \psi_{nm}(r) \delta_{\alpha \alpha} - \chi_{nm}(r) K_{nm}^{1D} \chi_{nm}(r).
\]

To express the 1D K-matrix in terms of the 3D K-matrix we use a frame transformation [21, 22, 23], 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 in his treatment of negative ion photodetachment in magnetic fields [24], we use the local frame transformation to relate our spherical free particle solutions, Eq. (4), to our harmonically confined cylindrical solutions, Eq. (10), through a nonorthogonal matrix \( U \):

\[
\psi_{nm}(r) = \sum_{l} F_{lm}(r) U_{ln} \quad \text{and} \quad \chi_{nm}(r) = \sum_{l} G_{lm}(r) (U^T)^{-1}_{ln}.
\]

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. (11) onto the spherical harmonics [24]. Using the transformation expressions, Eq. (11), in Eq. (10), the 1D K-matrix \( K_{1D} \) can be expressed in terms of \( K_{3D} \) at all energies:

\[
K_{1D} = U^T K_{3D} U.
\]

This relationship is essentially exact for any \( K_{3D} \), including multichannel cases, as long as \( r_c \ll a_\perp \).

Up to now, the cylindrical asymptotic wavefunction \( \Psi_\alpha(r) \), Eq. (11), is written in terms of the regular and irregular cylindrical functions solutions \( \psi_{nm}(r) \) and \( \chi_{nm}(r) \), 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 divergences must be eliminated. To do this, we use the approach of multichannel quantum defect theory and partition \( K_{1D} \) into a closed (“c”) and an open (“o”) subspace [16]:

\[
K_{1D} = \begin{pmatrix}
K_{cc}^{1D} & K_{oc}^{1D} \\
K_{oc}^{1D} & K_{oo}^{1D}
\end{pmatrix}.
\]

Eliminating the closed channels results in a “physical” K-matrix in the open channels, \( K_{oo}^{1D,\text{phys}} \):

\[
K_{oo}^{1D,\text{phys}} = K_{oo}^{1D} + iK_{oc}^{1D} (1 - iK_{cc}^{1D})^{-1} K_{oc}^{1D}.
\]
The corresponding asymptotic wavefunction $\Psi_{a,\text{phys}}^{\alpha}$ now denotes an open channel — having the correct physical boundary conditions in all channels involves a sum over only the open channels:

$$\Psi_{a,\text{phys}}^{\alpha}(r) = \sum_{n \in \text{open}} \Phi_{nm}(\rho, \phi) \left[ f_n(z) \delta_{n\alpha} - g_n(z) K_{n\alpha, \text{phys}} \right].$$

Equations (12), (14) and (15) provide a rigorous path from the full 3D scattering properties encapsulated in $K_{1D}^{\text{phys}}(E)$, to an effective 1D system, Eq. (15), whose scattering properties are given by $K_{1D, \text{phys}}^{\text{phys}}(E)$. Our framework shows that the closed channels contribute significantly to the effective 1D scattering properties at energies $E$ near closed channel resonances, where $\det(1 - iK_{1D}^{\text{phys}}(E)) \approx 0$ (see also (14)).

We now introduce an important simplification. When the 3D scattering properties are dominated by the phase shift $\delta_\alpha$ in a single partial wave $l$ ($K_{\alpha l}^{\text{phys}} = \delta_{\alpha l} \delta_{l \alpha} \rho \delta_l$), the 1D $K$-matrix, Eq. (12), becomes a rank one matrix,

$$K_{n\alpha} = (U^T)_n \delta_{\alpha l} U_{l\alpha}.$$  

Thus, the closed channel part of $K_{1D}$ also has rank one with a single eigenvalue $\lambda_c$:

$$\lambda_c = \text{Tr}K_{1D}^{\text{phys}} = \delta_{\alpha l} \sum_{n \in \text{closed}} (U_{nl})^2.$$  

This fact allows $K_{1D, \text{phys}}^{\text{phys}}$, Eq. (13), to be simplified by diagonalizing and inverting the matrix $[1 - iK_{1D}^{\text{phys}}]$ analytically:

$$K_{1D, \text{phys}}^{\text{phys}}(E) = \left[ 1 - i\lambda_c(E) \right]^{-1}.$$  

Equation (18) shows that the “bare” 1D $K$-matrix $K_{1D}$ 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 $K_{1D, \text{phys}}^{\text{phys}}$ 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 $a_s(E)/a_\perp = 0.6848$, 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 and multichannel cases suggests that a Tonks-like regime [13] can be realized experimentally in a “high-temperature” gas, $k_B T \gg \hbar \omega_\perp$. Further details regarding our results for bosons will be published elsewhere [25].

We now present an application of our framework to the low energy scattering ($m = 0$, $1 < E/\hbar \omega_\perp < 3$) of two spin-polarized fermions, whose 3D scattering properties are parameterized by a single parameter, the energy dependent scattering volume $V_p(E) = -\tan \delta_l(E)/k^2$. In this case, the resulting effective fermionic 1D $K$-matrix, Eq. (15), becomes:

$$K_{1D, \text{phys}}^{\text{phys}} = K_{1D}^{\text{phys}} = -\frac{6V_p}{a_\perp^2} q_0 a_\perp.$$  

Here, the Hurwitz zeta function $\zeta(\cdot, \cdot)$ [15] arises from the eigenvalue $\lambda_c$ of $K_{1D}^{\text{phys}}$. The $K$-matrix given in Eq. (19) along with the odd-parity wavefunction,

$$\Psi^-(z) \sim \frac{z}{2} \left[ \sin(q_0 |z|) + \cos(q_0 |z|) K_{1D, \text{phys}}^{\text{phys}} \right],$$

provides a complete scattering solution to the waveguide Hamiltonian, Eq. (1), when a single cylindrical channel is energetically open. The 1D $K$-matrix, Eq. (19), diverges when the scattering volume $V_p$ has the particular value

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

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

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. (20)], 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 [24]. Alternatively, we propose to map the fermionic $K_{1D, \text{phys}}^{\text{phys}}$, Eq. (19), to a bosonic 1D $K$-matrix (along with the corresponding wavefunctions). 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].

At low energies, the 1D scattering wavefunction $\Psi^-(z)$ for two fermions is given by Eq. (20) while that for two bosons reads:

$$\Psi^+(z) \sim \left[ \cos(q_0 |z|) - \sin(q_0 |z|) K_{1D, \text{phys}}^{\text{phys}} \right],$$

where $K_{1D, \text{phys}}^{\text{phys}}$ denotes the even parity 1D $K$-matrix. With the choice,

$$K_{1D, \text{phys}}^{\text{phys}} = -1/K_{1D, \text{phys}}^{\text{phys}},$$

the bosonic wavefunction can be written in terms of the fermionic one (and vice versa):

$$\Psi^+(z) = \frac{|z|}{z} \Psi^-(z)/K_{1D, \text{phys}}^{\text{phys}}.$$  

Application of the proposed mapping, Eqs. (20) and (24), to our effective 1D $K$-matrix for two fermions, Eq. (19), results in an equivalent system of two 1D bosons interacting through the potential $g_{1D}^{\text{map}} \delta(z)$, with the “mapped coupling constant”:

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


This remarkable result implies that two spin-polarized quasi-1D fermions with infinitely strong interactions [see Eq. (21)], can be mapped to a system of non-interacting bosons. More importantly, however, the mapped $g_{1D}^\text{map}$, Eq. (25), applies to any interaction strength $V_p$.

To confirm our analytical results we have performed numerical calculations for two spin-polarized fermions in a highly elongated trap interacting through a two-body model potential, $V_{2P}(r) = d/\cosh^2(r/b)$. We use a B-spline basis set to solve the 3D Schrödinger equation for the Hamiltonian given in Eq. (11) with the confining potential replaced by $\frac{\mu}{2}\omega_\perp^2 (p^2 + \lambda^2 z^2)$, where $\lambda = 0.01$. The antisymmetry of the fermionic wave functions is enforced by only including odd-parity states. Solid lines in Fig. 1 show the resulting energy spectrum, $E > \hbar \omega_\perp$, as a function of the two-body well depth $d$. Straight dotted lines indicate the energy levels of two non-interacting spin-polarized fermions, while straight dashed lines indicate those for two non-interacting bosons. As predicted analytically (and indicated by an arrow in Fig. 1), the full 3D energy levels coincide with that of two non-interacting bosons for well depths $d$ corresponding to $V_p = V_{p\text{crit}}$.

Figure 1 additionally shows the spectrum of the 1D bosonic Hamiltonian, Eq. (3), with the additional potential $\frac{\mu}{2}\lambda^2 \omega_\perp^2 z^2$, using the mapped coupling constant $g_{1D}^\text{map}$ [Eq. (25)] (asterisks). To account for the energy dependence of $g_{1D}^\text{map}$ we self-consistently solve for the scattering volume $V_p$ and the 1D energy levels for each well depth $d$ [27]; details will be published elsewhere [28]. 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 $\delta$-function potential with a mapped coupling strength $g_{1D}^\text{map}$, Eq. (25). We note that 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 paper.

In summary, this Letter develops a general framework for treating atom-atom scattering under quasi-1D confinement. The framework includes multichannel collisions at arbitrary energies and is limited only in the assumption that the characteristic length of the two-body potential is small compared to the confinement length $a_\perp$. Application of the framework to two spin-polarized fermions in a waveguide shows that the 3D scattering behavior, which is assumed to be characterized completely by the scattering volume $V_{p\text{crit}}$, is altered significantly due to the presence of the tight transverse confinement. Specifically, two quasi-1D fermions can have infinitely strong interactions for a finite 3D scattering volume. Finally, the system of two quasi-1D fermions can be mapped to a system of two 1D bosons.

Further study is required to understand the full implications of these results for the many body physics of quasi-1D spin-polarized fermions. At this point, we only mention that any many body theory will have to carefully account for the energy-dependence of the mapped coupling constant $g_{1D}^\text{map}$.

Discussions with Chris Greene and Mike Moore were helpful in this work. This work was supported by the NSF through a grant to ITAMP, Harvard-Smithsonian CFA. DB acknowledges additional funding by the NSF under grant 0331529.

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[27] E. L. Bolda, E. Tiesinga, and P. S. Julienne, quant-ph/0304001 (2003).

[28] The 1D $K$-matrix depends on our conventions chosen for $f_n(z)$ and $g_n(z)$, which follow ref. [20]. Other conventions exist in the literature (see, for example, ref. [21]).