Two-Body Scattering In The Absence And Presence Of Spin-Orbit Coupling Terms

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Outline Of This Lecture

Two-body scattering in free space.



Add waveguide: Confinement-induced resonances.



Additionally add one-dimensional spin-orbit coupling.



Quantum Degeneracy



BEC = DFG = Bose-Einstein Condensate Degenerate Fermi Gas

Bosons And Fermions: Atoms As Composite Particles

- Boson: Integer spin; e.g., photon, mesons (q, anti-q).
- Fermion: Half-integer spin; e.g., electron, quarks, baryons (q,q,q).
- Atoms: Composite bosons and fermions.



Bose Versus Fermi Statistics: Non-Interacting Particles

One-component Bose gas: 😳 😳 😳 😳 😳

One-component spin-polarized Fermi gas:

Two-component Fermi gas:



Start With Two-Body Potential: Van Der Waals Potential

- Hyperfine Hamiltonian couples singlet and triplet potential curves.
- In the vicinity of Fano-Feshbach resonance, scattering length tunable (here, tritium-tritium (BB) system).



Effective Parametrization Of Coupled-Channel Results



For what follows, assume negligible occupation of closed channel molecule.

Simple interaction models like zero-range and square-well potentials work.

Partial Wave Decomposition: Single Potential Curve

Insert $\Psi(\vec{r}) = \sum_{L,M} \frac{u_L(r)}{r} Y_{LM}(\hat{r})$ into relative Schroedinger equation with "short range" interaction potential $V(\vec{r})$.

Yields set of coupled radial equations:

$$\left(-\frac{\hbar^2}{2\mu} \frac{\partial^2}{\partial r^2} + \langle Y_{lm} | V(\vec{r}) | Y_{lm} \rangle + \frac{\hbar^2 l(l+1)}{2\mu r^2} \right) u_l(r)$$

= $-\sum_{LM \neq lm} \langle Y_{lm} | V(\vec{r}) | Y_{LM} \rangle u_{LM}(r) + E u_{lm}(r)$

Large *r*: $\Psi(\vec{r}) = F(\vec{r}) - G(\vec{r}) K(k)$ with $K_{lm,LM}(k) = \tan \delta_{lm,LM}(k)$, $F(\vec{r}) = \sum_{LM} j_L(kr) Y_{LM}(\hat{r})$, and $G(\vec{r}) = \sum_{LM} n_L(kr) Y_{LM}(\hat{r})$. $k = \sqrt{2\mu E/\hbar^2}$.

Partial Wave Decomposition

Large *r*:

 $\Psi(\vec{r}) = F(\vec{r}) - G(\vec{r}) K(k) \text{ with } K_{lm,LM}(k) = \tan \delta_{lm,LM}(k),$ $F(\vec{r}) = \sum_{LM} j_L(kr) Y_{LM}(\hat{r}), \text{ and } G(\vec{r}) = \sum_{LM} n_L(kr) Y_{LM}(\hat{r}).$

If $V(\vec{r}) = V_{hc}(r) + \frac{d^3(1-3\cos^2\theta)}{r^3}$, then *m* is a good quantum number and the K-matrix for each *m* contains off-diagonals (coupling between different orbital angular momentum channels).

If $V(\vec{r}) = V(r)$, then *l* and *m* are good quantum number and each (l,m) channel can be treated separately. l = 0: s-wave (two identical bosons; even spatial wave function). l = 1: p-wave (two identical fermions; odd spatial wave function).

Example: s-Wave Scattering Length For Square-Well Potential



Zero-Energy Wave Function At Unitarity



Inside solution depends on details of interaction potential.

Zero-Energy Wave Function For Various Scattering Lengths



Inside solution depends on details of interaction potential. These details are not being probed at low temperature (large de Broglie wave length).

Replace Interaction Potential By Bethe-Peierls Boundary Condition

Outside:

 $u_s(r) \propto \sin(kr) + \tan(\delta_s(k))\cos(kr).$

It follows:
$$\lim_{k \to 0} \frac{\frac{\partial}{\partial r} u_s(r)}{u_s(r)} \to \frac{k - \tan \delta_s(k) k^2 r}{kr + \tan \delta_s(k)} \xrightarrow[r \to 0]{} \frac{k}{\tan \delta_s(k)} = -\frac{1}{a_s(k)}$$

Enforcing the boundary condition at r = 0 implies working in the low energy limit:

It eliminates the "wiggles" at small r, which reflect the presence of deeper lying bound states.

The de Broglie wave length is so large that small scale features cannot be resolved (universal, low energy regime).

Boundary Condition Is Equivalent To Pseudopotential

Solve free-space Schroedinger equation and then enforce boundary condition at r = 0:

$$\Psi(\vec{r}) = \sum_{l,m} \frac{u_l(r)}{r} Y_{lm}(\hat{r})$$

$$\lim_{r\to 0} \frac{\frac{\partial}{\partial r} u_s(r)}{u_s(r)} \to -\frac{1}{a_s(k)}$$

Solve Schroedinger equation for zero-range Fermi-Huang pseudopotential:

$$V_{zr}(\vec{r}) = \frac{4\pi\hbar^2 a_s(k)}{m} \delta^{(3)}(\vec{r}) \frac{\partial}{\partial r} r$$
$$\delta^{(3)}(\vec{r}) = \frac{\delta(r)}{4\pi r^2}$$

Huang, Yang, PR 105, 767 (1957)

So far: Spherically symmetric s-wave interactions.

Can also be done for higher-partial wave channels. E.g., p-wave channel, d-wave channel. Need to be careful with math...

Input Into Mean-Field Gross-Pitaevskii Equation

One "test particle" moves in the mean-field (or background) created by the other N - 1 identical bosons.

Single-particle equation:

$$\left(\frac{-\hbar^2}{2m}\vec{\nabla}^2 + \frac{1}{2}m\omega^2\vec{r}^2 + (N-1)\frac{4\pi\hbar^2a_s}{m}|\boldsymbol{\Phi}(\vec{r})|^2\right)\boldsymbol{\Phi}(\vec{r}) = \mu\boldsymbol{\Phi}(\vec{r}).$$

GP equation yields energy shift $\Delta E/N = \frac{(N-1)}{2} \sqrt{\frac{2}{\pi} \frac{\hbar^2 a_s}{m a_{ho}^3}} + \cdots$

Microscopic Derivation Of Gross-Pitaevskii Equation

• Many-body Hamiltonian for *N* bosons under confinement:

$$H = \sum_{j=1}^{N} \left(\frac{-\hbar^2}{2m} \nabla_{\vec{r}_j}^2 + \frac{1}{2} m \omega^2 \vec{r}_j^2 \right) + \sum_{j=1}^{N-1} \sum_{k>j}^{N} V_{int}(\vec{r}_j - \vec{r}_k) \text{ SW, HS, PP, LJ, vdW,...}$$

- Single-particle Hartree product: $\Psi(\vec{r}_1, ..., \vec{r}_N) = \prod_{j=1} \Phi(\vec{r}_j)$
- ZR PP atom-atom potential: $V_{int}(\vec{r}) = \frac{4\pi\hbar^2 a_s}{m} \delta^{(3)}(\vec{r})$
- Plug V_{int} and Ψ into N-body SE \Rightarrow GP eq. for "single atom":

$$\left(\frac{-\hbar^2}{2m}\vec{\nabla}^2 + \frac{1}{2}m\omega^2\vec{r}^2 + (N-1)\frac{4\pi\hbar^2a_s}{m}|\boldsymbol{\Phi}(\vec{r})|^2\right)\boldsymbol{\Phi}(\vec{r}) = \mu\boldsymbol{\Phi}(\vec{r}).$$

Single atom feels effective potential/meanfield created by the other N - 1 bosons.

What Does The Gross-Pitaevskii Equation Predict?

Homogeneous system: periodic boundary condition, constant density.

Positive scattering length: Stable gas (not self-bound). Negative scattering length: Gas not stable;

collapse toward solid or liquid (self-bound).

Bosonic atoms in harmonic trap (mean-field GP treatment):

Positive scattering length: Effectively repulsive interaction. Negative scattering length: Effectively attractive interaction.

See, e.g., Dodd et al., PRA 54, 661 (1996)



Interpretation In Terms Of Hyperspherical Coordinates

- Linear SE: hyperradius R_{hyper} , (3N-4) hyperangles Ω , ZR interactions.
- Many-body symmetrized variational wave function: $F(R_{hyper})\Phi(\Omega)$.
- Effective potential: $V_{eff}(R_{hyper}) = c_1 R_{hyper}^{-2} + c_2 R_{hyper}^2 + c_3 a_s R_{hyper}^3$

Collapse prediction within ~20% of GP equation and experiment.

Figure from Bohn, Esry and Greene, PRA 58, 584 (1998)



Dramatic Changes In Presence Of Confinement



Two-Body s-Wave Scattering In Presence Of Waveguide



Write H as $H = H_{rel} + H_{cm}$.

$$H_{rel} = -\frac{\hbar^2}{2\mu} \vec{\nabla}^2 + \frac{2\pi\hbar^2 a_s(k)}{\mu} \delta(\vec{r}) \frac{\partial}{\partial r} r + \frac{1}{2}\mu\omega^2 \rho^2; a_s(k) = -\frac{\tan(\delta_s(k))}{k}.$$

Asymptotically (large $r; r \gg a_{ho}$): $\Psi(\vec{r}) \rightarrow F(\vec{r}) - G(\vec{r}) K^{1d}(k)$.

At
$$r = 0$$
: $\Psi(\vec{r}) = \mathcal{F}(\vec{r}) - \mathcal{G}(\vec{r})K^{3d}(k)$.
 $(K^{3d})_{st} = 0$ except for $(K^{3d})_{11} = \tan(\delta_s(k))$.

Goal: Find $K^{1d}(k)$ in terms of $K^{3d}(k)$; or $g_{1d}^{even}(k)$ in terms of $a_s(k)$

Confinement-Induced Resonances: Physical Picture

Confinement-induced resonances provide route toward realizing strongly interacting, effectively one-dimensional Bose and Fermi gases.

Naively: $V_{1d}(z) = \frac{2\pi\hbar^2 a_s}{\mu} \int |\Phi_{00}^{HO}(\rho, \varphi)|^2 \frac{\delta(\rho)}{2\pi\rho} \rho d\rho d\varphi \, \delta(z).$ $V_{1d}(z) = 2a_s \hbar \omega \, \delta(z).$

"Reality" [Olshanii, PRL 81, 938 (1998)]:

Particles are asymptotically in lowest oscillator mode.

During collision (at short distances), all HO modes $\Phi_{n,m}^{HO}(\rho, \varphi)$ are energetically accessible. Excited HO modes renormalize effect 1D coupling constant g_{1d}^{even} .

Frame Transformation: Pictorial Picture

Ζ

channels

closed n

2ħω

open

channel

Range of interaction is much smaller than transverse confinement: The confinement can be neglected during phase accumulation.

Project inner spherically symmetric solution, characterized by K_{3d} , onto cylindrically symmetric asymptotic (outer) solution that accounts for confinement and is characterized by K_{1d} .

Projection of one set of solutions onto the other leads to renormalization of effective 1d coupling constant.

Form Of The 1D K-Matrix

Asymptotically (large z): $\Psi \rightarrow F - G K$

 $\Psi, F, G, K \text{ are matrices:}$ $\begin{pmatrix} n_{\rho} = 0, n'_{\rho} = 0 & n_{\rho} = 0, n'_{\rho} = 1 & \dots \\ n_{\rho} = 1, n'_{\rho} = 0 & n_{\rho} = 1, n'_{\rho} = 1 & \dots \\ \vdots & \vdots & \ddots \end{pmatrix}$

Large K_{1d} matrix, corresponding to all transverse modes.

So far, asymptotic boundary condition has not yet been enforced. Need to somehow get rid of the closed channels.



Channel Elimination: Quantum Defect Treatment

QDT: Postpone imposing boundary condition as long as possible.

$$\begin{pmatrix} \Psi_{oo} & \Psi_{oc} \\ \Psi_{co} & \Psi_{cc} \end{pmatrix} = \begin{pmatrix} F_o & 0 \\ 0 & F_c \end{pmatrix} - \begin{pmatrix} G_o & 0 \\ 0 & G_c \end{pmatrix} \begin{pmatrix} K_{oo} & K_{oc} \\ K_{co} & K_{cc} \end{pmatrix}$$

Form new linear combination with the correct boundary condition. I.e., multiply by $(I \quad \mathcal{Y}_{co})^T$.

 $n_{o} = 0$

 $n_o >$

$$\begin{pmatrix} \Psi_{oo} + \Psi_{oc} \Psi_{co} \\ \Psi_{co} + \Psi_{cc} \Psi_{co} \end{pmatrix} = \begin{pmatrix} F_o - G_o K_{oo} - G_o K_{oc} \Psi_{co} \\ G_c K_{co} + F_c \Psi_{co} - G_c K_{cc} \Psi_{co} \end{pmatrix}$$

Set r.h.s. of second line to zero and solve for \mathcal{Y}_{co} . Insert result into first line.

Using $(G_c)^{-1}F_c = -\iota$, one finds $\Psi_{oo} + \Psi_{oc}\Psi_{co} = F_o - G_o K_{phys}$, where $K_{phys} = K_{oo} + \iota K_{oc}(1 - \iota K_{cc})^{-1}K_{co}$

Effective Even And Odd 1D Coupling Constants



Zero-Range Versus Finite-Range: Inclusion Of Energy-Dependence



Expand scattering wave function in terms of 2d HO channel functions.

Finite-range K-matrix obtained by propagating log-derivative matrix from z = 0 to z_{max} using Johnson algorithm.

$$V(r) = -\boldsymbol{v_0} \exp\left(-\frac{r^2}{2r_0^2}\right).$$

Excellent agreement!!!

Connection With (Virtual) Bound States



 g_{1d}^{even} diverges when scattering energy is equal to energy of virtual bound state. $E(virtual st.) = E(true \ b. st.) + 2\hbar\omega.$ Bergeman et al., PRL 91, 163201 (2003).

 g_{1d}^{odd} diverges when scattering energy is equal to energy of virtual bound state.

 $E(virtual st.) \neq E(true b. st.) + 2\hbar\omega.$ For $E = \hbar\omega$:

E(virtual st.) = E(true b. st.).Gao et al., PRA 91, 043622 (2015).

What's Exciting About Realizing 1D Systems?

Haller et al., Science 325, 1224 (2009): "Realization of an Excited, Strongly Correlated Quantum Gas Phase".





Adding 1D Rashba-Dresselhaus Spin-Orbit Coupling



Up to now:
$$H = \sum_{j=1}^{N} \frac{\vec{p}_{j}^{2}}{2m} + interactions + confinement$$



+ interactions + confinement

Alkali Atoms: Engineering The Single-Particle Dispersion



Why is this of interest? Expand E_{-} for large Ω and $\delta \neq 0$ around $p_{z,min}^{-}$:

$$E_{-} = const + \frac{\left(p_{z} - p_{z,min}^{-}\right)^{2}}{2m} + \cdots$$

Like a charged particle in a uniform vector potential \vec{A}^* : $\vec{eA}^* = p_{z,min}^- \vec{e}_z!$

Possibility to simulate physics of charged particles (e.g., fractional quantum Hall effect) with neutral atoms!

Modified Single-Particle Dispersion \rightarrow New Physics



Modified Single-Particle Dispersion: Time-Dependence

At the single-particle level, Rabi oscillations that depend on Ω and δ :



Raman lasers: $2\hbar k_{so}$ Corresponding energy is $4E_{so}$ Compensate for this energy by detuning δ

Time-Dependence: Add Trap Along z-Direction



What Happens When We Add Two-Body Interactions?

3D system with harmonic confinement along x and y and 1D SOC (spin-orbit coupling + Raman coupling + detuning).

Rewrite Hamiltonian in relative coordinates (\vec{r} and \vec{p} with reduced mass μ) and center-of-mass coordinates (\vec{R} and \vec{P} with total mass M):

$$H = H_{rel} + H_{cm}$$

$$H_{rel}(P_z)$$

$$= \frac{p_x^2 + p_y^2 + p_z^2}{2\mu} I_2^{(1)} \otimes I_2^{(2)} + \frac{\hbar k_{so} p_z}{\mu} \left(\sigma_z^{(1)} \otimes I_2^{(2)} - I_2^{(1)} \otimes \sigma_z^{(2)}\right)$$

$$+ \Omega \left(\sigma_x^{(1)} \otimes I_2^{(2)} + I_2^{(1)} \otimes \sigma_x^{(2)}\right) + \left(\delta + \frac{\hbar k_{so} P_z}{M}\right) \left(\sigma_z^{(1)} \otimes I_2^{(2)} + I_2^{(1)} \otimes \sigma_z^{(2)}\right)$$

$$+ (V_{2b}(r) + \mu \omega^2 \rho^2 / 2) I_2^{(1)} \otimes I_2^{(2)}$$
parametric dependence on CoM momentum

Non-Interacting Relative Dispersion Curves Along *z*



With SOC: Determining The K-Matrix

Asymptotically (large z): $\Psi \rightarrow F - G K$

F, G, K are matrices: $\begin{pmatrix}
n_{\rho} = 0, n'_{\rho} = 0 & n_{\rho} = 0, n'_{\rho} = 1 & \dots \\
n_{\rho} = 1, n'_{\rho} = 0 & n_{\rho} = 1, n'_{\rho} = 1 & \dots \\
\vdots & \vdots & \ddots
\end{pmatrix}$

Each block is 4x4 matrix due to four spin channels.

Renormalization due to closed $n_{
ho} = 0$ and $n_{
ho} \neq 0$ channels.

closed $n_{
ho} = 0$ channels

open channel



Two-Fermion Resonances In Presence Of Waveguide + 1D SOC



Singlet interactions only!

 $(k_{so})^{-1} \approx 3.54 a_{ho}$ and $\tilde{\delta} = 0$. Scattering energy $E = E_{th}$.

DM (double-minimum regime), K_{phys} is 2x2 matrix: Scattering lengths at which the eigen values $K_{phys}^{(1)}$ and $K_{phys}^{(2)}$ diverge are shown in blue and red.

SM (single-minimum regime), K_{phys} is 1x1 matrix: Scattering length at which K_{phys} diverges is shown in green.

Double-Minimum Regime: Tunability Even For Small Ω



Single-Minimum Regime: Modification Of Threshold Law



K^{odd}_{phys} even though we only have singlet interactions. SM regime: No singlet contribution to threshold state. In SM regime, emergence of new bound state is associated with divergence of K_{phys} .



Connection With Literature: Effective 1D 4x4 Model



 $\hbar\Omega/(\hbar\omega)$

Summary

Two-body scattering in free space.



Add waveguide: Confinement-induced resonances.



Additionally add one-dimensional spin-orbit coupling.



Thanks To Collaborators

Chris Greene: Scattering physics.

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