14.4 Thomas-Fermi Approximation

If $gN \gg \hbar\omega$, we neglect the kinetic energy term $\nabla^2\Psi$.

$$V(\mathbf{r}) + g|\Psi(\mathbf{r})|^2 = \mu \implies n(\mathbf{r}) = \max\left(0, \frac{\mu - V(\mathbf{r})}{g}\right) \tag{32}$$

For a harmonic trap $V(\mathbf{r}) = \frac{1}{2}m\omega^2 r^2$, the density profile $n(\mathbf{r})$ is an **inverted parabola**:

$$n(\mathbf{r}) = n_0\left(1 - \frac{r^2}{R_{TF}^2}\right), \quad R_{TF} = \sqrt{\frac{2\mu}{m\omega^2}} \tag{33}$$

where R_{TF} is the Thomas-Fermi radius where the density vanishes.

15 Class 10: Scattering theory g

In the many-body framework, the exact interaction energy expectation value is determined by the full N-particle wavefunction $\Psi(\mathbf{x}_1, \ldots, \mathbf{x}_N)$. This can be expressed using the two-particle density matrix $\rho^{(2)}(\mathbf{x}, \mathbf{x}')$, which represents the probability of finding a particle at $\mathbf{x}$ and another at $\mathbf{x}'$ simultaneously:

$$\langle \hat{U} \rangle = \frac{1}{2} \int \int V(\mathbf{x} - \mathbf{x}')\rho^{(2)}(\mathbf{x}, \mathbf{x}')\, d\mathbf{x}\, d\mathbf{x}' \tag{34}$$

In terms of field operators $\hat{\psi}(\mathbf{x})$, this is written as:

$$\langle \hat{U} \rangle = \frac{1}{2} \int \int \langle \hat{\psi}^\dagger(\mathbf{x})\hat{\psi}^\dagger(\mathbf{x}')V(\mathbf{x} - \mathbf{x}')\hat{\psi}(\mathbf{x}')\hat{\psi}(\mathbf{x})\rangle\, d\mathbf{x}\, d\mathbf{x}' \tag{35}$$

15.1 The Hartree Approximation

In the mean-field description of a Bose-Einstein Condensate, we assume that all particles occupy the same single-particle state (macro-orbital) $\psi(\mathbf{x})$. This is the **Hartree approximation**, where we neglect many-body correlations and approximate the two-particle density as a simple product of single-particle densities:

$$\rho^{(2)}(\mathbf{x}, \mathbf{x}') \approx |\psi(\mathbf{x})|^2|\psi(\mathbf{x}')|^2 \tag{36}$$

Substituting this into the energy functional gives the standard Hartree form used in GP theory:

$$\langle U \rangle_H = \frac{1}{2} \int \psi^*(\mathbf{x})\psi^*(\mathbf{x}')V(\mathbf{x} - \mathbf{x}')\psi(\mathbf{x}')\psi(\mathbf{x})\, d\mathbf{x}\, d\mathbf{x}' \tag{37}$$

15.2 Applying Contact Interactions

We start with a general two-body potential that depends only on the relative distance between atoms, $V(\mathbf{x} - \mathbf{x}') = V(r)$ where $r = |\mathbf{x} - \mathbf{x}'|$.

Before assuming a specific form for the potential, we take the functional derivative of the Hartree energy functional $\langle U \rangle_H$ with respect to $\psi^*(\mathbf{x})$. This yields a **non-local Gross-Pitaevskii equation**:

$$i\hbar\partial_t\psi(\mathbf{x}) = \left(-\frac{\hbar^2\nabla^2}{2m} + V_{ext}(\mathbf{x}) + \int V(\mathbf{x} - \mathbf{x}')|\psi(\mathbf{x}')|^2 d\mathbf{x}'\right)\psi(\mathbf{x}) \tag{38}$$

In this general form, the interaction term is a convolution: the evolution of the wavefunction at position $\mathbf{x}$ depends on the density $|\psi|^2$ at all other positions $\mathbf{x}'$, weighted by the potential V.

The Contact Approximation

At ultra-low temperatures, the de Broglie wavelength of the atoms is much larger than the range of the interatomic potential r_0. Because the wavefunction $\psi(\mathbf{x}')$ varies slowly over the range where V is non-zero, we can approximate the potential as a **contact interaction**:

$$V(\mathbf{x}-\mathbf{x}') \approx g\delta(\mathbf{x}-\mathbf{x}') \tag{39}$$

Substituting this delta-function into the integral, the convolution simplifies significantly:

$$\int g\delta(\mathbf{x}-\mathbf{x}')|\psi(\mathbf{x}')|^2 d\mathbf{x}' = g|\psi(\mathbf{x})|^2 \tag{40}$$

This reduction leads to the standard, **local Gross-Pitaevskii Equation**:

$$i\hbar\partial_t\psi = \left(-\frac{\hbar^2\nabla^2}{2m} + V_{ext}(\mathbf{r}) + g|\psi|^2\right)\psi \tag{41}$$

And the corresponding interaction energy becomes:

$$\langle U\rangle_H = \frac{g}{2}\int |\psi(\mathbf{x})|^4\, d\mathbf{x} \tag{42}$$

15.3 Scattering Wavefunction and Phase Shifts

To understand the interaction between two neutral atoms, we analyze the asymptotic behavior of the wavefunction as $r \to \infty$. We introduce three equivalent representations of the total wavefunction $\psi(\mathbf{r})$ to define the key quantities of scattering theory:

$$\begin{aligned}\psi(\mathbf{r}) &\approx e^{ikz} + f(\theta,k)\frac{e^{ikr}}{r} \\ &= \sum_{l=0}^{\infty} A_l(\theta)\left[\frac{\sin(kr - l\pi/2)}{kr} + f_l\frac{e^{i(kr-l\pi/2)}}{r}\right] \\ &= \sum_{l=0}^{\infty}\frac{A_l(\theta)}{2ikr}\left[e^{-i(kr-l\pi/2)} - S_l e^{i(kr-l\pi/2)}\right],\end{aligned} \tag{43}$$

where $A_l(\theta) = (2l+1)P_l(\cos\theta)$ is the spherical expansion coefficient.

1. Proper Definitions: $f(\theta,k)$, f_l, and S_l

These three forms allow us to distinguish between the global spatial distribution and the individual partial wave contributions:

- **Scattering Amplitude $f(\theta,k)$:** A spatial quantity that describes the scattered wave.$f(\theta,k) = 0$ for non-interacting particles.
- **Partial Wave Amplitude f_l:** The contribution of the l-th angular momentum component to the total amplitude, defined by the spherical expansion is $f(\theta,k) = \sum_{l=0}^{\infty}(2l+1)f_l P_l(\cos\theta)$. $f_l = 0$ for non-interacting particles.
- **Scattering Matrix S_l:** An operator-like scalar that represents the transformation of the incoming spherical wave into an outgoing one. $S_l = 1$ for non-interacting particles.

The fundamental difference is that S_l describes the **transformation** of the state, while f_l describes the **deviation** from free propagation. By comparing Eq. (2) and Eq. (3), we find the algebraic link:

$$f_l = \frac{S_l - 1}{2ik} \tag{44}$$

2. Elastic Scattering and Phase Shifts

In elastic scattering, particle number is conserved, meaning the flux of the outgoing wave must equal the flux of the incoming wave. This imposes the constraint $|S_l| = 1$. We can therefore parameterize S_l using a real **scattering phase shift** δ_l:

$$S_l = e^{2i\delta_l} \tag{45}$$

Substituting this into our expression for f_l, we obtain the standard form:

$$f_l = \frac{e^{2i\delta_l} - 1}{2ik} = \frac{e^{i\delta_l}\sin\delta_l}{k} \tag{46}$$

This shows that f_l is non-zero only if the potential induces a phase shift relative to the vacuum.

3. Pedagogical Argument: The Baseline Shift

The "Master Equation" in Eq. (3) provides the most intuitive pedagogical picture. It splits the radial wavefunction into two distinct physical parts:

1. **The Baseline:** $\frac{\sin(kr - l\pi/2)}{kr}$ represents the free-particle (vacuum) state where $V = 0$.
2. **The Deviation:** $f_l \frac{e^{i(kr - l\pi/2)}}{r}$ represents the purely scattered part—the "extra" wave generated by the potential.

If there is no interaction ($V = 0$), the phase shift $\delta_l = 0$, which leads to $S_l = 1$ and $f_l = 0$. The total wavefunction then collapses to the standard partial wave expansion of a plane wave.

When interactions are present, the potential either "pushes" or "pulls" the outgoing wave. Substituting $S_l = e^{2i\delta_l}$ back into Eq. (2) shows that the total radial wave is simply a sine wave shifted by δ_l:

$$\psi_{l,radial}(r) \propto \frac{\sin(kr - l\pi/2 + \delta_l)}{kr} \tag{47}$$

This confirms that the entire effect of the collision is encapsulated in this single phase angle δ_l.

The Schrödinger Equation Perspective

To find these values, we solve the radial Schrödinger equation for $u_l(r) = r\psi_l(r)$:

$$\left[\frac{d^2}{dr^2} + k^2 - \frac{l(l+1)}{r^2} - \frac{2\mu V(r)}{\hbar^2}\right] u_l(r) = 0 \tag{48}$$

The potential $V(r)$ modifies the wavefunction's curvature near the origin, which manifests as the phase shift δ_l in the asymptotic limit: $u_l(r) \propto \sin(kr - l\pi/2 + \delta_l)$.

15.4 Scattering Length a and the Effective Range Expansion

At ultra-low energies ($k \to 0$), we focus exclusively on the s-wave ($l = 0$) component. To characterize the interaction beyond the simplest limit, we expand the phase shift δ_0 in powers of the momentum k. This is the **effective range expansion**:

$$k \cot \delta_0 = -\frac{1}{a} + \frac{1}{2} r_{eff} k^2 + \mathcal{O}(k^4) \tag{49}$$

Here, a is the **s-wave scattering length** and r_{eff} is the **effective range**, which relates to the spatial extent of the potential $V(r)$.

The Scattering Length as a Wavefunction Offset

In the limit $k \to 0$, we can neglect the r_{eff} and higher-order terms. The definition of the scattering length then simplifies to:

$$a = -\lim_{k \to 0} \frac{\tan \delta_0}{k} \tag{50}$$

Physically, we examine the behavior of the radial wavefunction $u_0(r) \propto \sin(kr + \delta_0)$. For small k, we use the small-angle approximation $\sin(x) \approx x$:

$$u_0(r) \approx kr + \delta_0 = k\left(r + \frac{\delta_0}{k}\right) = k(r - a) \tag{51}$$

The scattering length a represents the **extrapolated node** of the zero-energy wavefunction.

- **Repulsive ($a > 0$):** The wavefunction is "pushed out" of the potential region, and the node is at a positive r.
- **Attractive ($a < 0$):** The wavefunction is "pulled in," and the extrapolated node lies at a negative r.

The s-wave Scattering Amplitude

Using the effective range expansion (neglecting r_{eff}), we can express the scattering amplitude f_0 directly in terms of a. Starting from $f_0 = 1/(k \cot \delta_0 - ik)$:

$$f_0(k) = \frac{1}{-1/a - ik} = -\frac{a}{1 + ika} \tag{52}$$

In the limit of vanishingly small momentum ($ka \ll 1$), the amplitude reduces to the constant value:

$$\lim_{k \to 0} f_0(k) = -a \tag{53}$$

This confirms that at absolute zero, the entire scattering process is encapsulated by the single parameter a, which is the assumption used to derive the coupling constant g for the Gross-Pitaevskii equation.

15.5 Linking a to the Coupling Constant g

We now have two ways to bridge the microscopic scattering length a to the macroscopic coupling constant $g = \int V(r) d^3r$.

Approach A: The Born Approximation (Perturbative)

The Born approximation assumes the potential is a small perturbation to the plane wave. The scattering amplitude is the Fourier transform of the potential:

$$f_0 \approx -\frac{\mu}{2\pi\hbar^2}\int V(\mathbf{r})d^3r = -\frac{m}{4\pi\hbar^2}g \tag{54}$$

In the $k \to 0$ limit, we define $f_0 = -a$. This leads directly to:

$$g = \frac{4\pi\hbar^2 a}{m} \tag{55}$$

Limitation: This is mathematically convenient but assumes the potential is "weak," which is often not true for real interatomic potentials.

Approach B: The Box Energy Shift (Intuitive)

Imagine two atoms in a large cubic volume L^3. The scattering length a shifts the wavefunction node, effectively changing the allowed wavevectors by $\Delta k \approx -\pi a/L^2$.

1. **Kinetic Energy Change:** This change in k results in a shift in the ground state energy:

$$\Delta E \approx \frac{\hbar^2}{m}\left(k_{shifted}^2 - k_{free}^2\right) \approx \frac{4\pi\hbar^2 a}{mL^3} \tag{56}$$

2. **Mean-Field Match:** In the GP equation, the interaction energy per particle is $g \times n$, where density $n = 1/L^3$. Matching the two gives:

$$g\left(\frac{1}{L^3}\right) = \frac{4\pi\hbar^2 a}{mL^3} \implies g = \frac{4\pi\hbar^2 a}{m} \tag{57}$$

Advantage: this shows that g is the physical energy cost of "pushing" the wavefunction by a distance a, regardless of the potential's internal shape.

Derivation of the Elastic Cross Section

The total elastic cross section σ_{el} is defined as the ratio of the total scattered flux to the incident flux. For identical bosons, we integrate the differential cross section $|f(\theta,k)+f(\pi-\theta,k)|^2$ over the hemisphere:

$$\sigma_{el} = \int_0^{2\pi} d\phi \int_0^{\pi/2} |f(\theta,k)+f(\pi-\theta,k)|^2 \sin\theta d\theta \tag{58}$$

In the s-wave limit ($l = 0$), the scattering amplitude f_0 is isotropic (independent of θ), so $f(\theta) = f(\pi-\theta) = f_0$. The integral simplifies to:

$$\sigma_{el} = 8\pi|f_0|^2 \tag{59}$$

Recalling the link between the amplitude and the phase shift, $f_0 = \frac{e^{i\delta_0}\sin\delta_0}{k}$, we substitute this into the expression:

$$\sigma_{el} = 8\pi\left|\frac{e^{i\delta_0}\sin\delta_0}{k}\right|^2 = \frac{8\pi}{k^2}\sin^2\delta_0 \tag{60}$$

The Effective Range Expansion

To find the k-dependence, we use the effective range expansion for the phase shift δ_0, which relates the scattering phase to the scattering length a:

$$k \cot \delta_0 \approx -\frac{1}{a} + \frac{1}{2} r_{eff} k^2 + \dots \tag{61}$$

Neglecting the effective range ($r_{eff} \approx 0$) for a dilute gas, we have $\cot \delta_0 = -1/ka$. Using the trigonometric identity $\sin^2 \delta = 1/(1 + \cot^2 \delta)$, we find:

$$\sin^2 \delta_0 = \frac{1}{1 + (-1/ka)^2} = \frac{k^2 a^2}{1 + k^2 a^2} \tag{62}$$

Substituting this back into the cross section formula yields the final form: [colback=blue!5, title=Elastic Cross Section for Identical Bosons]

$$\sigma_{el}(k) = \frac{8\pi a^2}{1 + k^2 a^2} \tag{63}$$

The Wigner Threshold Law

The physical significance of the complex part β becomes clear when we look at the low-energy limit of σ_{inel}. For small k, the S-matrix magnitude scales as $|S_0|^2 \approx 1 - 4k\beta$. Substituting this into the inelastic formula:

$$\sigma_{inel}(k) \approx \frac{2\pi}{k^2}(4k\beta) = \frac{8\pi\beta}{k} \tag{64}$$

This $1/k$ (or $1/v$) scaling is known as the **Wigner Threshold Law**. It tells us that while the elastic cross section reaches a constant value at zero temperature, the inelastic cross section *diverges*. This is why inelastic losses, such as three-body recombination, can remain a dominant factor in the lifetime of a BEC even at nanokelvin temperatures.

16 Lecture 11: From Scattering Poles to Feshbach Resonances

A bound state corresponds to a singularity (pole) in the scattering amplitude at a purely imaginary momentum $k = i\kappa$ ($\kappa > 0$). Setting the denominator of $f(k)$ to zero:

$$1 + i(i\kappa)a = 0 \implies \kappa = \frac{1}{a} \tag{65}$$

This leads to three physical regimes as the scattering length a is tuned:

- $a > 0$ **(Real Bound State):** The pole sits at $k = i/a$ on the physical sheet. The binding energy is $E_b = -\frac{\hbar^2 \kappa^2}{2\mu} = -\frac{\hbar^2}{2\mu a^2}$.
- $a \to \pm\infty$ **(Unitarity):** The pole sits at $k = 0$. The scattering cross-section $\sigma = 4\pi |f|^2$ diverges, limited only by the wavelength λ^2.
- $a < 0$ **(Virtual State):** The pole sits at $k = -i/|a|$ on the unphysical sheet. There is no bound state, but the system exhibits a large scattering length due to a "near-miss" bound state.

16.1 Potential Resonance: The Single Channel Square Well

A potential resonance occurs when the depth of a potential is tuned such that a new bound state is pulled down from the scattering continuum. Consider a single-channel square well potential of depth $-V_0$ and range r_0:

$$V(r) = \begin{cases} -V_0 & r < r_0 \\ 0 & r > r_0 \end{cases} \tag{66}$$

Defining the interior wavenumber $q = \sqrt{2\mu(E + V_0)/\hbar^2}$, the scattering phase shift δ is found by matching the boundary conditions at $r = r_0$. In the limit $k \to 0$, the scattering length is given by:

$$a = r_0 \left(1 - \frac{\tan q_0 r_0}{q_0 r_0}\right) \tag{67}$$

where $q_0 = \sqrt{2\mu V_0/\hbar^2}$.

- **Divergence condition:** As the potential depth V_0 increases, $q_0 r_0$ passes through values of $\pi/2, 3\pi/2, 5\pi/2, \ldots$.
- At these points, $\tan q_0 r_0 \to \infty$, causing the scattering length a to diverge to $\pm\infty$.
- This divergence marks the exact moment the potential becomes deep enough to support an additional bound state.

16.2 Poles and the Emergence of Bound States

A bound state corresponds to a singularity (pole) in the scattering amplitude at a purely imaginary momentum $k = i\kappa$ ($\kappa > 0$). Setting the denominator of $f(k)$ to zero:

$$1 + i(i\kappa)a = 0 \implies \kappa = \frac{1}{a} \tag{68}$$

This leads to three physical regimes as the scattering length a is tuned:

- $a > 0$ **(Real Bound State):** The pole sits at $k = i/a$ on the physical sheet. The binding energy is $E_b = \frac{\hbar^2}{2\mu a^2}$.
- $a \to \pm\infty$ **(Unitarity):** The pole sits at $k = 0$. The scattering cross-section $\sigma = 4\pi|f|^2$ diverges, limited only by the wavelength $1/k^2$.
- $a < 0$ **(Virtual State):** The pole sits at $k = -i/|a|$ on the unphysical sheet. There is no bound state, but the system exhibits a large scattering length.

17 Lecture 11: Multi-Channel Scattering and Feshbach Resonances

17.1 Definition of Scattering Channels

In the context of multi-channel scattering, a "channel" refers to a specific internal state (e.g., hyperfine or spin state) of the colliding particles. Channels are classified based on the relationship between the total energy E and the asymptotic potential energy V_∞ of that state.

- **Open Channel** ($E > V_\infty$)**:** A channel is considered open if the total energy of the system exceeds the energy of the atoms at infinite separation.

  - **Asymptotic Behavior:** The radial wavefunction $\psi(r)$ behaves as a superposition of traveling waves (oscillatory behavior) as $r \to \infty$.
  - **Physical Interpretation:** Atoms in this channel have sufficient kinetic energy to escape each other's potential and reach the detector as free particles.

- **Closed Channel ($E < V_\infty$):** A channel is closed if the total energy is lower than the energy threshold required for the atoms to be at infinite separation.
  - **Asymptotic Behavior:** The wavefunction $\psi(r)$ decays exponentially ($e^{-\kappa r}$) as $r \to \infty$, making the state non-propagating in the far field.
  - **Physical Interpretation:** While atoms cannot exist as free particles in this channel, it can support discrete **bound states** (molecules). A Feshbach resonance occurs when a bound state in a closed channel is tuned to the same energy as the scattering state in the open channel.

17.2 Model for Two-Channel Scattering

In multi-channel scattering, we consider two scattering channels. The interaction is described by a 2×2 scattering matrix $\mathbf{S}$, which connects the incoming and outgoing flux across both channels:

$$\mathbf{S} = \begin{pmatrix} S_{00} & S_{01} \\ S_{10} & S_{11} \end{pmatrix} \tag{69}$$

The requirement of probability conservation dictates that the $\mathbf{S}$-matrix must be unitary, satisfying $\mathbf{S}^\dagger \mathbf{S} = \hat{1}$. This imposes strict constraints on the magnitudes and phases of the matrix elements:

- **Diagonal Elements:** If we define the open-channel element as $S_{00} = \eta e^{2i\delta}$, where δ is the real scattering phase shift and η is the inelasticity parameter ($0 \leq \eta \leq 1$), unitarity requires that the closed-channel diagonal element has the same magnitude: $|S_{11}| = \eta$.

- **Off-Diagonal Elements:** The elements S_{01} and S_{10} describe the coupling between the two channels. Unitarity forces their magnitudes to be $|S_{10}| = |S_{01}| = \sqrt{1-\eta^2}$.

- **Phase Relationships:** To ensure row-column orthogonality ($S_{00}S_{10}^* + S_{01}S_{11}^* = 0$), the phases must be coupled. A general unitary form is:

$$\mathbf{S} = \begin{pmatrix} \eta e^{2i\delta} & i\sqrt{1-\eta^2} e^{i(\delta+\phi)} \\ i\sqrt{1-\eta^2} e^{i(\delta+\phi)} & \eta e^{2i\phi} \end{pmatrix} \tag{70}$$

The scattering matrix elements directly determine the observable scattering behavior:

- **Elastic Cross Section:** The probability that atoms scatter but remain in the open channel is $\sigma_{el} = \frac{\pi}{k^2}|1 - S_{00}|^2 = \frac{\pi}{k^2}|1 - \eta e^{2i\delta}|^2 = \sigma_{el} = \frac{\pi}{k^2}\left[(1-\eta)^2 + 4\eta \sin^2 \delta\right]$.

- **Inelastic Cross Section:** The loss of flux from the open channel due to transitions to the closed channel is $\sigma_{in} = \frac{\pi}{k^2}(1 - |S_{00}|^2) = \frac{\pi}{k^2}(1 - \eta^2)$.

- **Physical Interpretation:** $|S_{10}|^2$ represents the transition probability from channel 0 to channel 1. The "loss" in the elastic channel ($\eta < 1$) is exactly balanced by the emergence of the inelastic flux, ensuring total probability is conserved.

17.3 Potential vs. Feshbach Resonance

The scattering length a can be manipulated through two distinct resonance mechanisms:

- **Potential Resonance:** Occurs entirely within the **open channel**. As the depth of the open-channel potential $V_{open}(r)$ increases, the scattering length diverges whenever the potential becomes deep enough to support a new bound state at $E = 0$.
- **Feshbach Resonance:** Occurs due to coupling (ϵ) between the open channel and a bound state in the **closed channel**. When the energy of the closed-channel molecular state is tuned (e.g., via a magnetic field) to match the collision energy of the open channel, a diverges according to:
$$a(B) = a_{bg}\left(1 - \frac{\Delta B}{B - B_0}\right) \tag{71}$$

17.4 Reaction Matrix (K-Matrix)

While the **S**-matrix describes the transformation between incoming and outgoing traveling waves, the Reaction Matrix (**K**-matrix) provides an alternative framework based on real-valued standing waves, which is particularly useful for low-energy scattering calculations and for the derivation of scattering length near a Feshbach resonance.

For a single-channel s-wave scattering problem, the radial wavefunction at large distances ($r \to \infty$) is expressed as:
$$u(r) \propto e^{-ikr} - Se^{ikr} \propto \sin(kr) + K\cos(kr) \tag{72}$$
Comparing this to the standard phase-shifted form $\psi(r) \propto \sin(kr + \delta)$, we obtain the fundamental relation:
$$K = \tan\delta \tag{73}$$

In the multi-channel case, the radial wavefunction is represented as a vector $\mathbf{u}(r)$. To maintain consistency when some channels are closed, we define the wavefunction using the diagonal matrices of regular solutions $\mathbf{J}(r)$ and irregular solutions $\mathbf{N}(r)$:

$$\mathbf{u}(r) = [\mathbf{J}(r) + \mathbf{N}(r)\mathbf{K}]\,\mathbf{c} \tag{74}$$

For a two-channel system where channel 0 is open ($k_0 \in \mathbb{R}$) and channel 1 is closed ($k_1 = i\kappa$), the diagonal matrices are defined as:

$$\mathbf{J}(r) = \begin{pmatrix} \sin(k_0 r) & 0 \\ 0 & 0 \end{pmatrix}, \quad \mathbf{N}(r) = \begin{pmatrix} \cos(k_0 r) & 0 \\ 0 & e^{-\kappa r} \end{pmatrix} \tag{75}$$

where the coefficient vector $\mathbf{c} = (1, A_1)^T$ is chosen to satisfy the incident flux conditions. The components of the vector wavefunction are then expressed as:

- **Open Channel**: $u_0(r) = \sin(k_0 r) + (K_{00} + K_{01}A_1)\cos(k_0 r)$
- **Closed Channel**: $u_1(r) = (K_{10} + K_{11}A_1)e^{-\kappa r}$

In the closed channel, the "sine" term vanishes and the "cosine" term is replaced by the decaying exponential $e^{-\kappa r}$ to ensure $u_1(r) \to 0$ as $r \to \infty$. This formulation is consistent with research in atomic and molecular quantum gases, where the closed channel behaves as a virtual state rather than an oscillating wave.

The **K**-matrix is inherently Hermitian ($\mathbf{K}^\dagger = \mathbf{K}$) because it is constructed from the real, standing-wave solutions of the Schrödinger equation for a Hermitian Hamiltonian. Its connection to the **S**-matrix is given by the Cayley transform:

$$\mathbf{S} = \frac{\hat{1} + i\mathbf{K}}{\hat{1} - i\mathbf{K}}, \quad \mathbf{K} = i\frac{\hat{1} - \mathbf{S}}{\hat{1} + \mathbf{S}} \tag{76}$$

By solving the inverse relation, we derive the general form of the **K**-matrix elements:

$$\mathbf{K} = \frac{1}{D}\begin{pmatrix} \eta \sin 2\delta + \eta^2 \sin(2\delta - 2\phi) & \sqrt{1-\eta^2}\cos(\delta - \phi) \\ \sqrt{1-\eta^2}\cos(\delta - \phi) & \eta \sin 2\phi - \eta^2 \sin(2\delta - 2\phi) \end{pmatrix} \tag{77}$$

where the common denominator D is defined as:

$$D = 1 + \eta(\cos 2\delta + \cos 2\phi) + \eta^2 \cos(2\delta - 2\phi) \tag{78}$$

In the low-energy limit ($k \to 0$), the single-channel K-matrix element relates directly to the scattering length a:

$$K = \tan\delta \approx -ka \tag{79}$$

17.5 Derivation of scattering length $a(B)$ using K matrix

The magnetic field dependence of the scattering length $a(B)$ arises from the virtual population of the closed-channel bound state.

Step 1: Effective K-matrix for the Open Channel

The mixing amplitude A_1 in the closed channel is driven by the open-channel coupling K_{10} and restricted by the energy detuning from the bound state E_c. The consistency of the closed-channel response requires:

$$(E - E_c)A_1 = K_{10} + K_{11}A_1 \tag{80}$$

Solving for the amplitude A_1:

$$A_1 = \frac{K_{10}}{E - E_c - K_{11}} \tag{81}$$

Substituting this into the open-channel coefficient $K_{\text{eff}} = K_{00} + K_{01}A_1$, and using the Hermiticity property $K_{01} = K_{10}$, we find:

$$K_{\text{eff}} = K_{00} + \frac{K_{01}^2}{E - (E_c + K_{11})} \tag{82}$$

Step 2: Threshold Scaling and Resonance Width

In the limit $k \to 0$, we apply threshold scaling laws to relate the matrix elements to physical observables:

- $K_{\text{eff}} = -ka(B)$
- $K_{00} = -ka_{\text{bg}}$, where a_{bg} is the background scattering length
- $K_{01}^2 = C \cdot k$, representing the coupling strength

This yields:

$$-ka(B) = -ka_{\text{bg}} + \frac{C \cdot k}{E - E'_c} \implies a(B) = a_{\text{bg}} - \frac{C}{E - E'_c} \tag{83}$$

Step 3: Magnetic Field Tuning

Using the linear approximation for the magnetic detuning $E'_c - E \approx \Delta\mu(B - B_0)$, we recover the standard Feshbach formula:

$$a(B) = a_{\text{bg}} \left(1 - \frac{\Delta B}{B - B_0} \right) \tag{84}$$

where $\Delta B = C/(a_{\text{bg}}\Delta\mu)$ defines the resonance width.

Term	**Scattering**	**Definition** $u(r) = r\psi(r)$	**Scattering Length** a	**S-wave Cross section** σ
f	Amplitude	$\psi(r) \sim e^{ikz} + fe^{ikr}/r$	$-\lim_{k\to 0} f$	$4\pi\|f\|^2$
S	S-matrix	$u(r) \sim e^{-ikr} - Se^{ikr}$	$\lim_{k\to 0} \frac{1-S}{2ik}$	$\frac{\pi}{k^2}\|1-S\|^2$
δ	Phase shift	$S = e^{2i\delta}$	$-\lim_{k\to 0} \frac{\delta}{k}$	$\frac{4\pi}{k^2}\sin^2\delta$
K	K-matrix	$u(r) \sim \sin(kr) + K\cos(kr)$	$-\lim_{k\to 0} \frac{K}{k}$	$\frac{4\pi}{k^2}\frac{K^2}{1+K^2}$
T	T-matrix	$u(r) = \phi + G_0 T\phi$	$\frac{\pi}{k}\text{Im}(T)$	$(\frac{2\pi}{k})^2\|T\|^2$

Table 4: Mathematical properties and low-energy limits of fundamental scattering variables.

Comparison of fundamental scattering quantities and their mathematical properties.

17.6 Scattering of Alkali Atoms: Hyperfine and Exchange Interactions

A realistic description of two alkali atoms in their ground states requires a Hamiltonian that accounts for both internal and inter-atomic degrees of freedom:

$$H = H_{HF} + H_{ex} \tag{85}$$

- **Hyperfine Interaction (H_{HF}):** Dominates at **large separation** ($r \to \infty$). The appropriate basis is $|f_1, m_{f1}; f_2, m_{f2}\rangle$ or the coupled basis $|F, M_F\rangle$, where $\mathbf{F} = \mathbf{f_1} + \mathbf{f_2}$.
- **Exchange Interaction (H_{ex}):** Dominates at **short distance** where electron clouds overlap. The physics is governed by the total electron spin $\mathbf{S} = \mathbf{s_1} + \mathbf{s_2}$ (Singlet $S = 0$ or Triplet $S = 1$) and total nuclear spin $\mathbf{I} = \mathbf{i_1} + \mathbf{i_2}$. The basis here is $|S, I; F, M_F\rangle$.

The transition between these bases as atoms approach each other allows the external magnetic field to tune the relative energy of the channels, facilitating the Feshbach resonances used in modern quantum gas experiments.

18 Lecture 12 Short-Range Exchange and Channel Mixing

18.1 The Two-Zone Physical Picture

To solve the multi-channel scattering problem, we divide the interatomic distance r into two distinct regions where different interactions dominate.

- **Short Range ($r < r_0$):** The electronic exchange interaction is the strongest force. The individual electronic spins $\mathbf{s}_1, \mathbf{s}_2$ and nuclear spins $\mathbf{i}_1, \mathbf{i}_2$ decouple, making the total electronic spin $\mathbf{S} = \mathbf{s}_1 + \mathbf{s}_2$ (Singlet $S = 0$ or Triplet $S = 1$) the "good" quantum number.

- **Long Range ($r > r_0$):** The exchange interaction vanishes. The Hamiltonian is dominated by the hyperfine interaction $H_{hf} = a_{hf}(\mathbf{s}_1 \cdot \mathbf{i}_1 + \mathbf{s}_2 \cdot \mathbf{i}_2)$ and the Zeeman effect. The good quantum numbers are the projections of the total atomic spins $f_{1,2}$.

18.2 Frame Transformation and the Mixing Mechanism

The "mixing" between open and closed channels that leads to a Feshbach resonance occurs because the eigenstates of the short-range potential do not coincide with the eigenstates of the long-range Hamiltonian.

We handle this transition using a **Frame Transformation Matrix** $U_{S,\alpha}$. This matrix projects the short-range singlet/triplet states $|S\rangle$ onto the long-range hyperfine/Zeeman channels $|\alpha\rangle$:

$$|\alpha\rangle_{long} = \sum_{S\in\{0,1\}} U_{S,\alpha}|S\rangle_{short} \tag{86}$$

18.3 The Coupling Operator $\hat{W}$

Because the singlet potential $V_S(r)$ and triplet potential $V_T(r)$ are different, an atom in a specific hyperfine channel $|\alpha\rangle$ experiences a "mixed" potential. The coupling that allows an atom to jump from an **open channel** (P) to a **closed channel** (Q) is proportional to the difference potential:

$$\hat{W}_{PQ} \propto \langle \Phi_Q|V_T(r) - V_S(r)|\Psi_P\rangle \tag{87}$$

Given the coupling, we can directly solve the Schrödinger equation for the multi-channel radial wavefunction. We expand the total wavefunction $|\Psi\rangle$ in the channel basis $\{|\alpha\rangle\}$:

$$|\Psi(r)\rangle = \frac{1}{r}\sum_{\alpha} \psi_\alpha(r)|\alpha\rangle \tag{88}$$

Substituting this into the Schrödinger equation $\hat{H}|\Psi\rangle = E|\Psi\rangle$ and projecting onto a specific channel $|\alpha\rangle$ yields a set of coupled second-order differential equations:

$$\left[-\frac{\hbar^2}{2\mu}\frac{d^2}{dr^2} + \frac{\ell(\ell+1)\hbar^2}{2\mu r^2} + V_{\alpha\alpha}(r) - E\right]\psi_\alpha(r) = -\sum_{\beta\neq\alpha} V_{\alpha\beta}(r)\psi_\beta(r) \tag{89}$$

Where the diagonal and off-diagonal potential matrix elements are defined as:

$$V_{\alpha\beta}(r) = \langle\alpha|\hat{V}_{exchange}(r) + \hat{H}_{hf} + \hat{H}_Z|\beta\rangle \tag{90}$$

As we discussed, at short range, the coupling is driven by the exchange interaction. If we simplify to an open channel (P) and a closed channel (Q), the coupling term $V_{PQ}(r)$ is:

$$V_{PQ}(r) \propto [V_T(r) - V_S(r)] \times \text{(Spin-Mixing Coefficient)} \tag{91}$$

Physically, the term on the right-hand side of the radial equation acts as a **source/sink term**. The open-channel wavefunction $\psi_P(r)$ "feeds" into the closed-channel $\psi_Q(r)$ in the region where the singlet and triplet potentials differ most.

To find the scattering length, we integrate these equations numerically from $r = 0$ out to the long-range region:

1. **At $r \to 0$:** The wavefunctions must vanish, $\psi_\alpha(0) = 0$.

2. **At** $r \to \infty$**:** The closed-channel wavefunction must decay exponentially, $\psi_Q(r) \to e^{-\kappa r}$.

3. **At** $r \to \infty$**:** The open-channel wavefunction takes the asymptotic form:

$$\psi_P(r) \propto \sin(kr + \delta) \approx k(r - a) \quad \text{(for } k \to 0\text{)} \tag{92}$$

By matching the numerically integrated solution to this asymptotic form, we directly extract the scattering length a. When the magnetic field tunes the closed-channel bound state near E, the "leakage" into the closed channel causes the phase shift δ to change rapidly, leading to the characteristic divergence of a.

- **T-matrix:** Efficient for calculating cross-sections and identifying resonance positions analytically.

- **Radial Integration:** Provides the actual **spatial distribution** of the atoms. This is crucial for understanding the "size" of the Feshbach molecule and the validity of the zero-range approximation in your Hubbard model simulations.

18.4 Weak Coupling Limit: Perturbative Treatment of the Wavefunction

18.5 Hamiltonian Partitioning

We consider a two-channel system consisting of an open channel (P) and a closed channel (Q). The total Hamiltonian $\hat{H}$ is partitioned into a diagonal part $\hat{H}_0$ and an off-diagonal coupling operator $\hat{W}$:

$$\hat{H} = \hat{H}_0 + \hat{W} = \begin{pmatrix} \hat{H}_P & 0 \\ 0 & \hat{H}_Q \end{pmatrix} + \begin{pmatrix} 0 & \hat{V}_{PQ} \\ \hat{V}_{QP} & 0 \end{pmatrix} \tag{93}$$

where:

- $\hat{H}_P = -\frac{\hbar^2}{2\mu}\frac{d^2}{dr^2} + V_{PP}(r)$ is the open-channel Hamiltonian.

- $\hat{H}_Q = -\frac{\hbar^2}{2\mu}\frac{d^2}{dr^2} + V_{QQ}(r)$ is the closed-channel Hamiltonian.

- $\hat{V}_{PQ} = \hat{V}_{QP}^\dagger$ is the coupling potential (typically the exchange interaction).

18.6 Zeroth-Order Solution

We assume the system is prepared in the open channel at collision energy E. The zeroth-order wavefunction $|\Psi^{(0)}\rangle$ satisfies $(\hat{H}_0 - E)|\Psi^{(0)}\rangle = 0$:

$$|\Psi^{(0)}\rangle = \begin{pmatrix} \phi_k(r) \\ 0 \end{pmatrix} \tag{94}$$

where $\phi_k(r)$ is the background scattering state in the potential V_{PP}.

18.7 First-Order: Closed-Channel Occupation

The first-order correction $|\Psi^{(1)}\rangle$ is found via the inhomogeneous equation:

$$(E - \hat{H}_0)|\Psi^{(1)}\rangle = \hat{W}|\Psi^{(0)}\rangle \tag{95}$$

Expanding the matrix components:

$$\begin{pmatrix} E - \hat{H}_P & 0 \\ 0 & E - \hat{H}_Q \end{pmatrix} \begin{pmatrix} \psi_P^{(1)} \\ \psi_Q^{(1)} \end{pmatrix} = \begin{pmatrix} 0 \\ \hat{V}_{QP}\phi_k \end{pmatrix} \tag{96}$$

The bottom row provides the equation for the closed-channel component:

$$(E - \hat{H}_Q)\psi_Q^{(1)}(r) = \hat{V}_{QP}(r)\phi_k(r) \tag{97}$$

Expanding $\psi_Q^{(1)}$ in terms of the closed-channel bound state $\phi_b(r)$ (where $\hat{H}_Q\phi_b = E_b\phi_b$):

$$\psi_Q^{(1)}(r) \approx \frac{\langle \phi_b|\hat{V}_{QP}|\phi_k\rangle}{E - E_b}\phi_b(r) \tag{98}$$

Definition: $\langle \phi_b|\hat{V}_{QP}|\phi_k\rangle = \int_0^\infty \phi_b^*(r)\hat{V}_{QP}(r)\phi_k(r)dr$ is the coupling matrix element.

18.8 Second-Order: Open-Channel Correction

The second-order correction satisfies $(E - \hat{H}_0)|\Psi^{(2)}\rangle = \hat{W}|\Psi^{(1)}\rangle$:

$$\begin{pmatrix} E - \hat{H}_P & 0 \\ 0 & E - \hat{H}_Q \end{pmatrix} \begin{pmatrix} \psi_P^{(2)} \\ \psi_Q^{(2)} \end{pmatrix} = \begin{pmatrix} \hat{V}_{PQ}\psi_Q^{(1)} \\ 0 \end{pmatrix} \tag{99}$$

The top row describes the ”back-coupling” into the open channel:

$$(E - \hat{H}_P)\psi_P^{(2)}(r) = \hat{V}_{PQ}(r)\psi_Q^{(1)}(r) \tag{100}$$

To solve for $\psi_P^{(2)}$, we use the Green's function $G_P(r, r'; E) = \langle r|(E - \hat{H}_P)^{-1}|r'\rangle$:

$$\psi_P^{(2)}(r) = \int_0^\infty G_P(r, r'; E)\hat{V}_{PQ}(r')\psi_Q^{(1)}(r')dr' \tag{101}$$

Substituting the first-order result for $\psi_Q^{(1)}$:

$$\psi_P^{(2)}(r) = \frac{\langle \phi_b|\hat{V}_{QP}|\phi_k\rangle}{E - E_b}\int_0^\infty G_P(r, r'; E)\hat{V}_{PQ}(r')\phi_b(r')dr' \tag{102}$$

18.9 Final Result

The total open-channel wavefunction to second order is:

$$\psi_P(r) \approx \phi_k(r) + \frac{\langle \phi_b|\hat{V}_{QP}|\phi_k\rangle}{E - E_b}\int_0^\infty G_P(r, r'; E)\hat{V}_{PQ}(r')\phi_b(r')dr' \tag{103}$$

18.9.1 Scattering Length

The second-order term modifies the asymptotic phase of the wavefunction. By analyzing the long-range behavior of the integral, we find that the phase shift δ is modified by:

$$\tan(\delta) = \tan(\delta_{bg}) - \frac{\pi|\langle\phi_b|V_{QP}|\phi_k\rangle|^2}{E - E_b} \tag{104}$$

This confirms that even weak coupling can lead to a massive change in the scattering length a because the correction is **resonantly enhanced** by the energy denominator $(E - E_b)^{-1}$.

Summary of the Perturbative Cycle

- **Order 0:** Atoms scatter off the background potential V_{PP}.
- **Order 1:** Atoms "probe" the closed channel bound state ϕ_b.
- **Order 2:** The bound state "re-radiates" back into the scattering channel, shifting the asymptotic phase and diverging the scattering length.

18.10 Implications for Feshbach Resonances

1. **Existence:** If $V_S(r) = V_T(r)$, the channels would remain uncoupled, and no Feshbach resonances would occur regardless of the magnetic field.
2. **Resonance Width ΔB:** The width of the resonance is determined by the overlap between the open-channel scattering wavefunction and the closed-channel bound state, weighted by the difference potential $V_T - V_S$.
3. **Quantum Defect:** The short-range phase shifts δ_S and δ_T (the quantum defects) provide the boundary conditions that determine the background scattering length a_{bg} at long range.

18.11 Summary Table: Basis Comparison

Feature	**Short Range ($r \ll x_{vdW}$)**	**Long Range ($r \gg x_{vdW}$)**
Dominant Energy	Electrostatic Exchange	Hyperfine & Zeeman
Good Basis	Singlet/Triplet (S, M_S)	Hyperfine (f, m_f)
Potentials	$V_S(r)$ and $V_T(r)$	$1/r^6$ van der Waals tail

Fermion-Mediated Pairing of Heavy Bosons

1. Physical Constants and Parameters

We consider a mixture of heavy bosons and light fermions (e.g., Cs-Li):

- m_B, m_F: Masses of the boson and fermion, respectively.
- $R = \frac{m_B}{m_F}$: Mass ratio ($R \approx 22.1$ for Cs-Li).
- a_{BB}: Background boson-boson s-wave scattering length.
- a_{BF}: Interspecies s-wave scattering length.
- k_F: Fermi momentum of the fermion gas.
- $g_{BF} \approx \frac{2\pi\hbar^2 a_{BF}}{m_F}$: Interspecies coupling constant (valid for $m_B \gg m_F$).

2. The Mediated Potential (V_{ind})

In the static Born-Oppenheimer limit, the induced interaction between two bosons is given by the spatial Fourier transform of the fermion polarizability:

$$V_{ind}(r) = -\frac{g_{BF}^2 m_F k_F^4}{\pi^3 \hbar^2} F(2k_F r) \tag{105}$$

where the spatial profile $F(x)$ is the RKKY function:

$$F(x) = \frac{\sin x - x\cos x}{x^4} \tag{106}$$

Substituting the definition of g_{BF} yields:

$$V_{ind}(r) = -\frac{4\hbar^2 a_{BF}^2 k_F^4}{\pi m_F} F(2k_F r) \tag{107}$$

3. The Zero-Energy Schrödinger Equation

The threshold for the first bound state occurs at energy $E = 0$. The radial equation for the relative motion of two bosons (reduced mass $\mu = m_B/2$) is:

$$u''(r) = \frac{m_B}{\hbar^2} V_{ind}(r) u(r) \tag{108}$$

Defining the dimensionless strength $\Lambda = \frac{4Ra_{BF}^2 k_F^4}{\pi}$:

$$u''(r) + \Lambda F(2k_F r) u(r) = 0 \tag{109}$$

4. Threshold Derivation

At the unitarity limit ($a_{eff} \to \infty$), we integrate the equation from 0 to ∞ subject to the boundary conditions:

1. **Short-range:** $u(0) = -a_{BB}$ and $u'(0) = 1$.
2. **Long-range:** $u'(\infty) = 0$ (wavefunction flattens at the binding threshold).

Integrating the curvature $u''(r)$:

$$\int_0^\infty u''(r)dr = u'(\infty) - u'(0) = -1 \tag{110}$$

Substituting the radial equation:

$$1 = \frac{m_B}{\hbar^2} \int_0^\infty |V_{ind}(r)| u(r) dr \tag{111}$$

Expanding the overlap integral $J = \int_0^\infty F(x)u(x)dx$ for small $k_F a_{BB}$:

$$J \approx I_1 - (2k_F a_{BB}) I_2 \tag{112}$$

where $I_1 \approx 0.40$ and $I_2 \approx 0.12$.

5. The Critical Formula

Rearranging for a_{BF} and grouping numerical coefficients α and β:

$$|a_{BF}^c| \approx \frac{1}{k_F\sqrt{R}}\sqrt{\alpha + \beta(k_F a_{BB})} \tag{113}$$

Numerical fitting yields $\alpha \approx 2.5$ and $\beta \approx 3.1$.

6. Numerical Application: Cs-Li Mixture

Parameters: $R \approx 22.1$, $k_F = 3.5\ \mu\text{m}^{-1} \approx 1.85 \times 10^{-4}\ a_0^{-1}$, and $a_{BB} = 200\ a_0$.

1. **Repulsion term:** $k_F a_{BB} \approx 0.037$.
2. **Calculation:**

$$|a_{BF}^c| = \frac{1}{(1.85 \times 10^{-4})\sqrt{22.1}}\sqrt{2.5 + 3.1(0.037)}$$

$$|a_{BF}^c| \approx 1858\ a_0$$

Result: The pairing threshold is approximately 1860 a_0.