

7810 Scattering in Quantum Gases
University of Colorado, Boulder (Fall 2019)

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This is graduate course on quantum scattering theory in the ultracold regime taught at the university of Colorado, Boulder by [Jose P. D’Incao](#). The course webpage can be found [here](#). An overview of the topics covered are as follows.

1. Basics of Scattering Theory.
2. Scattering of Particles with Molecule Structures.
3. Collisions in Periodic External Fields (Floquet Theory).

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Chapter 1

Introduction

In this class, we aim to take Hamiltonians and derive scattering solutions. To develop intuitions and technical skills about scattering in the ultracold (mostly) regimes. We will be starting out with the basics of scattering theory, which will prepare us for applying these concepts to more complex and interesting systems. Scattering is when a system with initially with no interaction, enters a regime of significant interaction and exits this regime to no interaction once again. As in all of physics, it is essential that we know the system we're dealing with. In our case, these are cold gases. This thus entails 1) short-range interactions 2) low energies. We will start off by looking a little into what these really mean.

§1.1 Short-Range Interactions

Consider a system of 2 interacting particles, separated by a distance r . The potential between them can be written as $V(r)$. We then define short-range interactions by:

$$\boxed{\lim_{r \rightarrow \infty} r^2 V(r) = 0} \quad (1.1)$$

Short-range interactions would then imply that our system would have a **finite** number of bound states. There is in fact a very quick back of the envelope way to estimate the number of bound states for a given potential. We do this with the relation:

$$N \approx \frac{1}{\pi} \int_{r_i}^{r_k} dr \sqrt{\frac{2\mu}{\hbar^2} (E - V(r))} \quad (1.2)$$

where r_i is the distance to the first turning point of the potential-well, and r_k the distance to the second turning point.

Example:

Consider a system with the potential:

$$V(r) = \begin{cases} +\infty, & r < r_i \\ -\frac{C_\alpha}{r^\alpha}, & r \geq r_i \end{cases} \quad (1.3)$$

The first thing we do is to set $E = 0$, which grants us that:

$$r_k = \left(\frac{C_\alpha}{|E|} \right)^{1/\alpha} = \infty \quad (1.4)$$

This renders our approximation integral as:

$$N \approx \frac{1}{\pi} \int_{r_i}^{\infty} dr \sqrt{\frac{2\mu}{\hbar^2} \left(\frac{C_\alpha}{r^\alpha} \right)} = \frac{\sqrt{8\mu C_\alpha}}{\pi \hbar} \left(\frac{r_i^{1-\alpha/2}}{\alpha - 2} \right) \quad (1.5)$$

for $\alpha > 2$, which tells us that N is finite when $\alpha > 2$! This means that we can define a *range of interaction*, that is approximately when we have some form of the “kinetic” and “potential” energies equate:

$$\frac{\hbar^2}{2\mu r_\alpha^2} = \frac{C_\alpha}{r_\alpha^\alpha} \quad (1.6)$$

$$\Rightarrow r_\alpha = \frac{1}{2} \left(\frac{2\mu C_\alpha}{\hbar^2} \right)^{\alpha-2} \quad (1.7)$$

We say that r_α grants us some measure of length scales at which particles no longer interact significantly.

The next concept we would like to establish is the idea of *low-energy*.

§1.2 Low-Energy Scales

What exactly do we mean when we say “*low-energy*”? For all intends and purposes, we take a low-energy regime as being:

$$E \ll \frac{\hbar^2}{2\mu r_\alpha^2} \quad \Rightarrow \quad \lambda_{\text{de broglie}} \gg r_\alpha \quad (1.8)$$

In this regime, scattering observables depend **only** on a few *partial waves* (which is something that we will come back to later on in the class). This also implies some sort of universality to these systems (also touched on more later).

It is useful to note that in order to establish an energy, length and time scale, we only need to know the length and mass scales. The rest can be derived from these 2 quantities. For a gas, the length scale would be the average interatomic distances:

$$l_n = n^{-1/3} \quad (1.9)$$

where n is the atomic density. From this, we get:

$$E_n = \frac{\hbar^2}{2ml_n^2} = \frac{\hbar^2}{2m} n^{2/3} \quad (1.10)$$

As for timescales, we will take these as:

$$t_n = \frac{\hbar}{E_n} \sim n^{-2/3} \quad (1.11)$$

and we will see later that the regime of *quantum degeneracy* occurs when (phase transition from a thermal gas to a condensate):

$$\boxed{\frac{k_B T}{E_n} \ll 1} \quad (1.12)$$

where E_n is the characteristic energy of the system. What we want to do now is look at typical values for several gases.

- Rubidium-85 gas as an example. This gas has an average density of $n = 10^{14} \text{cm}^{-3}$. Then at $T = 1 \text{nK}$, we will find that:

$$\frac{k_B T}{E_n} \approx 0.017 \quad (1.13)$$

- Air has about a density of $n \sim 10^{21} \text{cm}^{-3}$, and at $T = 273 \text{K}$, we find that:

$$\frac{k_B T}{E_n} \approx 10^6 \quad (1.14)$$

- Neutron star has $n \sim 10^{35} \text{cm}^{-3}$ and at $T \sim 10^6 \text{K}$, we find that:

$$\frac{k_B T}{E_n} \approx 0.04 \quad (1.15)$$

So what really affects quantum degeneracy is a long wavelength.

Chapter 2

Single Channel Scattering

Here, we are about to explore a regime of scattering known as single channel scattering. This regime generally entails that you are scattering particles off an infinitely massive scattering center. Either that or you're considering a scattering system in the center of mass frame such that there is no center of mass movement. However, what single channel scattering really means is that the particles we are scattering do not have any internal structure. We will see later that including internal structures allows particles to be in different energy states (internal energy configurations), these energy states are known as “channels”, hence multiple energy states imply multi-channel scattering. But for now, let's focus our efforts to understanding single channel scattering.

§2.1 Collisions

Before we get into scattering systems, we first want to get a grasp of what collisions are. A widely used measure of collisions is the *scattering cross-section*. Going back to classical mechanics, consider a particle incoming with velocity v onto a scattering center (another infinitely massive stationary particle). Key parameters that describe this system are the impact parameter a and the deflection angle after collision θ . This can be visualized in figure 2.1 below.

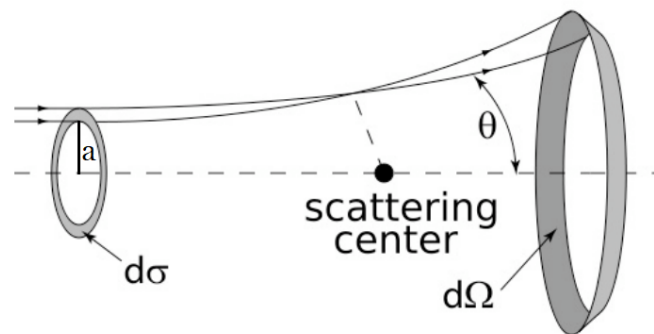


Figure 2.1: Classical Scattering ()

We see that the impact parameter a will tell us how far we can deviate from the scattering axis before there is no longer deflection pass the scattering center. With this, idea, we want the scattering cross-section to be an indication of the area within which we will observe scattering effects:

$$\boxed{\sigma \sim a^2} \quad (2.1)$$

To give a clearer picture of the collision process, some other relevant parameters are listed below.

1. **Collision Rate:** $\kappa = \frac{\hbar k}{m} \sigma$
2. **Interaction strength:** $E_n / \left(\frac{\hbar^2}{2\mu a^2} \right)$. We are in the regime of strong interactions when $na^3 \gg 1$, and the converse would be weak interactions
3. **Collision Time:** $t_c = \frac{1}{n\kappa} \Rightarrow \frac{t_n}{t_c} \sim \frac{1}{a^2}$
4. **s-wave Scattering Length:** a . This is analogous to the impact parameter in classical mechanics.

In most introductory courses on quantum mechanics, we heavily study bound states in boundary conditions that constitute some sort of potential well. The question now is, what kind of boundary conditions would be necessary for a scattering problem? We can always say that our initial state is a plane wave, or at least some superposition of plane waves e^{ikz} , whereas our final state after scattering would have to be characterized by angles θ and ϕ , but in principle can scatter in any direction (spherical wave) off the scattering center with amplitudes as a function of angular position. For the pedagogical purposes, let's assert a few assumptions (which can be generalized later on).

1. *Short Range Potential:* $V(\vec{r}) = 0, r \gg r_0$
2. *Isotropic Potential:* $V(\vec{r}) = V(r)$

where r_0 is the *range of the potential* (can be taken to be the *Van der Waals radius*). With these in mind, we can safely write the total solution of an incoming plane wave scattering off a scattering center to be:

$$\psi(\vec{r}) = e^{ikz} + f(\theta, \phi) \frac{e^{ikr}}{r} \quad (2.2)$$

where $f(\theta, \phi)$ is called the *scattering amplitude*. We came up with the scattering term by means of writing the most general solution (to get a more comprehensive explanation of this ansatz, refer to appendix A) which works at long ranges (large r). This ansatz is illustrated in figure 2.2 below.

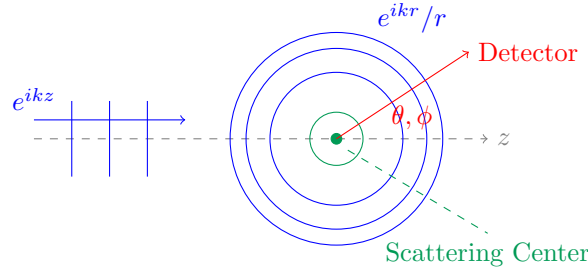


Figure 2.2: Scattering Stationary Solution

The goal now is to decompose the scattering term into a *partial wave expansion* as this allows us to extract some relevant physics.

§2.1.1 Partial Wave Expansion

Let us first rewrite the Schrödinger equation in a more explicit way:

$$\left[-\frac{\hbar^2}{2\mu} \left(\frac{d^2}{dr^2} + \frac{2}{r} \frac{d}{dr} \right) + \frac{\hat{L}^2(\theta, \phi)}{2\mu r^2} + V(r) - E \right] \psi(\vec{r}) = 0 \quad (2.3)$$

We know:

$$\hat{L}^2(\theta, \phi) Y_{l,m}(\theta, \phi) = l(l+1) \hbar^2 Y_{l,m}(\theta, \phi) \quad (2.4)$$

where $Y_{l,m}$ are the spherical harmonics.

Note: The spherical harmonics are eigenstates of the angular momentum operator and would be a natural basis.

With this, we have the most general solution for isotropic potentials to be:

$$\psi(\vec{r}) = \sum_{l,m} A_{l,m} \frac{u_{E,l}(r)}{r} Y_{l,m}(\theta, \phi) \quad (2.5)$$

This is known as the *partial wave expansion*. This expansion can tell us about the scattering at all ranges of r , but this solution doesn't tell us anything yet about our scattering until we connect the first scattering solution to this solution.

Note: Note that Bosons have $l = \text{even}$ ($\psi(\vec{r}) = \psi(-\vec{r})$) while Fermions have $l = \text{odd}$ ($\psi(\vec{r}) = -\psi(-\vec{r})$).

First, putting this into the Schrödinger equation:

$$\begin{aligned} & \left[-\frac{\hbar^2}{2\mu} \left(\frac{d^2}{dr^2} + \frac{2}{r} \frac{d}{dr} \right) + \frac{\hat{L}^2(\theta, \phi)}{2\mu r^2} + V(r) - E \right] \left(\sum_{l,m} A_{l,m} \frac{u_{E,l}(r)}{r} Y_{l,m}(\theta, \phi) \right) = 0 \\ \Rightarrow & \sum_{l,m} A_{l,m} \left[-\frac{\hbar^2}{2\mu} \left(\frac{d^2}{dr^2} + \frac{2}{r} \frac{d}{dr} \right) + \frac{\hat{L}^2(\theta, \phi)}{2\mu r^2} + V(r) - E \right] \frac{u_{E,l}(r)}{r} Y_{l,m}(\theta, \phi) = 0 \\ \Rightarrow & \sum_{l,m} A_{l,m} Y_{l,m}(\theta, \phi) \left[-\frac{\hbar^2}{2\mu} \left(\frac{d^2}{dr^2} + \frac{2}{r} \frac{d}{dr} \right) + \frac{l(l+1)\hbar^2}{2\mu r^2} + V(r) - E \right] \frac{u_{E,l}(r)}{r} = 0 \\ \Rightarrow & \left[-\frac{\hbar^2}{2\mu} \frac{d^2}{dr^2} + \frac{l(l+1)\hbar^2}{2\mu r^2} + V(r) - E \right] u_{E,l}(r) = 0 \end{aligned} \quad (2.6)$$

which is known as the *Schrödinger radial equation*. We also define the *effective potential* as:

$$V_{\text{eff}}(r) = V(r) + \frac{l(l+1)\hbar^2}{2\mu r^2} \quad (2.7)$$

which will elucidate some notions on scattering. Now let's take a WKB (semi-classical) approximation. To do this, we add a term called the *Langer correction* to the effective potential, which now becomes:

$$\tilde{V}_{\text{eff}}(r) = V(r) + \frac{l(l+1)\hbar^2}{2\mu r^2} + \frac{\hbar^2/4}{2\mu r^2} \quad (2.8)$$

The Langer correction term is added for 3D spherically symmetric problems and is heuristically a factor that arises due to the range of the radial Schrödinger equation being restricted from 0 to ∞ . With this correction, we can consider the classical means of scattering off the angular momentum barrier:

$$\begin{aligned} \frac{l(l+1)\hbar^2}{2\mu r^2} + \frac{\hbar^2/4}{2\mu r^2} &= E \\ \Rightarrow r_c &= \frac{(l+1/2)^2}{k} \end{aligned} \quad (2.9)$$

where $k^2 = 2\mu E/\hbar^2$ and r_c gives us the classical scattering turning point for low energy analysis. A question we can now ask is what is the probability that 2 particles collide? To get this probability, we utilize the general result from the WKB approximation:

$$\psi(r) = \frac{N}{\sqrt{p(r)}} \exp \left\{ \pm \frac{i}{\hbar} \int_{r_0}^r p(r') dr' \right\} \quad (2.10)$$

Having that the spatially varying momentum is:

$$\begin{aligned} p(r) &= \sqrt{2\mu [E - V_{\text{eff}}(r)]} \\ &= \sqrt{2\mu \left[V_{\text{eff}}(r) + \frac{\hbar^2/4}{2\mu r^2} \right]} \end{aligned} \quad (2.11)$$

where we take the energy of the particle to be effectively zero (low energy analysis), causing the probability to evaluate to:

$$\mathbb{P}(\text{2 particle collision}) \sim \exp \left\{ -2 \int_{r_0}^{r_c} \sqrt{\frac{2\mu}{\hbar^2} \left[V_{\text{eff}}(r) + \frac{\hbar^2/4}{2\mu r^2} \right]} dr \right\} \quad (2.12)$$

To solve this, we are going to split the integral up to integrating across some r^* such that

$r_0 < r^* < r_c$ and $V(r^*) = 0$:

$$\begin{aligned}
 \mathbb{P}(2 \text{ particle collision}) &\sim \exp \left\{ -2 \int_{r_0}^{r^*} \sqrt{\frac{2\mu}{\hbar^2} \left[V_{\text{eff}}(r) + \frac{\hbar^2}{4} \right]} dr - 2 \int_{r^*}^{r_c} \sqrt{\frac{2\mu}{\hbar^2} \left[V_{\text{eff}}(r) + \frac{\hbar^2}{4} \right]} dr \right\} \\
 &\sim \exp \left\{ -2 \int_{r_0}^{r^*} \sqrt{\frac{2\mu}{\hbar^2} \left[V_{\text{eff}}(r) + \frac{\hbar^2}{4} \right]} dr \right\} \exp \left\{ 2 \int_{r^*}^{r_c} \sqrt{\frac{2\mu}{\hbar^2} \left[V_{\text{eff}}(r) + \frac{\hbar^2}{4} \right]} dr \right\} \\
 &\sim A \exp \left\{ -2 \int_{r^*}^{r_c} \sqrt{\frac{2\mu}{\hbar^2} \left[V_{\text{eff}}(r) + \frac{\hbar^2}{4} \right]} dr \right\} \\
 &\sim k^{2l+1}
 \end{aligned} \tag{2.13}$$

This tells us that the probability of scattering falls off with higher order partial waves, making partial waves a practical tool for scattering analysis.

§2.2 Asymptotic Solutions

Let us now consider solutions whereby $r \gg r_0$ and $V(r) \approx 0$. That renders our radial equation as:

$$\left[-\frac{\hbar^2}{2\mu} \frac{d^2}{dr^2} + \frac{l(l+1)\hbar^2}{2\mu r^2} - \frac{\hbar^2 k^2}{2m} \right] u_{E,l}(r) = 0 \tag{2.14}$$

This produces 2 possible solutions which are spherical Bessel and Neumann functions:

$$f_{El}(r) = \sqrt{\frac{2\mu}{\pi \hbar^2 k}} (kr) j_l(kr), \quad \text{regular at } r = 0 \tag{2.15}$$

$$g_{El}(r) = \sqrt{\frac{2\mu}{\pi \hbar^2 k}} (kr) n_l(kr), \quad \text{irregular at } r = 0 \tag{2.16}$$

Bessel and Neumann functions are really just oscillatory functions with a decay envelop (figure 2.3 below).

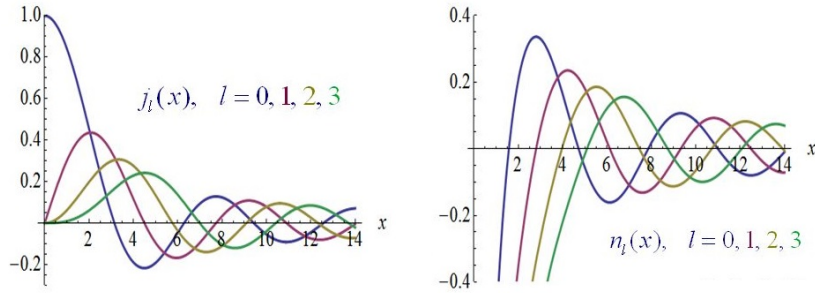


Figure 2.3: Spherical Bessel and Neumann functions.

These solutions are **not** normalizable since they are scattering solutions, and so the pre-factors ($\sqrt{2\mu/\pi\hbar^2k}$) in front of these solutions are there for *energy normalization*. These solutions are orthonormal with respect to different energies:

$$\begin{aligned}\int f_{El}(r)f_{E'l}(r)dr &= \delta(E - E') \\ \int g_{El}(r)g_{E'l}(r)dr &= \delta(E - E')\end{aligned}\tag{2.17}$$

In the region where $r \gg r_0$, there will be a regime whereby $kr \ll 1$ (low-energy and $r \gg r_0$ but not large enough to make kr large) and another where $kr \gg 1$ (low-energy and r large enough to make kr large). This is illustrated in figure 2.4 below.

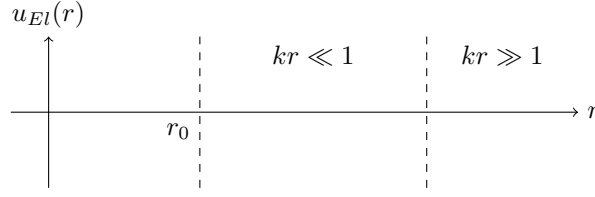


Figure 2.4: Regions of interest for $u_{El}(r)$.

In both these regimes, we can find very good approximate analytical solutions to f_{El} and g_{El} . First note that our radial solution can then be written as:

$$\begin{aligned}u_{El} &= A_l f_{El}(r) + B_l g_{El}(r) \\ &= C_l [f_{El}(r) \cos \delta_l + g_{El}(r) \sin \delta_l]\end{aligned}\tag{2.18}$$

where $a_l = \sqrt{A_l^2 + B_l^2}$ and $\tan \delta_l = -B_l/A_l$. It turns out that the 2 forms above are completely equivalent.

Note: The zero energy solution of the radial equation is given by:

$$u_{0l}(r) = \alpha r^{l+1} + \frac{\beta}{r^l}\tag{2.19}$$

Now we list the solutions in the corresponding regimes below.

1. $kr \ll 1$ regime:

$$(kr)j_l(kr) \approx \frac{(kr)^{l+1}}{(2l+1)!!}\tag{2.20}$$

$$(kr)n_l(kr) \approx \frac{(2l-1)!!}{(kr)^l}\tag{2.21}$$

Substituting our analytical approximations, we get:

$$u_{El}(r) \approx C_l \sqrt{\frac{2\mu}{\pi\hbar^2k}} \left[\frac{(kr)^{l+1}}{(2l+1)!!} \cos \delta_l + \frac{(2l-1)!!}{(kr)^l} \sin \delta_l \right]\tag{2.22}$$

Then if we impose $u_{El}(kr \ll 1) = u_{0l}$, we arrive at:

$$\alpha = C_l \frac{(k)^{l+1}}{(2l+1)!!} \cos \delta_l, \quad \beta = -C_l \frac{(2l-1)!!}{(k)^l} \sin \delta_l \quad (2.23)$$

$$\Rightarrow \tan \delta_l = -\frac{\beta}{\alpha} \left(\frac{k^{2l+1}}{(2l+1)!!(2l-1)!!} \right) \quad (2.24)$$

where we have $k^{2l+1}/(2l+1)!!(2l-1)!!$ is universal whereas β/α depends on the regime we are in. This is known as the *Wigner's threshold law*.

2. $kr \gg 1$ regime:

$$(kr)j_l(kr) \approx \sin \left(kr - \frac{\pi l}{2} \right) \quad (2.25)$$

$$(kr)n_l(kr) \approx \cos \left(kr - \frac{\pi l}{2} \right) \quad (2.26)$$

Substituting our analytical approximations, we get:

$$u_{El} = C_l \sqrt{\frac{2\mu}{\pi \hbar^2 k}} \sin \left(kr - \frac{\pi l}{2} + \delta_l \right) \quad (2.27)$$

Which are oscillatory solutions, much like a plane wave scattering off a hard wall in 1D.

We call δ_l the *scattering phase shift*, because this just tells us that at large distances, scattering off the scattering center simply results in a phase shift between the incoming and outgoing wavefunction. Looking again at the $kr \ll 1$ regime, we had:

$$u_{El} \sim \frac{1}{(2l+1)!!} - \frac{\tan \delta_l / k^{2l+1}}{r^{2l+1}} \quad (2.28)$$

$$\Rightarrow \boxed{(a_l)^{2l+1} = - \lim_{k \rightarrow 0} \frac{\tan \delta_l}{k^{2l+1}}} \quad (2.29)$$

where in the boxed equation above, we call a_l the *l -wave scattering length* (l is a variable and could represent any order of scattering, s, p, d, f, \dots), with the definition simply stemming from the fact that we notice a length dimensional quantity and take the low-energy limit of it.

§2.2.1 The Born Approximation

We will no not be going through the derivation of the *Born approximation* result in this class but simply present it as follows:

$$\tan \delta_l \approx -\frac{2\mu k}{\hbar^2} \int_0^\infty [j_l(kr)]^2 V(r) r^2 dr \quad (2.30)$$

This is valid when $a_l \sim r_0$ (small scattering length). This grants us that:

1. $V(r) > 0 \Rightarrow \delta_l < 0 \Rightarrow a_l > 0$
2. $V(r) < 0 \Rightarrow \delta_l > 0 \Rightarrow a_l < 0$

which grants us a language to talk about different forms of scattering by referencing the scattering length. Let's now look at the general form of single channel scattering solutions. The first bit of intuition is that when we have a very deep potential well, the wavefunction would oscillate greatly (\sim due to high kinetic energies). Let's look again at our radial solutions at long ranges in the 2 possible regimes of kr :

$$(kr \ll 1) : u_{El}(r) \sim \left[\frac{1}{(2l+1)!!} + \frac{a_l^{2l+1}}{r^{2l+1}} \right] r^{l+1} \quad (2.31)$$

$$(kr \gg 1) : u_{El} \sim \sin \left(kr - \frac{\pi l}{2} + \delta_l \right) \quad (2.32)$$

So we can look at the $l = 0$ case, and have a solution that which takes a form that looks something that presented in figure 2.5 below.

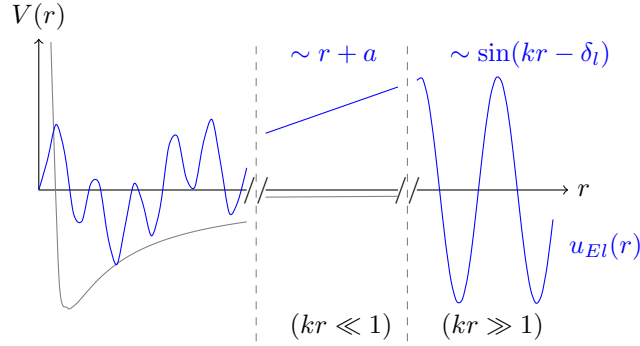


Figure 2.5: $l = 0$ form of solution

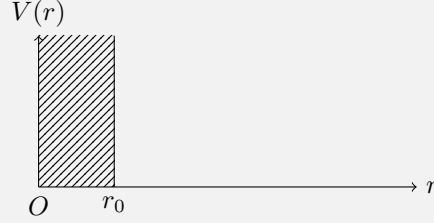
where in the case of negative scattering length ($a < 0$, corresponding to attractive potentials), we just have the slope in the region where $kr \ll 1$ being negative (downward sloping). In practice, to get solutions to the wavefunction in the region where r is around the range of r_0 , we use numerical methods (e.g. Runge-Kutta 4th order solver) given initial conditions $\{u_{El}, u'_{El}\}$. In general, we have the expression:

$$\frac{u'_{El}(r)}{u_{El}(r)} = \frac{f'_{El}(r) \cos \delta_l - g'_{El} \sin \delta_l}{f_{El}(r) \cos \delta_l - g_{El} \sin \delta_l} \Big|_{r=r^*} \quad (2.33)$$

$$\Rightarrow \boxed{\tan \delta_l = \frac{W[f_{El}, u_{El}]}{W[g_{El}, u_{El}]} \Big|_{r=r^*}} \quad (2.34)$$

where $W[,]$ is the *Wronskian* defined as $W[a, b] = ab' - a'b$ and r^* is known as the *matching distance*, that is the distance beyond which the asymptotic solutions become good approximations.

Note: With this, we can prove the *Wigner threshold law* which tells us that as $k \rightarrow 0$, then $\tan \delta_l \sim k^{2l+1}$.

Example 1:**Figure 2.6:** 1D Hard-Wall Potential

Consider a hard wall potential at r_0 :

$$V(r) = \begin{cases} \infty, & r \leq r_0 \\ 0, & r > r_0 \end{cases} \quad (2.35)$$

The solutions for $r \leq r_0$ are trivial since they must be vanishing ($u_{El} = 0$). As for $r > r_0$, we must look for the Bessel function solutions:

$$f_{El}(r) = \sqrt{\frac{2\mu}{\pi\hbar^2 k}}(kr)j_l(kr) \quad (2.36)$$

$$g_{El}(r) = \sqrt{\frac{2\mu}{\pi\hbar^2 k}}(kr)n_l(kr) \quad (2.37)$$

The tangent of the phase shift at $r = r_0$ is then:

$$\begin{aligned} \tan \delta_l &= \frac{W[f_{El}, u_{El}]}{W[g_{El}, u_{El}]} \\ &= \frac{f_{El}(r_0)u'_{El}(r_0)}{g_{El}(r_0)u'_{El}(r_0)} \\ &= \frac{j_l(kr_0)}{n_l(kr_0)} \end{aligned} \quad (2.38)$$

which grants us that in the regime where $kr_0 \ll 1$, we have:

$$\begin{aligned} \tan \delta_l &= -\frac{(kr_0)^{2l+1}}{(2l+1)!!(2l-1)!!} \\ \Rightarrow (a_l)^{2l+1} &= \frac{r_0^{2l+1}}{(2l+1)!!(2l-1)!!} \end{aligned} \quad (2.39)$$

Example 2:

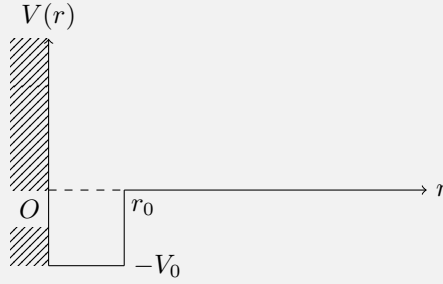


Figure 2.7: 1D Square-Well Scattering Potential

Consider the potential now with a hard wall and attractive square-well:

$$V(r) = \begin{cases} \infty, & r < 0 \\ -V_0, & 0 \leq r \leq r_0 \\ 0, & r > r_0 \end{cases} \quad (2.40)$$

For this question, we will be looking at the analysis for $l = 0$. We will split analysis for this into 2 parts, one where $E > 0$ and the other for $E < 0$. Consider first the case where the energy is $E > 0$.

1. $E > 0$:

For this problem, we will have 2 wave numbers:

$$r > r_0 : \quad k^2 = \frac{2\mu E}{\hbar^2} \quad (2.41)$$

$$r \leq r_0 : \quad \kappa^2 = \frac{2\mu(E + V_0)}{\hbar^2} \quad (2.42)$$

So we have that:

$$r \leq r_0 : \quad u_{E0}(r) = \sqrt{\frac{2\mu}{\pi\hbar^2\kappa}}(\kappa r)j_0(\kappa r) \quad (2.43)$$

$$\begin{aligned} r > r_0 : \quad f_{E0}(r) &= \sqrt{\frac{2\mu}{\pi\hbar^2k}}(kr)j_0(kr) \\ g_{E0}(r) &= \sqrt{\frac{2\mu}{\pi\hbar^2k}}(kr)n_0(kr) \end{aligned} \quad (2.44)$$

because in the $r < r_0$ region, we must have that the wavefunction be regular at $r = 0$. So taking the Wronskian formula once again to find the phase shift, we get the expression for $k \rightarrow 0$ to be:

$$\tan \delta_0 = -kr_0 + \frac{k}{\kappa_0} \tan(\kappa_0 r_0) \quad (2.45)$$

$$\Rightarrow \boxed{a = r_0 - \frac{\tan(\kappa_0 r_0)}{\kappa_0}} \quad (2.46)$$

where $\kappa_0^2 = 2\mu V_0/\hbar^2$. This expression tells us that a diverges whenever $\kappa_0 r_0 = n\pi + \pi/2$, which corresponds to creation of bound states in the potential well. Note that increasing values of κ_0 implies that we are making the potential well deeper.

2. $E < 0$:

Now we consider $E < 0$ solutions (when $l = 0$). We use the same procedure but now:

$$r \leq r_0 : u_{E0}(r) = A \sin(\kappa r) \quad (2.47)$$

$$r > r_0 : h_{E0}(r) = B e^{-kr} \quad (2.48)$$

where now, $k^2 = 2\mu|E|/\hbar^2$ and we just named another function h_{E0} since it is not the Bessel function solution. Then plugging into the Wronskian formula for the phase shift, we get:

$$\sqrt{\kappa_0^2 - k^2} \cot \left[r_0 \sqrt{\kappa_0^2 - k^2} \right] = -k \quad (2.49)$$

This is a transcendental equation and number of intersections between the functions on the RHS and LHS of the expression above gives us the number bound states. Notice that in the limit where $\kappa_0 \gg k$, we get:

$$\begin{aligned} -k &\approx \kappa_0 \cot [\kappa_0 r_0] \\ \Rightarrow \tan(\kappa_0 r_0) &\approx -\frac{\kappa_0}{k} \\ \Rightarrow a \approx r_0 - \frac{1}{\kappa_0} \left(-\frac{\kappa_0}{k} \right) \\ \Rightarrow k &\approx \frac{1}{a - r_0} \end{aligned} \quad (2.50)$$

From this, we plug this into the equation for the energy involving k which gives us:

$$\begin{aligned} E &= -\frac{\hbar^2 k^2}{2\mu} \\ &\approx -\frac{\hbar^2}{2\mu(a - r_0)^2} \end{aligned} \quad (2.51)$$

Then if we further assert that the s-wave scattering length a is much larger than the range of the potential r_0 , we get:

$$\boxed{E = -\frac{\hbar^2}{2\mu a^2}} \quad (2.52)$$

This is in fact a “*universal*” result.

That is to say, whenever we have a single channel scattering system which incoming particle having an energy close to zero in relation to the depth of the potential well, then the energy would go like $\sim 1/a^2$ as long as the scattering length is much greater than the range of the potential.

States with $l = 0$ for which majority of the wavefunction exists outside the classically forbidden region (due to the lack of an angular momentum barrier) despite having insufficient energy classically are known as *halo states*.

§2.3 Effective Range Expansion

We are now going to talk about the concept of *effective range*. From the definition of the scattering length, and then adding correction terms when we don't take the limit of $k \rightarrow \infty$, we get:

$$-k \cot \delta = \frac{1}{a} - \frac{1}{2} r_{\text{eff}} k^2 + \dots \quad (2.53)$$

where r_{eff} is known as the effective range. This let's us determine how much our observable will change when we vary the energy (what the energy dependence of the system is since it is attached to k^2). We can actually compute this analytically for the square-well scattering problem. This works out to be:

$$r_{\text{eff}} = r_0 \left[1 - \frac{r_0^2}{3a^2} - \frac{1}{\kappa_0^2 a r_0} \right] \quad (2.54)$$

The effective range will also allow us a way to characterize resonances (e.g. Feshbach resonances) later.

§2.3.1 Inelastic Scattering and Absorbing Potentials

Let's now go back to our square-well scattering potential and add a small imaginary potential as illustrated in figure 2.8 below.

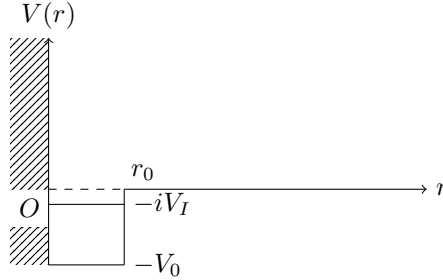


Figure 2.8: 1D Square-Well Scattering Potential with Imaginary Part

Physically, what this imaginary part corresponds to is an *absorbing (optical) potentials*, which let's us model a 2-channel scattering system. For more information on this, refer to “*Physics Of Atoms And Molecules*” - Bransden & Joachain (pg 657). This is a theoretical amendment to the potential which allows it to absorb some amount of probability from the incoming wavefunction (probability is loss to the second channel). We thus write:

$$V(r) = V_R(r) + iV_I(r) \quad (2.55)$$

where $V_I < 0$ in order to prevent the probability from exceeding unity. The Schrödinger's equation then becomes:

$$\left[-\frac{\hbar^2}{2\mu} \frac{d^2}{dr^2} + \frac{l(l+1)}{2\mu r^2} - \frac{\hbar^2 k^2}{2\mu} + V_R(r) + iV_I(r) \right] u_{El}(r) = 0 \quad (2.56)$$

This allows us to separate our solution into real and imaginary parts as well:

$$u_{El}(r) = u_{El}^R(r) + iu_{El}^I(r) \quad (2.57)$$

$$\Rightarrow \begin{cases} \left[-\frac{\hbar^2}{2\mu} \frac{d^2}{dr^2} + \frac{l(l+1)}{2\mu r^2} - \frac{\hbar^2 k^2}{2\mu} + V_R(r) \right] u_{El}^R(r) = V_I(r) u_{El}^I(r) \\ \left[-\frac{\hbar^2}{2\mu} \frac{d^2}{dr^2} + \frac{l(l+1)}{2\mu r^2} - \frac{\hbar^2 k^2}{2\mu} + V_R(r) \right] u_{El}^I(r) = -V_I(r) u_{El}^R(r) \end{cases} \quad (2.58)$$

which is a couple system of equations. Writing the coupled system in matrix notation, we get:

$$\left(\left[-\frac{\hbar^2}{2\mu} \frac{d^2}{dr^2} + \frac{l(l+1)}{2\mu r^2} - \frac{\hbar^2 k^2}{2\mu} \right] \mathbb{I} + \begin{bmatrix} V_R & V_I \\ -V_I & V_R \end{bmatrix} \right) \begin{bmatrix} u_{El}^R \\ u_{El}^I \end{bmatrix} = \vec{0} \quad (2.59)$$

Since we had the solution of $u_{El}(r)$ being:

$$u_{El} = C_l \sqrt{\frac{2\mu}{\pi \hbar^2 k}} \sin \left(kr - \frac{\pi l}{2} + \delta_l \right) \quad (2.60)$$

this then implies that we **must** allow complex phase shifts! This then implies that the scattering length is also going to have real and imaginary parts:

$$a = \text{Re}\{a\} + i \text{Im}\{a\} \quad (2.61)$$

where the imaginary part of this gives us a measure of the rate $\kappa_{\text{inelastic}}$ [cm^3/s] at which the probability will decay to zero:

$$\boxed{\kappa_{\text{inelastic}} = -\frac{\hbar}{2\mu} \text{Im}\{a\}} > 0 \quad (2.62)$$

Note: In the case where we have an exact relationship for the scattering length and phase shifts (like in the square-well scattering problem $a = f(\delta = \kappa_0 r_0)$), then we can equivalently construct the same coupled equations by adding a small imaginary part to the phase:

$$\begin{aligned} \kappa_0 r_0 &\rightarrow \kappa_0 r_0 - i\eta \\ \Rightarrow a &\rightarrow \left[r_0 - \frac{1}{\kappa_0} \frac{\sin \kappa_0 r_0 \cos \kappa_0 r_0}{\cos^2 \kappa_0 r_0 + \sinh^2 \eta} \right] - i \left[\frac{1}{2\kappa_0} \frac{\sinh(2\eta)}{\cos^2 \kappa_0 r_0 + \sinh^2 \eta} \right] \end{aligned} \quad (2.63)$$

This results in a suppression of the poles of the scattering length against the phase shifts (does not diverge anymore).

§2.4 Time-Delay in Scattering

A good reference for time-delays is *Friedrich (sections 1.4.2 and 1.4.3)*. The concept of time-delay alludes to that of resonances, where there is some localization of probability within the potential well for some significant time-scale before most of the probability is outside the well.

Definition 2.4.1. Time-Delay *The “extra time” spent by a wave packet near the scattering center due to interactions (difference between scattering time with and without interaction).*

Some initial papers on this are [Wigner, PR 98, 145 \(1955\)](#) and [Smith, PR 118, 349 \(1960\)](#). We will skip over the derivation here but the useful result for time-delay is:

$$Q_l = 2\hbar \frac{d}{dE} \delta_l(E) \quad (2.64)$$

This is essentially what you would expect from perfectly elastic scattering of point particles.

Example 1:

In the case of no interaction, we have $\delta_l = 0$, which gives us that:

$$Q_l = 0 \quad (2.65)$$

Example 2:

In the case of a hard sphere, we have that the phase-shift is $\delta_0 = -kr_0$ with $k = \sqrt{2\mu E/\hbar^2}$, which gives us that:

$$Q_l = -\frac{2r_0\mu}{\hbar k} = \frac{2\mu}{v} \quad (2.66)$$

which is actually exactly the time it takes to go back and forth in $r \in [0, r_0]$ with velocity $v = \hbar k/\mu$.

§2.4.1 Time-Delay Near Resonances

There are several types of resonances, some of which are listed below.

1. **Shape Resonances:** Resonances due to the potential well having a bump, which increases the probability of the particle to stay within the well even when $E > 0$.
2. **Feshbach Resonances:** Occurs in multi-channel problems, which creates several potential curves based on the internal states. These resonances are when a molecular state is realized in an internal state with a higher potential state than in the incoming channel.
3. **Potential Resonances:** When $E < 0$, if a molecular state occurs via tunneling, then this will lead to the particle staying within the well with some significant probability.

It turns out that phase shifts near resonances increase by π via the *Breit-Wigner line shape* relation:

$$\delta_l(E) = \delta_{bg} + \tan^{-1} \left(\frac{-\Gamma/2}{E - E_{\text{res}}} \right) \quad (2.67)$$

where Γ is the reciprocal of the resonance (molecular) lifetime and δ_{bg} is the *background scattering phase shift* (discussed further below).

Note: The above expression holds for well-separated resonances. Resonances with interference between scattering amplitudes result in other line shapes such as *Fano line-shapes*.

This causes the time-delay near resonances to be:

$$Q_l = \frac{\hbar\Gamma}{(E - E_{\text{res}})^2 + (\Gamma/2)^2} \quad (2.68)$$

which has the shape of a Lorentzian. It is worth noting that:

$$Q_l^{\text{max}} = \frac{4\hbar}{\Gamma} \quad (2.69)$$

which tells us that the sharper the resonance is, the larger the time-delay.

§2.5 Scattering Cross-Sections

Earlier we have seen that to derive scattering, we first look at the wavefunction in the very large limit ($kr \gg 1$), where we arrived at the partial wave expansion expression:

$$\psi_E \approx r^{-1} \sum_{l,m} A_{l,m} Y_l^m(\theta, \phi) \left(\frac{2\mu}{\pi\hbar^2 k} \right)^{1/2} \sin\left(kr - \frac{l\pi}{2} + \delta_l\right) \quad (2.70)$$

The goal of writing this was to compare this result to specific scattering problems (also in the $kr \gg 1$ regime) which would take the general form:

$$\psi_E = e^{i\vec{k} \cdot \vec{r}} + f(\hat{k}', \hat{k}) \frac{e^{ikr}}{r} \quad (2.71)$$

which similar form we have seen before but less generalized. Above, the prime on \hat{k}' indicates the post scattering momentum direction and we have $\hat{k} = \hat{r}$. The scattering amplitude function would now have matrix elements $\langle \hat{k}' | f(\hat{k}', \hat{k}) | \hat{k} \rangle$. It turns out that we can write:

$$e^{i\vec{k} \cdot \vec{r}} = 4\pi \sum_{l,m} i^l Y_{lm}^*(\hat{k}) Y_{lm}(\hat{r}) j_l(kr) \quad (2.72)$$

which, in the $kr \gg 1$ regime:

$$e^{i\vec{k} \cdot \vec{r}} \approx 4\pi \sum_{l,m} i^l Y_{lm}^*(\hat{k}) Y_{lm}(\hat{r}) \frac{\sin(kr - \frac{l\pi}{2})}{kr} \quad (2.73)$$

Substituting this into the general scattering solution and equating it to the partial wave expansion, we get:

$$4\pi \sum_{l,m} i^l Y_{lm}^*(\hat{k}) Y_{lm}(\hat{r}) \frac{\sin(kr - \frac{l\pi}{2})}{kr} + f(\hat{k}', \hat{k}) \frac{e^{ikr}}{r} = \frac{1}{r} \sum_{l,m} A_{l,m} Y_l^m(\theta, \phi) \left(\frac{2\mu}{\pi \hbar^2 k} \right)^{1/2} \sin\left(kr - \frac{l\pi}{2} + \delta_l\right) \quad (2.74)$$

Now we define:

$$Y_l^m(\hat{r}) \equiv \langle \hat{k}' | l, m \rangle, \quad Y_{lm}^*(\hat{k}) \equiv \langle l, m | \hat{k} \rangle \quad (2.75)$$

$$\Rightarrow f(\hat{k}', \hat{k}) \frac{e^{ikr}}{r} = \frac{1}{r} \sum_{l,m} \langle \hat{k}' | l, m \rangle \left[A_{l,m} \left(\frac{2\mu}{\pi \hbar^2 k} \right)^{1/2} \sin\left(kr - \frac{l\pi}{2} + \delta_l\right) - 4\pi i^l \langle l, m | \hat{k} \rangle \frac{\sin(kr - \frac{l\pi}{2})}{kr} \right] \quad (2.76)$$

In the above expression, the left-hand side only has outgoing waves whereas on the right-hand side, there are both incoming and outgoing waves, which we can force to vanish. This grants us that:

$$A_{lm} = 4\pi i^l e^{i\delta_l} \langle l, m | \hat{k} \rangle \left(\frac{2\mu}{\pi \hbar^2 k} \right)^{-1/2} \quad (2.77)$$

which now allows us to find the scattering amplitude:

$$\begin{aligned} \langle \hat{k}' | f(\hat{k}', \hat{k}) | \hat{k} \rangle &= \sum_{lm} \langle \hat{k}' | l, m \rangle \frac{4\pi}{2ik} i^l (e^{2i\delta_l} - 1) \langle l, m | \hat{k} \rangle \\ &= \frac{1}{2ik} \sum_l (2l+1) P_l(\cos\theta) (e^{2i\delta_l} - 1) = f_k(\theta) \\ &= \sum_l \frac{2l+1}{k \cot \delta_l - ik} P_l(\cos\theta) = f_k(\theta) = \sum_l f_l(\theta) \end{aligned} \quad (2.78)$$

So this allows us to compute the distribution of scattered particles based on phase shifts! With this, we define the outgoing flux of scattered waves through a solid angle $d\Omega$ as:

$$\frac{\hbar k}{\mu} |f(\Omega)|^2 d\Omega \quad (2.79)$$

with units of $[\sim L^3/T]$ where $\hbar k/\mu$ acts as a velocity term. The incoming flux through a solid angle $d\Omega$ would then simply be $\hbar k/\mu [\sim L/T]$. The differential cross section $d\sigma$ is then:

$$d\sigma = \frac{\text{outgoing flux}}{\text{incoming flux}} = |f(\Omega)|^2 d\Omega \quad (2.80)$$

The total cross-section is then:

$$\begin{aligned} \sigma &= \int_0^{2\pi} d\phi \int_0^\pi \sin\theta |f(\Omega)|^2 d\theta \\ &= \frac{\pi}{k^2} \sum_l (2l+1) |e^{2i\delta_l} - 1|^2 \\ &= \frac{4\pi}{k^2} \sum_l (2l+1) \sin^2 \delta_l \equiv \sum_l \sigma_l \end{aligned} \quad (2.81)$$

This allows us another means to see why only s -wave scattering is dominant in the low energy ($k \ll 1$) limit. We saw earlier that $\delta_l \sim k^{2l+1}$ in the low energy regime, so we get;

$$\sigma = \sum_l \sigma_l \sim 1 + c_1 k^4 + c_2 k^8 + \dots \quad (2.82)$$

and since $k \ll 1$, all the higher order terms drop out and only the $l = 0$ term is relevant. Now consider the probability flux:

$$\vec{J} = \frac{\hbar}{2\mu i} [\psi \nabla \psi^* - \psi^* \nabla \psi] \quad (2.83)$$

the incoming flux for $\psi_{\text{incoming}} = e^{ikz}$ would be given by:

$$\vec{J}_{\text{incoming}} = -\frac{\hbar k}{2\mu} \hat{z} \quad (2.84)$$

whereas for the outgoing wave $\psi_{\text{outgoing}} = f(\theta, \phi) e^{ikr}/r$, the flux would be:

$$\vec{J}_{\text{outgoing}} = |f(\theta, \phi)|^2 \frac{\hbar k}{2\mu r^2} \hat{r} \quad (2.85)$$

So we get:

$$\frac{d\sigma}{d\Omega} = \frac{r^2 |\vec{J}_{\text{outgoing}} \cdot \vec{r}|}{\|\vec{J}_{\text{incoming}}\|} \quad (2.86)$$

§2.6 Fano Line-Shapes with Resonant Scattering

For more references on this, refer to (Bransdon & Joachim, pg 593-599). In 1961, Fano was studying the interference between background and resonant scattering. He found that this interference could produce asymmetric (time-delay against energy) line-shapes. As a hand-wavey description, *background scattering* is the scattering that happens if there were no resonances occurring. *Resonant scattering* on the other hand is what we discussed earlier in section 2.4.1. With resonances, a phase will be accumulated due to it being “stuck” in the potential well for some significant time-scale. Due to this, this creates interference effects between the resonant and background scattering waves. To derive this rigorously, we recall the phase shift formula:

$$\tan \delta_l = \frac{W[f_{El}, u_{El}]}{W[g_{el}, u_{El}]} \quad (2.87)$$

The goal is now to separate the phase shift computed above into 2 parts:

$$\delta_l = \delta_{bg} + \delta_{res} \quad (2.88)$$

To do this, we simplify the Wronskian definition above to:

$$\begin{aligned}\tan \delta_l &= \frac{f_{El}u'_{El} - f'_{El}u_{El}}{g_{el}u'_{El} - g'_{el}u_{El}} \\ &\equiv \frac{f_{El}\gamma'_{El} - f'_{El}}{g_{el}\gamma'_{El} - g'_{el}}, \quad \text{where } \gamma_{El} = \frac{u'_{El}}{u_{El}}\end{aligned}\quad (2.89)$$

Then looking at $e^{2i\delta_l}$ because it appears in the scattering cross-section, we get:

$$\begin{aligned}e^{2i\delta_l} &= \frac{-f'_{El} + ig'_{El} + (f_{El} - ig_{El})\gamma_{El}}{f'_{El} + ig'_{El} + (f_{El} - ig_{El})\gamma_{El}} \\ &= \left[\frac{f_{El} - ig_{El}}{f_{El} + ig_{El}} \right] \times \left[\frac{(-f'_{El} + ig'_{El})/(f_{El} - ig_{El}) + \gamma_{El}}{(f'_{El} + ig'_{El})/(f_{El} + ig_{El}) + \gamma_{El}} \right] \\ &\equiv e^{2i\delta_{bg}} \times e^{2i\delta_{res}}\end{aligned}\quad (2.90)$$

It turns out that the background scattering phase-shift is **slowly varying** with energy, whereas the resonant scattering phase-shift as we saw earlier will be the arctan of a Breit-Wigner line-shape:

$$\delta_{res} = \arctan \frac{\Gamma/2}{E_{res} - E} \quad (2.91)$$

where Γ_{res} is the lifetime of the molecular state. Background scattering can be thought of as the phase shift that is present in the absence of resonant scattering (usually in another channel) i.e. the long-range effect scattering. Now if we plug in the decomposed phase shift above into each partial wave cross-section, we get:

$$\begin{aligned}\sigma_l &= \frac{4\pi}{k^2} (2l+1) |1 - e^{2i\delta_l}|^2 \\ &= \frac{4\pi}{k^2} (2l+1) \left[\frac{1}{1+q^2} \right] \left[\frac{(q+\varepsilon)^2}{1+\varepsilon^2} \right]\end{aligned}\quad (2.92)$$

where:

$$q = -\cot \delta_{bg} \quad \text{and} \quad \varepsilon = \frac{E - E_{res}}{\Gamma/2} \quad (2.93)$$

So we see that we have again been able to decompose the cross-section into a product of terms that are affected by background and resonant scattering:

$$\begin{aligned}\text{background contribution : } & \frac{1}{1+q^2} \\ \text{resonant contribution : } & \frac{(q+\varepsilon)^2}{1+\varepsilon^2}\end{aligned}\quad (2.94)$$

This allows us to see that we do not have significant resonant effects when $\varepsilon \gg 1$. Some other interesting properties are listed below.

1. ($\varepsilon = -q \Rightarrow \sigma_l = 0$) i.e. ($E = E_{res} - q\Gamma/2 \Rightarrow \sigma_l = 0$)

2. ($\varepsilon = 1/q \Rightarrow \sigma_l = 4\pi(2l+1)/k^2 \equiv \sigma_l^{\max}$). This is known as the *unitary limit*.
3. Strong background scattering: $q = 0 \Rightarrow \sigma_l = \frac{4\pi}{k^2}(2l+1) \left[\frac{\varepsilon^2}{1+\varepsilon^2} \right]$. In this regime, we have that $\sigma_l = 0$ when $E = E_{res}$, known as a *window resonance* (fully non-interacting system!).
4. Breit-Wigner (no background) resonance: $q \rightarrow \infty, \Rightarrow \sigma_l = \frac{4\pi(2l+1)}{k^2} \frac{(\Gamma/2)^2}{(E-E_{res})^2 + (\Gamma/2)^2}$. In this regime, we see that when $E = E_{res}$, we get $\sigma_l = \sigma_l^{\max}$.

Note: If we just consider the l -wave scattering cross-section without the prefactor:

$$\begin{aligned} |e^{2i\delta_l} - 1|^2 &= |1 - S|^2 \\ &= \left[\frac{1}{1+q^2} \right] \left[\frac{(q+\varepsilon)^2}{1+\varepsilon^2} \right] \end{aligned} \quad (2.95)$$

We have that S are the S -matrix terms $S = e^{2i\delta_l}$. Plotting $|1 - S|^2$ against ε give us asymmetric line-shapes except for certain specific regimes (e.g. $q = 0, q \rightarrow 0$).

Having touched a little on scattering involving more than 1 channel, we are now ready to proceed to multi-channel scattering problems.

Chapter 3

Multi-Channel Scattering

So far, we have looked at single channel problems. That is, we looked at problems where the interaction was anisotropic so that there will never be transitions between different total angular momentum ℓ states. However for more general scenarios, we have that the channels “talk to each other” leading to off-diagonal terms in relevant scattering matrices as we will see. We start off with a survey of relevant scattering matrices.

§3.1 Scattering Matrices

We will now be looking at several matrices that are relevant to scattering processes. These will allow us to analyze scattering systems in an elegant and powerful way. The first scattering matrix we will be looking at is the *transition-matrix*, more commonly referred to as the *T-matrix*.

Note: Be careful when looking at nuclear physics literature because they often use this name for other processes

§3.1.1 T-Matrix

Recall that for single-channel scattering, we had:

$$f(\theta, \phi) = \frac{4\pi}{k} \left(\frac{e^{2i\delta_l} - 1}{2i} \right) \quad (3.1)$$

As such, in the multi-channel regime, we can generalize this definition into a matrix of entries being the scattering amplitudes. The elements of this matrix are thus defined as:

$$\langle \hat{k}' | f(\theta, \phi) | \hat{k} \rangle \equiv \frac{4\pi}{k} \sum_{l,m} \sum_{l',m'} \langle \hat{k}' | l', m' \rangle \langle l', m' | \hat{T} | l, m \rangle \langle l, m | \hat{k} \rangle \quad (3.2)$$

$$\Rightarrow \boxed{\hat{T} \equiv \frac{4\pi f(\theta, \phi)}{k}} \quad (3.3)$$

Comparing this to the **single-channel** expression (2.78) we derived earlier, we get:

$$\left[\hat{T}\right]_{l,l',m,m'} = \langle l', m' | \hat{T} | l, m \rangle = \delta_{l,l'} \delta_{m,m'} \frac{e^{2i\delta_l} - 1}{2i} \quad (3.4)$$

So we get a purely diagonal T -matrix because there is no interaction between channels in this case (effectively a system of single-channels with no interaction). The single-channel assumptions holds for single-channel isotropic interactions. With this intuition, we can say that the T -matrix represents the probability of transitioning from one channel to another. The general expression for the scattering cross-section in terms of the T -matrix is then:

$$\sigma = 4\pi \sum_{l,m} \sum_{l',m'} \frac{|T_{l,l',m,m'}|^2}{k^2} \quad (3.5)$$

The result above is a result of quantum mechanical *elastic scattering*. In quantum mechanical scattering, when the internal state **changes** ($|l, m\rangle \rightarrow |l', m'\rangle$), the process is known as *inelastic scattering* (except when the internal states are degenerate). This holds true even when the total kinetic energy of the 2 colliding particles are conserved, which deviates away from the classical definition.

§3.1.2 S-Matrix

Recall that in the $kr \gg 1$ regime, we had the radial equation behaving like:

$$u_{El}(r) = A_l \left(\frac{2\mu}{\pi \hbar^2 k} \right)^{1/2} \sin \left(kr - \frac{l\pi}{2} - \delta_l \right) \quad (3.6)$$

$$\sim \exp \left\{ -i \left(kr - \frac{l\pi}{2} \right) \right\} - S \exp \left\{ +i \left(kr - \frac{l\pi}{2} \right) \right\} \quad (3.7)$$

where we have defined $S \equiv e^{2i\delta_l}$. This is in fact the S -matrix element for a single-channel system ($\langle l', m' | \hat{S} | l, m \rangle = \delta_{l,l'} \delta_{m,m'} e^{2i\delta_l}$). Generalizing this to the multi-channel scenario, we have:

$$\boxed{\hat{S} = 1 + 2i\hat{T}} \quad (3.8)$$

This matrix allows us to find useful things such as the poles of the S matrix being resonances (e.g. transmission resonances).

§3.1.3 Reaction Matrix

Again in the regime where $kr \gg 1$, for single-channel scattering, we have that:

$$u_{El}(r) \sim \sin \left(kr - \frac{l\pi}{2} \right) + K \cos \left(kr - \frac{l\pi}{2} \right) \quad (3.9)$$

allowing us to define:

$$K = \tan \delta_l \quad (3.10)$$

So for multi-channel systems (as a matrix), we have this definition generalized to:

$$\hat{K} = \frac{1}{i}(\hat{S} - \mathbb{I})(\hat{S} + \mathbb{I})^{-1} = \hat{T}(1 + i\hat{T})^{-1} \quad (3.11)$$

This is known as the *reaction matrix* or the *K-matrix*.

§3.1.4 Time-Delay and Phase Shift Matrices

Here are 2 other matrices relevant to scattering problems.

1. *Time-delay matrix*:

$$\hat{Q} = i\hbar \hat{S} \frac{d}{dE} \hat{S}^\dagger \quad (3.12)$$

2. *Phase-shift matrix*:

$$\hat{\delta} = \frac{1}{2i} \ln(\hat{S}) = \tan^{-1}(\hat{K}) \quad (3.13)$$

where remember that these \ln and \tan^{-1} definitions are on matrices which dictate the expansion definitions, hence the 2 possible different definitions depend on the kr regime we are in.

§3.2 Scattering of Particles with Internal Structure

Consider a particle with an internal structure (multiple internal levels of pseudo-spin S) of eigenbasis $|S\rangle$ and associated energy eigenvalues ε_S . As such, we have the eigenvalue equation:

$$\hat{H}_A |S\rangle = \varepsilon_S |S\rangle \quad (3.14)$$

where \hat{H}_A is the Hamiltonian, keeping in mind that since this corresponds to the internal structure, it has **no** kinetic energy term. As such in a 2-particle scattering system, the total Hamiltonian of the system would be:

$$\hat{H} = -\frac{\hbar^2 \nabla^2}{2\mu} + \hat{V}(r) + \hat{H}_A^{(1)} + \hat{H}_A^{(2)} \quad (3.15)$$

where $\hat{V}(r)$ is the interaction potential between the 2 particles. We have that the interaction potential now being a matrix since each atom can be in different internal states (figure 3.1 below):

$$\hat{V}(r) = \sum_{\alpha, \alpha'} |\alpha\rangle V_{\alpha, \alpha'}(r) \langle \alpha'|, \quad \text{where } |\alpha\rangle = |S^{(1)}\rangle \otimes |S^{(2)}\rangle \quad (3.16)$$

The diagonal entries of the above potential matrix are called the *channels* (which is finally where this formal name of multi-channel scattering comes from).



Figure 3.1: 2 particles with internal structure.

So we have that the $V_{\alpha,\alpha}(r)$ diagonal entries are called the *direct interactions* and $V_{\alpha,\alpha'}(r)$ for $\alpha \neq \alpha'$ are the *inter-channel couplings*. Because these $|\alpha\rangle$ states are tensor product states, we can define:

$$\left[\hat{H}_A^{(1)} + \hat{H}_A^{(2)} \right] |\alpha\rangle = \left[\varepsilon_\alpha^{(2)} + \varepsilon_\alpha^{(1)} \right] |\alpha\rangle \equiv \varepsilon_\alpha |\alpha\rangle \quad (3.17)$$

where we note here that $\hat{H}_A^{(1)} = \hat{H}_A^{(1)} \otimes \mathbb{I}$ and $\hat{H}_A^{(2)} = \mathbb{I} \otimes \hat{H}_A^{(2)}$ (for lighter notation).

Note: If each particle has N possible pseudo-spin internal states, the 2 **distinguishable** particle system would have N^2 possible states.

In this case of 2-particle scattering, we would expect that the **total** wavefunction solution would have a part that is spatially dependent, and the other which is dependent on the pseudo-spin:

$$|\Psi\rangle = |\psi_{\text{spatial}}(\vec{r})\rangle \otimes |\alpha\rangle \quad (3.18)$$

§3.2.1 Identical Particles

Asserting that the particles are identical, then each state could be written as either of the 2 following symmetric (s) or antisymmetric (a) states:

$$|\alpha_s\rangle = (1 + \delta_{S_1, S_2}) \frac{|S_1 S_2\rangle + |S_2 S_1\rangle}{\sqrt{2}} \quad (3.19)$$

$$|\alpha_a\rangle = (1 - \delta_{S_1, S_2}) \frac{|S_1 S_2\rangle - |S_2 S_1\rangle}{\sqrt{2}} \quad (3.20)$$

where δ_{S_1, S_2} is the Kronecker-delta function, and is required for normalization. The number of states for each case would then be:

$$N_s = \frac{N(N+1)}{2} \quad (3.21)$$

$$N_a = \frac{N(N-1)}{2} \quad (3.22)$$

Symmetry and antisymmetry of parity is associated to the quantum statistics of the particles (Fermions vs Bosons), but with stricter conditions for such particles as not just pseudo-spins would have to obey this parity property, but also the spatial portion of the wavefunction. As such, we have:

$$\text{Bosons : } |\Psi\rangle = |\Psi_s\rangle = |\psi_{s,\text{spatial}}(\vec{r})\rangle \otimes |\alpha_s\rangle \quad \text{or} \quad |\psi_{a,\text{spatial}}(\vec{r})\rangle \otimes |\alpha_a\rangle \quad (3.23)$$

$$\text{Fermions : } |\Psi\rangle = |\Psi_a\rangle = |\psi_{a,\text{spatial}}(\vec{r})\rangle \otimes |\alpha_s\rangle \quad \text{or} \quad |\psi_{s,\text{spatial}}(\vec{r})\rangle \otimes |\alpha_a\rangle \quad (3.24)$$

Recall that the spatial wavefunction can be written as a sum of partial waves:

$$\begin{aligned} \psi_{\text{spatial}}(\vec{r}) &= \sum_{l,m} A_{l,m} \frac{u_{E,l}(r)}{r} Y_{l,m}(\theta, \phi) \\ \Rightarrow \Psi(\vec{r}, \alpha) &= \sum_{\alpha} \sum_{l,m} A_{l,m}^{(\alpha)} \frac{u_{E,l}^{(\alpha)}(r)}{r} Y_{l,m}(\theta, \phi) |\alpha\rangle \end{aligned} \quad (3.25)$$

For the symmetric case (Bosons), we require that l runs only over even numbers, whereas for Fermions, we have it run only over odd numbers. Plugging this into the Schrödinger's equation, we get:

$$\sum_{l,m,\alpha} A_{l,m}^{(\alpha)} \left[-\frac{\hbar^2}{2\mu} \frac{d^2}{dr^2} + \frac{l(l+1)}{2\mu r^2} + \sum_{\tilde{\alpha}, \tilde{\alpha}'} |\tilde{\alpha}\rangle V_{\tilde{\alpha}, \tilde{\alpha}'}(r) \langle \tilde{\alpha}'| + \sum_{\tilde{\alpha}} (|\tilde{\alpha}\rangle E_{\tilde{\alpha}} \langle \tilde{\alpha}| - E) \right] u_{E,l}^{(\alpha)}(r) Y_{l,m}(\theta, \phi) |\alpha\rangle = 0 \quad (3.26)$$

Which then gives us the radial equation:

$$\boxed{\left[-\frac{\hbar^2}{2\mu} \frac{d^2}{dr^2} + \frac{l(l+1)}{2\mu r^2} \right] u_{E,l}^{(\alpha)}(r) + \sum_{\alpha, \alpha'} V_{\alpha, \alpha'}(r) u_{E,l}^{(\alpha')}(r) + (E_{\alpha} - E) u_{E,l}^{(\alpha)}(r) = 0} \quad (3.27)$$

Which is in fact an N -coupled system of 2nd order differential equations indexed by $\alpha = 1, 2, \dots, N$. More concisely, we can write this as the “eigenvalue” matrix equation:

$$\begin{aligned} & \left[\hat{T}_r + \hat{E}_{th} + \hat{V} \right] \vec{u} = E \vec{u} \\ \text{where } & [\hat{T}_r]_{\alpha, \alpha'} = \left[-\frac{\hbar^2}{2\mu} \frac{d^2}{dr^2} + \frac{l(l+1)}{2\mu r^2} \right] \delta_{\alpha, \alpha'} \\ & [\hat{E}_{th}]_{\alpha, \alpha'} = E_{\alpha} \delta_{\alpha, \alpha'} \\ & [\hat{V}]_{\alpha, \alpha'} = V_{\alpha, \alpha'} \\ & [\vec{u}]_{\alpha'} = u_{E,l}^{(\alpha')}(r) \end{aligned} \quad (3.28)$$

Even though this system has N 2nd order differential equations, there will only be N **degenerate** eigenstate solutions (instead of $2N$) because we only except the solutions that are well-behaved at the origin. Also, this system is not a traditional eigenvalue problem because E is a fixed value, so we are working to find the eigenvectors given the eigenvalue. We will adopt the index ν to denote the eigenstate index.

Note: **Only** the potential matrix is not diagonal with off-diagonal entries called the *inter-channel couplings*, since it encodes the interactions between the different channels.

Note: The eigenstates ψ_E^ν , of the system of differential equations is in general a combination of various $|\alpha\rangle$ states (*spin-admixture*).

Generally, if a particle with energy E is in an excited channel state such that given its energy, it would be a bound state, this is known as a *meta-stable* state since it is likely that the particle could transit into a lower energy channel and cause the molecular state to decay.

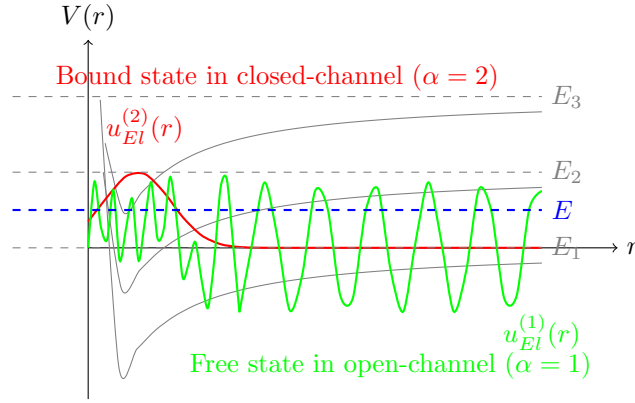


Figure 3.2: Multi-channel meta-stable state.

§3.2.2 Multi-Channel Asymptotic Solutions

We now consider the regime in which the particles are taken to be very far apart from one another ($r \rightarrow \infty$). When this occurs, we should have that the interaction potential vanishes $\hat{V}(r) \rightarrow 0$, which reduces the multi-channel Schrödinger radial equation to:

$$\left[-\frac{\hbar^2}{2\mu} \frac{d^2}{dr^2} + \frac{l(l+1)}{2\mu r^2} + (E_\alpha - E) \right] u_{E,l}^{(\alpha)}(r) = 0 \quad (3.29)$$

This should grants us solutions that are analogous to those found in the single channel regime (section 2.2) which could have been written as:

$$u_{E,l}(r) = A_l [f_{E,l}(kr) + \tan \delta_l g_{E,l}(kr)] \quad (3.30)$$

We take this solution and generalize it to the multi-channel scattering case to get:

$$u_{E,l}^{(\alpha,\nu)}(r) = A_l^{(\alpha,\nu)} \left[\delta_{\alpha,\nu} f_{E,l}^{(\alpha)}(k_\alpha r) + K_l^{(\nu,\alpha)} g_{E,l}^{(\alpha)}(k_\alpha r) \right] \quad (3.31)$$

where $\delta_{\alpha,\nu}$ is the Kronecker-delta function, $k_\alpha = \sqrt{2\mu(E - E_\alpha)/\hbar^2}$ and $K_l^{(\nu,\alpha)}$ here is in fact the reaction matrix we introduced in section 3.1.3 above. The delta-function is present as that term

describes the incoming wave, which will always only have separate channel contributions. The upper indices α and ν denote the following.

- α index: Vector component (spin, channel) index.
- ν index: Degenerate eigenstate (with energy E) index.

As such, we can write the eigenstates in a matrix form with entries indexed by α and ν , that is:

$$[\hat{u}_{El}] = u_{El}^{(\alpha,\nu)}(r) \quad (3.32)$$

This grants us that each energy eigenstate with **total** energy E is found by taking the sum over the index α :

$$u_{E,l}^{(\nu)}(r) = \sum_{\alpha} B^{(\alpha)} u_{E,l}^{(\alpha,\nu)}(r) \quad (3.33)$$

It works out that the fundamental matrix of solutions $u_{E,l}^{(\alpha,\nu)}(r)$ is unitary such that when applied to the Hamiltonian as follows:

$$(\hat{u}_{E,l}) \hat{H} (\hat{u}_{E,l})^{\dagger} \quad (3.34)$$

it produces a diagonal matrix (diagonal entries being the E_{α} energies). We recall that the radial asymptotic solutions are Bessel and Neumann functions, so in the multi-channel case, they become:

$$\begin{aligned} f_{E,l}(k_{\alpha}r) &= \left(\frac{2\mu}{\pi \hbar^2 k_{\alpha}} \right)^{1/2} (k_{\alpha}r) j_l(k_{\alpha}r) \\ g_{E,l}(k_{\alpha}r) &= \left(\frac{2\mu}{\pi \hbar^2 k_{\alpha}} \right)^{1/2} (k_{\alpha}r) n_l(k_{\alpha}r) \end{aligned} \quad (3.35)$$

Notice that if for anyone of the eigen-energies E_{α} , we had $E < E_{\alpha}$, this would make k_{α} imaginary. This of course would result in decaying exponential solutions when exiting that respective α channel. As such, in the asymptotic region where $r \gg r_0$, the probability of finding the particle becomes negligibly small such that we can treat that channel as “closed off”. As such, we adopt the language of calling channels with *opened* or *closed*.

- **Closed-Channel**: $E < E_{\alpha}$
- **Open-Channel**: $E > E_{\alpha}$

We denote the number of open-channels for a given energy E as N_o and that for closed-channels N_c . As such, we will have that the reaction matrix $K^{(\nu,\alpha)}$ would have effectively on $N_o \times N_o$ non-trivial entries that are group as a block matrix within the $N \times N$ total K -matrix, since all the closed-channel entries would simply be 0. This is illustrated below:

$$\hat{K}_{\nu,\alpha} = \begin{pmatrix} \begin{array}{c|ccc} & & & \\ \hline & \text{non-trivial} & & \\ & \text{entries} & & \\ \hline & & & \\ \vdots & \vdots & & \\ 0 & \dots & \dots & \dots & 0 \end{array} & \begin{array}{ccc} \dots & 0 & 0 \\ \dots & 0 & 0 \\ \vdots & & \\ \vdots & & \end{array} \end{pmatrix}_{\alpha,\nu} \quad (3.36)$$

where we take that the lower the index of α , the lower the energy ($E_\alpha < E_{\alpha'}$ if $\alpha < \alpha'$). The ν indices are arranged such that the resulting non-trivial entries form a block matrix as shown above. We can see this a little more explicitly with an example.

Example:

Consider a system of 2 colliding particles, each with 3 channels. In general, we have:

$$\hat{u} = \begin{bmatrix} u^{(11)} & u^{(12)} & u^{(13)} \\ u^{(21)} & u^{(22)} & u^{(23)} \\ u^{(31)} & u^{(32)} & u^{(33)} \end{bmatrix} \quad (3.37)$$

Let's now say that we have channel 3 is **closed**, this would simplify our matrix to:

$$\begin{aligned} \hat{u} &= \begin{bmatrix} u^{(11)} & u^{(12)} & u^{(13)} \\ u^{(21)} & u^{(22)} & u^{(23)} \\ 0 & 0 & 0 \end{bmatrix} \\ &= \begin{bmatrix} f^{(11)} & 0 & 0 \\ 0 & f^{(22)} & 0 \\ 0 & 0 & 0 \end{bmatrix} + \begin{bmatrix} K^{(11)} & K^{(12)} & K^{(13)} \\ K^{(21)} & K^{(22)} & K^{(23)} \\ K^{(31)} & K^{(32)} & K^{(33)} \end{bmatrix} \begin{bmatrix} g^{(11)} & 0 & 0 \\ 0 & g^{(22)} & 0 \\ 0 & 0 & +\infty \end{bmatrix} \end{aligned} \quad (3.38)$$

where we get that the $f^{(33)}$ (vanishing for $r \gg r_0$) and $g^{(33)}$ (diverging for $r \gg r_0$) solutions are the non-physical solutions. Multiplying out the K -matrix with the outgoing solutions and dropping the unphysical terms, we get:

$$\begin{bmatrix} K^{(11)} & K^{(12)} & K^{(13)} \\ K^{(21)} & K^{(22)} & K^{(23)} \\ K^{(31)} & K^{(32)} & K^{(33)} \end{bmatrix} \begin{bmatrix} g^{(11)} & 0 & 0 \\ 0 & g^{(22)} & 0 \\ 0 & 0 & +\infty \end{bmatrix} = \begin{bmatrix} g^{(11)} K^{(11)} & g^{(22)} K^{(12)} & 0 \\ g^{(11)} K^{(21)} & g^{(22)} K^{(22)} & 0 \\ g^{(11)} K^{(31)} & g^{(22)} K^{(32)} & 0 \end{bmatrix} \quad (3.39)$$

Comparing this with the first matrix of vanishing channel-3 terms, we get the conditions:

$$\begin{aligned} u^{(13)} &= u^{(23)} = 0 \\ K^{(31)} &= K^{(32)} = 0 \\ \Rightarrow \hat{u} &= \begin{bmatrix} f^{(11)} & 0 & 0 \\ 0 & f^{(22)} & 0 \\ 0 & 0 & 0 \end{bmatrix} + \begin{bmatrix} K^{(11)} & K^{(12)} & 0 \\ K^{(21)} & K^{(22)} & 0 \\ 0 & 0 & 0 \end{bmatrix} \begin{bmatrix} g^{(11)} & 0 & 0 \\ 0 & g^{(22)} & 0 \\ 0 & 0 & 0 \end{bmatrix} \\ \Rightarrow \hat{u} &= \begin{bmatrix} f^{(11)} & 0 \\ 0 & f^{(22)} \end{bmatrix} + \begin{bmatrix} K^{(11)} & K^{(12)} \\ K^{(21)} & K^{(22)} \end{bmatrix} \begin{bmatrix} g^{(11)} & 0 \\ 0 & g^{(22)} \end{bmatrix} \end{aligned} \quad (3.40)$$

So this tells us that the effective dimensions of any scattering system would be equal to **only** the number of open-channels $\dim\{\hat{K}\} = N_o$.

Note: In our example above, we dropped all the unphysical terms but in actual fact, the K -matrix terms would not vanish as they encode the couplings between the channels regardless of the channels being closed.

§3.3 Calculating Scattering Matrices

We have seen the reaction matrix popping up in the multi-channel solution, but we have not seen how to compute it explicitly as of yet. To learn how to do this, we first recall how we computed phase-shifts (the single-channel analog of the multi-channel regime) in the single-channel case. We computed the tangent of the phase shift using the Wronskian formula:

$$\tan \delta_l = \frac{W[f_{El}, u_{El}]}{W[g_{el}, u_{El}]} \quad (3.41)$$

The idea in the multi-channel scattering case is very similar, just that now we are working with objects with indices (matrices), which has to get us using matrix inverses instead. This grants us:

$$\hat{K} = (\hat{f}_{El} - \hat{f}'_{El} \hat{\gamma}_{El})(\hat{g}_{El} - \hat{g}'_{El} \hat{\gamma}_{El})^{-1}, \quad \hat{\gamma}_{El} \equiv \hat{u}_{El}(\hat{u}'_{El})^{-1} \quad (3.42)$$

where the primes denote derivatives with respect to the radial coordinate. Having this form, we can then easily derive the S and T -matrices using the formulas relating them to the reaction matrix we saw in section 3.1. Some properties of these matrices are as follows.

1. The K -matrix is **real symmetric**.
2. The S and T matrices are **unitary** ($\hat{S}\hat{S}^\dagger = \hat{T}\hat{T}^\dagger = \mathbb{I}$).
3. **Probability flux conservation** dictates:

$$\sum_i |\hat{S}]_{ij}|^2 = \sum_i |\hat{T}]_{ij}|^2 = 1 \quad (3.43)$$

4. $\dim \hat{S} = \dim \hat{T} = \dim \hat{K} = N_o$

§3.3.1 Multi-Channel Scattering Cross-Sections

Now, let us consider the scattering boundary conditions which is going to give us the general solution (generalizing from the single-channel scattering case):

$$\psi_E^{(\nu)} = \sum_{\alpha} B_{\alpha}^{(\nu)} \left[e^{i\vec{k}_{\alpha} \cdot \vec{r}} \delta_{\alpha, \nu} + f_{\nu, \alpha}(\theta, \phi) \frac{e^{ik_{\alpha} r}}{r} \right] |\alpha\rangle \quad (3.44)$$

This allows us to compare this solution to the one we have using equation (3.31):

$$\psi_E^{(\nu)} = \sum_{\alpha} \sum_{l, m} \frac{1}{r} \left[A_l^{(\alpha, \nu)} \left[\delta_{\alpha, \nu} f_{E, l}^{(\alpha)}(k_{\alpha} r) + K_l^{(\nu, \alpha)} g_{E, l}^{(\alpha)}(k_{\alpha} r) \right] \right] Y_{l, m}(\theta, \phi) |\alpha\rangle \quad (3.45)$$

as we did in the single-channel case to find the scattering amplitudes $f_{\nu, \alpha}(\theta, \phi)$. From here, following a very similar derivation, we find that for elastic scattering, the scattering cross-section would be:

$$\sigma_{elastic}^{\alpha} = 4\pi \sum_{l_{\alpha}} \frac{(2l+1)}{k_{\alpha}^2} \left| [\hat{T}^{(l_{\alpha})}]_{\alpha, \alpha} \right|^2 \quad (3.46)$$

and for the inelastic cross-section, this would be:

$$\sigma_{inelastic}^{\alpha} = 4\pi \sum_{l_{\alpha}} \sum_{\alpha'} \frac{(2l+1)}{k_{\alpha}^2} \left| [\hat{T}^{(l_{\alpha})}]_{\alpha',\alpha} \right|^2 \quad (3.47)$$

These grant us the respective reaction matrices:

$$\boxed{\hat{K}_j^{(\alpha)} = \frac{\hbar k_{\alpha}}{\mu} \sigma_j^{\alpha}} \quad (3.48)$$

where j indicates elastic and inelastic scattering. It turns out that we in fact have $\dot{n}(t) = -K_{inelastic} \cdot n(t)$ where $n(t)$ is the density of the gas. So the inelastic reaction matrix elements tell us about the rate of decrease in the density of a gas, which is intuitive because we see that the reaction matrix consists of a velocity $\hbar k_{\alpha}/\mu$ and the cross-section, which in the inelastic case, is a measure of the probability for transitions to another (likely lower energy) channel. As a result, a larger reaction matrix grants us a larger effective particle velocity which results in lower gas densities.

Note: In the limit that $k \rightarrow 0$, we have that:

$$a_{\alpha} = \frac{\ln [\hat{S}]_{\alpha,\alpha}}{2\alpha} = -\frac{[\hat{K}]_{\alpha,\alpha}}{k_{\alpha}} \quad (3.49)$$

§3.4 Pathway Analysis

We will now be looking at how to analyze collisions via a formalism known as *pathway analysis*. This means of scattering analysis was in fact how Fano approached many scattering problems. We start by considering the elastic pathways, which is where the incoming and outgoing pathways are the same. This also allows a diagrammatic means of visualizing the different channel transitions a particle in collision could undergo.

§3.4.1 Elastic Collision Pathways

Elastic collisions are collisions in which the incoming and outgoing channels are the same. Consider 3 energies E_1 , E_2 and E_3 which are the 3 lowest energy levels in a multi-channel system. Consider that the incoming particle is in the channel with energy E_2 . There are several possible pathways here. These are listed below.

1. One possibility (the simplest one) is that the now channel-transitions occur and the particle simply exits the scattering potential in the same channel it entered (figure 3.3).
2. Alternatively, we could have the incoming particle transit to the channel with energy E_1 and the transit back up to exit in the same pathway (figure 3.4).
3. Lastly, we could have the particle enter, transit to channel E_3 , transit back down to channel E_2 and exit (figure 3.5).

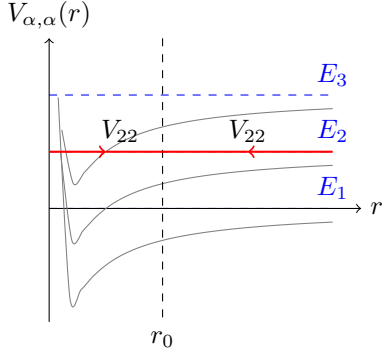


Figure 3.3: Pathway 1 of elastic scattering.

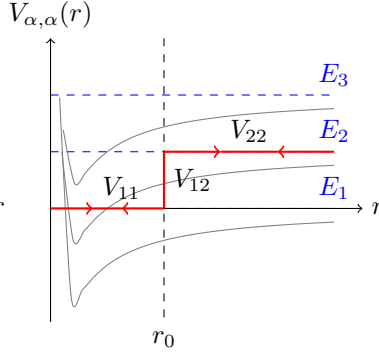


Figure 3.4: Pathway 2 of elastic scattering.

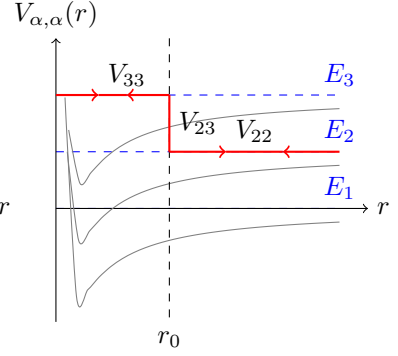


Figure 3.5: Pathway 3 of elastic scattering.

The scattering cross-section that describe these pathways is then given by summing over all the partial waves of channel 2 labelled by l_2 :

$$\sigma_{elastic}^{(2)} = 4\pi \sum_{l_2} (2l_2 + 1) \frac{|T_{22}^{(2)}|^2}{k_2^2} \quad (3.50)$$

§3.4.2 Inelastic Collision Pathways

In the system we have set-up, inelastic collisions would occur when the outgoing pathway has an energy lower than that of the incoming pathway. As such, we must have the particle exiting in channel E_1 . So we have the following scenarios.

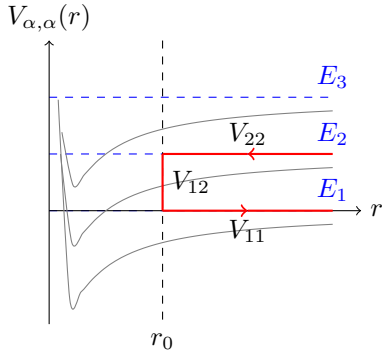


Figure 3.6: Pathway 1 of inelastic scattering.

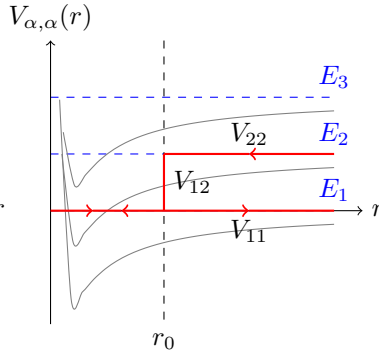


Figure 3.7: Pathway 2 of inelastic scattering.

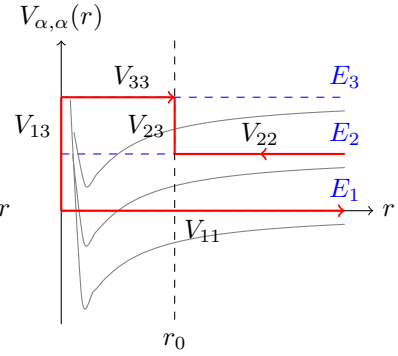


Figure 3.8: Pathway 3 of inelastic scattering.

The scattering cross-section that describes these pathways is then given by summing over all the partial waves of channel 2 labelled by l_2 and also over all off-diagonal elements in the T

matrix:

$$\sigma_{inelastic}^{(2)} = 4\pi \sum_{l_2} \left[(2l_2 + 1) \sum_{\alpha'} \frac{|T_{\alpha',2}^{(2)}|^2}{k_2^2} \right] \quad (3.51)$$

Note: All other transitions are treated as higher order terms which have very small probabilities of occurring. As such, we do not consider these cases in our analysis.

In general then (for both elastic and inelastic scattering), we get that the T -matrix entries are computed via taking the sum over the probabilities of these pathways.

$$|\hat{T}_{12}|^2 = \sum_{i=1}^{\infty} \mathbb{P}_i \quad (3.52)$$

where i indexes the pathways.

Note: The probabilities \mathbb{P}_i are the probability for the i -th total pathway. That is, \mathbb{P}_i encompasses the probability of entering channel α , making the channel transitions specified by the i -th pathway and finally exiting channel α' .

§3.4.3 Bound-States

Bound states in a multi-channel system are states whereby the energy E of the incoming particle is less than the energy of **lowest** channel energy ($E < E_1$). If we have a situation where $E < E_j$ for $j > 1$, this could allow for resonant states like we saw earlier but **not** bound states. Recall that in the single-channel scattering regime, we had the scattering amplitude partial waves is given by:

$$f_l(\theta, \phi) = \frac{2l + 1}{k \cot(\delta_l(k)) - ik} P_l(\cos \theta) \quad (3.53)$$

in which bound-state solutions are found by solving for the poles of these scattering amplitudes:

$$k \cot(\delta_l(k)) - ik = 0 \quad (3.54)$$

The solutions for k from the equation above grant us the binding energies. Now to generalize this to the mutli-channel case, we generalize $k\delta_l(k)$ to a matrix $\hat{M}(k)$ such that we have the equation:

$$\det\{\hat{M}(k) - ik\mathbb{I}\} = 0 \quad (3.55)$$

where the matrix entries are defined as:

$$M_{\alpha\nu} = \frac{k_\alpha}{K_{\alpha\nu}(k)}, \quad k_\alpha^2 = \frac{2\mu(E - E_\alpha)}{\hbar^2} \quad (3.56)$$

$K_{\alpha,\nu}$ being the reaction matrix we saw earlier.

§3.5 Contact Interaction

Before we continue on our analysis of multi-channel systems, we take a small detour toward an understanding of *contact interactions*. This is important for non-finite range ($r = 0$) interaction regimes, and is a valuable tool for many applications such as many-body physics. To derive the form of this potential, we look to the *Fermi contact potential* as proposed by Fermi in 1934.

$$V(r) = \frac{4\pi\hbar^2 a}{2\mu} \delta(\vec{r}), \quad \delta(\vec{r}) = \frac{\delta(r)}{4\pi r^2} \quad (3.57)$$

This potential arises by taking a square-well of width r_0 and depth V_0 , and taking the limits as $r_0 \rightarrow 0$ and $V_0 \rightarrow \infty$ (illustrated in figure 3.9 below).

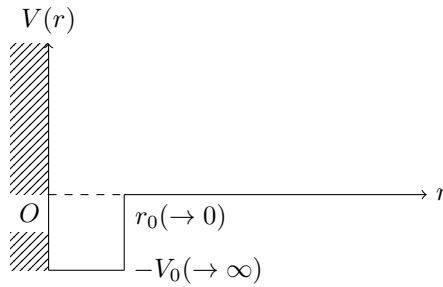


Figure 3.9: Fermi-pseudopotential

However, this potential leads to some less than desirable behaviour (too singular) for certain applications. This was fixed by Huang and Yang in 1957 (PR 105, 767) via the form:

$$V(r) = \frac{4\pi\hbar^2 a}{2\mu} \delta(\vec{r}) \frac{d}{dr}(r) \quad (3.58)$$

where the parenthesis on the r after the derivative indicates that the derivative and r act together as an operator:

$$V(r)\psi(r) = \frac{4\pi\hbar^2 a}{2\mu} \delta(\vec{r}) \frac{d}{dr}(r\psi(r)) \quad (3.59)$$

This is known as a *regularized Fermi pseudopotential*.

Note: The regularized Fermi pseudopotential for contact interactions we have above can also be written as:

$$V(r) = \frac{4\pi\hbar^2 a}{2\mu} \delta(\vec{r}) \left[1 + r \frac{d}{dr} \right] \quad (3.60)$$

if the notation with r after the derivative is confusing.

One thing that is interesting about contact interactions is that it can be decomposed into the following simple form:

$$V(r) = \sum_{l,m} |l, m\rangle V_l(r) \langle l, m| \quad (3.61)$$

where the matrix $V_l(r)$ is diagonal because we are considering isotropic interactions. So in principle, this is a sum that we can truncate in cold collisions:

$$V(r) \approx |0, 0\rangle V_0(r) \langle 0, 0| + \dots \quad (3.62)$$

In general, we have that the matrix entries are written as:

$$V_l(r) = \frac{4\pi\hbar^2}{2\mu} (a_l)^{2l+1} \frac{(2l+1)!!}{l!2^l} \frac{\delta(r)}{r^l} \frac{d^{2l+1}}{dr^{2l+1}} (r^{l+1}) \quad (3.63)$$

where the *Bethe-Peierls boundary condition* asserts that:

$$\left(\left(\frac{(2l+1)!!}{(2l)!!} \frac{d^{2l+1}}{dr^{2l+1}} r^{l+1} \right) \frac{u(r)}{r} \right) \Big|_{r=0} = - \frac{r^{l+1}}{(a_l)^{2l+1}} \frac{u(r)}{r} \Big|_{r=0} \quad (3.64)$$

which allows us to determine the coefficients of our scattering ansatz. So for the situation that $l = 0$, we get:

$$\frac{1}{u} \frac{du(r)}{dr} \Big|_{r=0} = -\frac{1}{a} \quad (3.65)$$

The contact potential only acts at the point where $r = 0$, but for any other position $r \neq 0$, we have the Schrödinger equation reducing to:

$$\begin{aligned} \left[\frac{d^2}{dr^2} + k^2 \right] u(r) &= 0 \\ \Rightarrow u(r) &= A \sin(kr + \delta) \end{aligned} \quad (3.66)$$

given that the energy is $E > 0$. So matching these boundary conditions, we get:

$$\begin{aligned} \frac{1}{u} \frac{du(r)}{dr} \Big|_{r=0} &= \frac{1}{u} \frac{du(r)}{dr} \Big|_{r=0+} \\ \Rightarrow \boxed{\delta = -ka} \end{aligned} \quad (3.67)$$

Note: Contact interactions do **not** satisfy *Levinson's theorem* (relation between the number of bound states of a potential to the difference in phase of a scattered wave at zero and infinite energies) because they are a pseudopotential.

As for energies $E < 0$, we get:

$$\begin{aligned} & \left[\frac{d^2}{dr^2} - \kappa^2 \right] u(r) = 0 \\ \Rightarrow & u(r) = Ae^{-\kappa r} \\ \Rightarrow & \boxed{\kappa = \frac{1}{a}} \end{aligned} \tag{3.68}$$

Contact interactions work best in the regime where the scattering length is much larger than the interatomic/intermolecular interactions. Ross and Shawn in 1961 generalized the idea of the contact interaction potential for multi-channel systems so that we have the potential as a matrix:

$$\boxed{\hat{V}_s(r) = \frac{4\pi\hbar^2}{2\mu} \hat{A} \delta(\vec{r}) \frac{d}{dr}(r)} \tag{3.69}$$

where the subscript s on the potential indicates only s -wave scattering, and \hat{A} is the scattering length matrix with elements $\hat{A}_{\alpha,\nu} = a_{\alpha,\nu}$. The boundary conditions for this are then:

$$\boxed{\left. \frac{d}{dr} u_{\alpha,\nu} \right|_{r=0} = - \sum_{\alpha'} \frac{u_{\alpha',\nu}}{a_{\alpha',\nu}}} \tag{3.70}$$

Example (Channel-Coupled Contact Interaction):

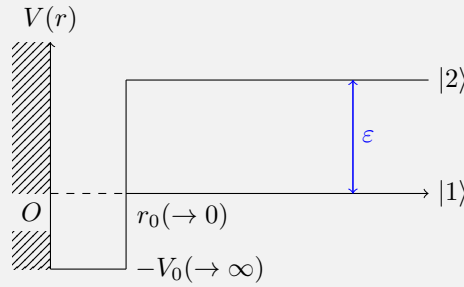


Figure 3.10: 2-channel Fermi-pseudopotential

Consider again the contact interaction pseudopotential (square-well and hard-wall potential of width r_0 which we take to 0) with 2 channels. Each channel has associated scattering lengths a_j and energy levels ε_j where $\varepsilon_2 = \varepsilon$ and $\varepsilon_1 = 0$ for convenience. We

can write without loss of generality that:

$$V_s = \frac{4\pi\hbar^2}{2\mu} \begin{bmatrix} a_1 & 1/\beta \\ 1/\beta & a_2 \end{bmatrix} \delta(\vec{r}) \frac{d}{dr}(r) \quad (3.71)$$

where β are the channel couplings. We can then ask, what the scattering length of the system as a whole is, given that we know the scattering lengths of the individual channels and their couplings. Consider the case where $0 < E < \varepsilon$. Having $a_2 < 0$ would not be interesting since this would not allow any molecular states. However, for $a_2 > 0$, we have the energy:

$$E_{bare} = \varepsilon - \frac{\hbar^2}{2\mu a_2^2} \quad (3.72)$$

where “bare” means no coupling. So by varying the energy such that it gets close to a resonance, we will get some interesting behaviours and resonant states. Alternatively, we could fix $E = 0$ and vary ε . These would actually allow at some value of ε such that the $E = 0$ line intersects the E_{bare} curve (plotting E vs ε) resulting in a molecular state. This is known as a *Feshbach resonance*.

Recall that if $a > 0$, we can have 1 bound-state associated with energy $-\hbar^2/(2\mu a^2)$. However, $a < 0$ would produce no bound-states. In the case of our system here, we would have several possible regimes.

1. $a_j < 0$ for all j : 0 bound-states.
2. $a_1 > 0, a_2 < 0$: 1 bound-states.
3. $a_j > 0$ for all j : 1 bound-states + 1 bound-state if $\varepsilon - \hbar^2/(2\mu a_2^2) < 0$.

There are 2 things we can do to study this.

1. Fix ε and vary the energy E . This would allow us to get Fano-lineshape and study the resonant behaviour through the plot.
2. Fix $E = 0$ and ε . This would allow us to look at the closed-channel state when it becomes bound (Feshbach resonances), and the channel (β) couple behaviours.

$E < 0$:

Consider first the case where $E < 0$ (no open-channels). This would result in the radial wavefunction:

$$\begin{aligned} u(r) &= u^{(1)}(r) |1\rangle + u^{(2)}(r) |2\rangle \\ &= A e^{-\kappa r} |1\rangle + B e^{-\tilde{\kappa} r} |2\rangle \end{aligned} \quad (3.73)$$

where $\kappa^2 = 2\mu|E|/\hbar^2$ and $\tilde{\kappa}^2 = 2\mu(\varepsilon + |E|)/\hbar^2 = k_\varepsilon^2 + \kappa^2$. At this point, we do not know the values of these wave-numbers but we do know that it is a bound-state. Let us first

solve for the constants A and B using the Bethe-Peierl boundary conditions:

$$\begin{aligned}
 \frac{d}{dr} \begin{bmatrix} u^{(1)} \\ u^{(2)} \end{bmatrix} &= - \begin{bmatrix} 1/a_1 & \beta \\ \beta & 1/a_2 \end{bmatrix} \begin{bmatrix} u^{(1)} \\ u^{(2)} \end{bmatrix}_{r=0} \\
 \Rightarrow \begin{bmatrix} -A\kappa \\ -B\tilde{\kappa} \end{bmatrix} &= - \begin{bmatrix} 1/a_1 & \beta \\ \beta & 1/a_2 \end{bmatrix} \begin{bmatrix} A \\ B \end{bmatrix} \\
 \Rightarrow \begin{bmatrix} 1/a_1 - \kappa & \beta \\ \beta & 1/a_2 - \tilde{\kappa} \end{bmatrix} \begin{bmatrix} A \\ B \end{bmatrix} &= \begin{bmatrix} 0 \\ 0 \end{bmatrix} \\
 \Rightarrow \boxed{\left(\frac{1}{a_1} - \kappa \right) \left(\frac{1}{a_2} - \sqrt{\kappa^2 + k_\varepsilon^2} \right) - \beta^2 = 0}
 \end{aligned} \tag{3.74}$$

This is a transcendental equation in κ since all other parameters would be provided to us. To first gain more analytical insight and check if this equation makes sense, we first turn off the coupling $\beta = 0$ which grants us 2 solutions for κ :

$$\kappa = \frac{1}{a_1} \quad \text{or} \quad \sqrt{\frac{1}{a_2^2} - k_\varepsilon^2} \tag{3.75}$$

$$\Rightarrow E = -\frac{\hbar^2}{2\mu a_1^2} \quad \text{or} \quad E = \varepsilon - \frac{\hbar^2}{2\mu a_2^2} \tag{3.76}$$

The first of these solutions is only valid if $a_1 > 0$, and the second when $a_2 > 0$ since we know that $\kappa \geq 0$ by definition. This makes physical sense because we wanted to study bound states anyways which already asserts this restriction on a_j . These energy relations allow us to plot E vs ε which without coupling, grant us linear curves. However, once coupling is turned on, we get *level repulsion* (separation of the eigenvalues of each channel). The level repulsion can be seen in a numerical plot as in figure 3.11 below.

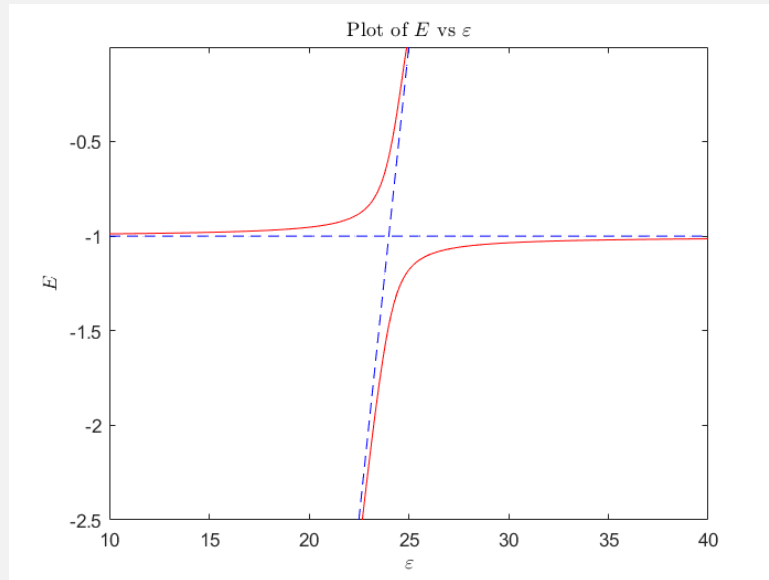


Figure 3.11: Plot of E vs ε .

For the numerics, the parameters $a_1 = 1, a_2 = 0.2, \beta = 0.1, \mu = 0.5, \hbar = 1$ were used. The red lines are the energy curves while the horizontal blue dotted line is the line of $-\hbar^2/(2\mu a_1^2)$, while the positive gradient blue dotted line is the line of $\varepsilon - \hbar^2/(2\mu a_2^2)$.

Now consider the case where we set $\kappa = 0$ (zero energy solution with non-zero coupling), this would grant us:

$$\begin{aligned} k_\varepsilon &= \frac{1 - a_1 a_2 \beta^2}{a_2} \\ \Rightarrow \quad \varepsilon &= \frac{\hbar^2}{2\mu a_2^2} (1 - a_1 a_2 \beta^2)^2 \end{aligned} \quad (3.77)$$

So we see that when there is a non-zero coupling, we need a value of ε that is slightly off $\hbar^2/(2\mu a_2^2)$ to get a zero-energy bound-state.

$0 < E < \varepsilon$:

Now consider the regime where $0 < E < \varepsilon$. This would grant us the solutions:

$$\begin{aligned} u(r) &= u^{(1)}(r) |1\rangle + u^{(2)}(r) |2\rangle \\ &= A \sin(kr + \delta) |1\rangle + B e^{-\kappa r} |2\rangle \end{aligned} \quad (3.78)$$

Again applying the Bethe Peierls boundary condition, we end up with the linear system:

$$\begin{aligned} \begin{bmatrix} Ak \cos \delta \\ B \end{bmatrix} &= - \begin{bmatrix} 1/a_1 & \beta \\ \beta & 1/a_2 \end{bmatrix} \begin{bmatrix} A \sin \delta \\ B \end{bmatrix} \\ \Rightarrow \quad \tan \delta &= -k \left(\frac{1}{a_1} - \frac{a_2 \beta^2}{1 - a_2 \kappa} \right) \\ \Rightarrow \quad a &= - \lim_{k \rightarrow 0} \tan \delta \\ &= \left(\frac{1}{a_1} - \frac{a_2 \beta^2}{1 - a_2 k_\varepsilon} \right)^{-1} \end{aligned} \quad (3.79)$$

If we want to know the limit to which a diverges ($a \rightarrow \infty$, implying a resonance), we have:

$$\begin{aligned} \frac{1}{a_1} &= \frac{a_2 \beta^2}{1 - a_2 k_\varepsilon} \\ \Rightarrow \quad k_\varepsilon &= \frac{1 - a_1 a_2 \beta^2}{a_2}, \quad \varepsilon_0 = \frac{\hbar^2}{2\mu a_2^2} (1 - a_1 a_2 \beta^2)^2 \end{aligned} \quad (3.80)$$

where ε_0 is the separation corresponding to the resonant scattering length. A good check of this result is to look at the case where the channel separation is very large, granting us an effective single-channel scattering system. To do this, we take k_ε to be very large, which indeed grants us $a = a_1$. Notice that when we take $k_\varepsilon \rightarrow \infty$, we get that the scattering length is just $a = a_1$, telling us that a_1 is the background scattering (off-resonant scattering length).

Fano Lineshapes

Now consider the Fano lineshapes of this scattering system. Recall that these are the plots of

$$\begin{aligned} F(\tilde{\varepsilon}, q) &= |e^{2i\delta_l} - 1|^2 \\ &= |1 - S|^2 \\ &= \left[\frac{1}{1 + q^2} \right] \left[\frac{(q + \tilde{\varepsilon})^2}{1 + \tilde{\varepsilon}^2} \right] \end{aligned} \quad (3.81)$$

where:

$$q = -\cot \delta_{bg} \quad \text{and} \quad \tilde{\varepsilon} = \frac{E - E_{res}}{\Gamma/2} \quad (3.82)$$

Since we know the scattering-phase shift, this gives us that the Fano lineshape goes like:

$$F(E) = \frac{k^2}{\left(\frac{1}{a_2} - \frac{a_2 \beta^2}{1 - a_2 \kappa} \right)^2 + k^2} \quad (3.83)$$

$$q = \frac{1 - a_1 a_2 \beta^2}{a_1 k_\varepsilon} \quad (3.84)$$

$$E_{res} = \varepsilon - \frac{\hbar^2}{2\mu a_2^2} + \frac{\hbar^2}{2\mu a_2^2} \left(\frac{2a_1 a_2 \beta^2}{1 + a_1^2 k_\varepsilon^2} \right) + \dots \quad (3.85)$$

What is interesting is that when we have $\varepsilon \approx \varepsilon_0$, the lineshapes become very odd (not the typical Fano lineshape). Because near this threshold regime, we can no longer consider the background and resonant scattering as separate processes as they interfere in a significantly different way than before.

$E \geq \varepsilon$:

For this regime, we once again do a similar procedure but now, having to use Bessel function solutions.

Chapter 4

Scattering in External Fields

We are now going to move into applying external fields to scattering events. In these note, we will be focusing on Alkali atoms since they have a single outermost electron which allows us to use weaker fields to perturb and probe the system. It turns out that external fields appear in the one-body Hamiltonian, and does not necessary play such a big role in the collision processes between particles. So we are going to start by looking at the internal structure of single particles subject to external fields.

§4.1 Internal Atomic Structure

We will mostly be working in regimes where the external is weak, such that it does not affect so much the electronic structure of the atom below the valence electron. The important quantum numbers we will need to describe this system are

1. Principle quantum number $\{n\}$
2. Orbital angular momentum and its projection $\{l, m_l\}$
3. Nuclear spin and its projection $\{i, m_i\}$
4. Valence electron spin and its projection $\{s, m_s\}$

Then to know the energy levels of this system, we have to write down the effective Hamiltonian that describes the system:

$$\hat{H}_A = \hat{H}_{Born} + A_{so} \hat{\vec{L}} \cdot \hat{\vec{S}} + A_{hf} \hat{\vec{I}} \cdot (\hat{\vec{S}} + \hat{\vec{L}}) - \mu_B (g_s \hat{\vec{S}} + g_i \hat{\vec{I}} + g_l \hat{\vec{L}}) \cdot \vec{B} \quad (4.1)$$

where the subscripts correspond to A (atomic), so (spin-orbit) and hf (hyperfine). The n, l quantum numbers are associated to the \hat{H}_{Born} term (below-valence electronic structure), the $A_{so} \hat{\vec{L}} \cdot \hat{\vec{S}}$ term is responsible for the fine spin-orbit coupling structure, the $A_{hf} \hat{\vec{I}} \cdot (\hat{\vec{S}} + \hat{\vec{L}})$ term is responsible for the hyperfine nuclear/electron spin-orbit coupling, and the last term is known as the *Zeeman Hamiltonian* which is responsible for the spin coupling with the magnetic field. g_s and g_i known as the *gyromagnetic numbers* and μ_B is *Bohr's magneton*.

To analyze this Hamiltonian, we first pick a basis where \hat{H}_{Born} is purely diagonal, so that we can effectively treat it as a number $E_{n,l}$. One way to write the eigenstates of this system is:

$$|\alpha\rangle = |l, m_l\rangle \otimes |s, m_s\rangle \otimes |i, m_i\rangle \quad (4.2)$$

However, this representation gives a horribly dense matrix which is not a wise choice of basis. So a better choice would be to consider the operator $\hat{J} = \hat{L} + \hat{S}$, which grants the eigenstates:

$$|j, m_j; l, s\rangle = \sum_{m_l, m_s} \langle s, m_s, l, m_l | j, m_j; l, s \rangle (|s, m_s\rangle \otimes |l, m_l\rangle) \quad (4.3)$$

This basis allows the $A_{so}\hat{L} \cdot \hat{S}$ term to also be diagonal. Additionally, we want to include the nuclear spins in this basis such that we can create a nice representation, so we consider the operator $\hat{J} + \hat{I} = \hat{F}$ which grants the eigenstates:

$$|f, m_f; l, s, i\rangle = \sum_{m_j, m_i} \langle i, m_i, j, m_j | f, m_f; l, s, i \rangle (|i, m_i\rangle \otimes |j, m_j; l, s\rangle) \quad (4.4)$$

The notation we will adopt for these states can be written as:

$${}^{2s+1}_n l_j(f) \quad (4.5)$$

Before we perform the analysis for an atom in an external magnetic field, we consider an example. Rubidium-87 in an external magnetic field with quantum numbers $n = 5, i = 5/2, s = 1/2$ has the energy level diagram given in figure 4.1 below.

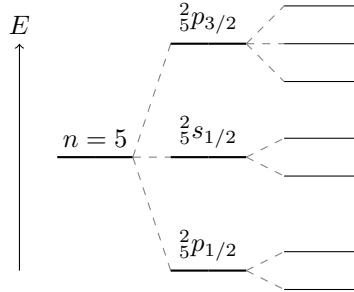


Figure 4.1: Energy splitting up to the Zeeman effect.

So we see that the Zeeman structure (due to the Zeeman Hamiltonian term) produces energy splittings of about 3-orders of magnitude less than those due to spin-orbit coupling. What this Zeeman effect corresponds to is a breaking of the symmetry of the problem, which results in a splitting of the degeneracies (as seen in perturbation theory). So in the ultracold regime, these are the energy transitions we are concerned with since all other energy transitions will require too much energy to excite (i.e. multi-channel scattering in the ultracold regime arises due to the Zeeman splitting of energy states, which grant us pseudospin states labelled by $|\alpha\rangle = |f, m_f\rangle$).

Now let's turn on the external field. We get the Hamiltonian in the “brute-force basis” we originally as:

$$\hat{H}_A = E_{nl}\mathbb{I} + \frac{A_{so}}{2} \left(\hat{J}^2 - \hat{L}^2 - \hat{S}^2 \right) + \frac{A_{hf}}{2} \left(\hat{F}^2 - \hat{I}^2 - \hat{J}^2 \right) - \mu_B \left(g_s \hat{S}_z + g_i \hat{I}_z \right) B_z \quad (4.6)$$

First, we consider the case when $l = 0$ and setting $E_{n,0} = 0$ in the brute-force basis:

$$\begin{aligned} & \langle s, m_s; i, m_i | \hat{H}_A | s, m'_s; i, m'_i \rangle \\ &= \frac{A_{hf}}{2} \langle s, m_s; i, m_i | \hat{F}^2 | s, m'_s; i, m'_i \rangle \\ & - \left\{ \frac{A_{hf}}{2} [i(i+1) + s(s+1)] + \mu_B [g_s m_s + g_i m_i] B_z \right\} \delta_{m_i, m'_i} \delta_{m_s, m'_s} \end{aligned} \quad (4.7)$$

The only non-diagonal term is that relating to the \hat{F}^2 operator, which we can insert a complete basis set to get:

$$\langle s, m_s; i, m_i | \hat{F}^2 | s, m'_s; i, m'_i \rangle = \sum_{f, m_f} \langle s, m_s; i, m_i | f, m_f \rangle f(f+1) \langle f, m_f | s, m'_s; i, m'_i \rangle \quad (4.8)$$

We know from the Clebsch-Gordan coefficients that we only have non-trivial terms when we have:

$$|i - s| \leq f \leq i + s \quad (4.9)$$

$$m_s + m_i = m_f \quad (4.10)$$

by the *selection rules*. Similarly for the primed quantum numbers as well. This in general is an off-diagonal, dense matrix. So these would admit eigenstates:

$$|\alpha\rangle = |\alpha; (s, l), i, m_f\rangle = \sum_{m_s, m_i} c_{m_s, m_i} |s, m_s; i, m_i\rangle \quad (4.11)$$

§4.2 2-Body Hamiltonians

What happens now, when we start to get interaction between 2-atoms? First of all, let us consider an abstract notion of the number of states in a 2-atom system. Let's say that each atom has N internal states. If the atoms are identical, we would expect a total of $N^2/2$ possible states for the coupled system of 2-atoms. However, we are only concerned with a subspace of all these states which deals with the interactions. We now aim to gain a better understanding of this subspace and how to find it. We can write the 2-body Hamiltonian in general as:

$$\hat{H} = \hat{H}_m + \hat{H}_A^{(1)} + \hat{H}_A^{(2)} \quad (4.12)$$

where \hat{H}_m is called the molecular Hamiltonian responsible for the interactions between atoms, and $\hat{H}_A^{(j)}$ is the individual atomic Hamiltonian for atom j . In general, the molecular Hamiltonian is

going to be very complex due to all the internal structure and inter-atomic structure interactions. We can effectively decompose these as follows:

$$\hat{H}_m = \hat{T}_r + \hat{T}_{r_e} + \hat{V}_{ee} + \hat{V}_{e_1N} + \hat{T}_{e_2N} + \hat{T}_{NN} \quad (4.13)$$

where the r subscript stands for the distance between nuclei, r_e is the distance between valence electrons, e stands for the electron terms and N for nuclear terms. The wave function for such a system would be:

$$\psi_M(\vec{r}, \vec{r}_1, \vec{r}_2) = \psi(\vec{r})\phi(\|\vec{r}\|, \vec{r}_1, \vec{r}_2) \quad (4.14)$$

where \vec{r}_j is the radius between the nucleus and electron in atom j . This generally would require the Bohr-Oppenheimer approximation, but however, we are not concerned with the electronic degrees of freedom, so we “*integrate out*” such effects to get the effective Hamiltonian:

$$\hat{H}_N(r) \equiv \langle \psi_{ee} | \hat{H}_m | \psi_{ee} \rangle \quad (4.15)$$

where $|\psi_{ee}\rangle$ is electron interaction wavefunction. After integrating out these electron dependencies, we are left only with the nuclear degrees of freedom which we can write an effective Hamiltonian of this entire system to be:

$$\hat{H} = \left[-\frac{\hbar^2}{2\mu} \left(\frac{d^2}{dr^2} + \frac{2}{r} \frac{d}{dr} \right) + \frac{\hat{L}^2}{2\mu r^2} + \hat{V}_{int}(r) \right] + \left[\hat{H}_A^{(1)} + \hat{H}_A^{(2)} \right] \quad (4.16)$$

where $\hat{V}_{int}(r)$ is the interaction potential which accounts for an effective treatment of all the electronic degrees of freedom and \hat{L} is the angular momentum operator for the entire system. The results above are taken from many-body theory and are the concern mostly in chemical physics. We also want to write the interaction potential in the spin basis so that we can account for the spin interactions:

$$\hat{V}_{int}(r) = \sum_{s, m_s} |s, m_s\rangle V_s(r) \langle s, m_s| \quad (4.17)$$

such that the $V_s(r)$ are the eigenvalues of the electronic Hamiltonian. We now look at how these $V_s(r)$ terms would look like as functions for r . First, we consider an ansatz for the wavefunction for our effective Hamiltonian, which reads:

$$\psi_E(\vec{r}) = \sum_{\alpha} \left(\sum_{l, m} \frac{u_{E,l}^{(\alpha)}(r)}{r} Y_{l,m}(\vec{r}) \right) |\alpha\rangle \quad (4.18)$$

This allows us to consider just the radial portion of our effective Schrödinger equation from the Hamiltonian above to get:

$$\left[-\frac{\hbar^2}{2m} \frac{d^2}{dr^2} + \frac{l(l+1)\hbar^2}{2\mu r^2} - (E - \varepsilon_{\alpha}) \right] u_{E,l}^{(\alpha)}(r) + \sum_{\alpha'} V_{\alpha, \alpha'}(r) u_{E,l}^{(\alpha)}(r) = 0 \quad (4.19)$$

where we defined $V_{\alpha,\alpha'}(r) = \sum_{s,m_s} \langle \alpha | s, m_s \rangle V_s(r) \langle s, m_s | \alpha' \rangle$. It works out that in the long-range regime ($r \gg r_0$), the potential matrix elements go like:

$$V_{\alpha,\alpha} \rightarrow -\frac{C_6}{r^6} \quad (4.20)$$

$$V_{\alpha,\alpha'} \sim e^{-r/\beta} \rightarrow 0 \quad (4.21)$$

In the case of alkali atoms in their ground states ($l = 0, s = 1/2$) which we are looking at, we would have $s = s_1 + s_2 = 0$ or 1 ($s = 0$ corresponds to the single anti-parallel state, and $s = 1$ corresponds to the triplet parallel state). Recall the singlet and triplet states are given by:

$$\begin{aligned} \text{Singlet : } & \left\{ \begin{array}{l} |\downarrow\uparrow\rangle - |\uparrow\downarrow\rangle \end{array} \right. \\ \text{Triplet : } & \left\{ \begin{array}{l} |\downarrow\uparrow\rangle + |\uparrow\downarrow\rangle \\ |\downarrow\downarrow\rangle \\ |\uparrow\uparrow\rangle \end{array} \right. \end{aligned} \quad (4.22)$$

So the sum in $\sum_{s,m_s} \langle \alpha | s, m_s \rangle V_s(r) \langle s, m_s | \alpha' \rangle$ would only run over $s = 0, 1$. These potentials would have wells due to the electron-nucleus attraction, however the triplet state would have a shallower well due to the Pauli exclusion principle of the electronic spins (parallel spins do not want to share the same state). The Pauli exclusion takes effect at short distances, but at large distances, these 2 spin s states look the same and follow the [Buckingham potential](#) ($\sim 1/r^6$) and is visualized in figure 4.2 below (using 2 Rubidium-85 atoms). In the molecular Hamiltonian, we have that \hat{S}^2 and \hat{I}^2 are conserved.

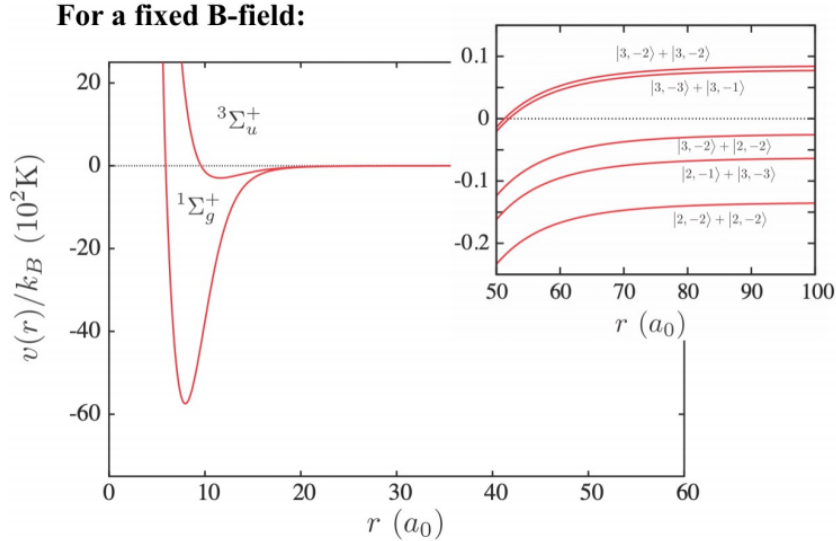


Figure 4.2: Potential Curves for 2 Rubidium-85 atoms with effective spins (J.P. D’Incao, 2019).

Now let’s look at the atomic portion of the 2-body Hamiltonian. In fact, just having this Hamiltonian will already be useful in the long-range regime where there is little inter-atomic

interaction. If we consider the case where $l_1 = l_2 = 0$, choosing the zero-point energy such that $E_{n,0}^{(1)} + E_{n,0}^{(2)} = 0$ and having $\vec{B} = B\hat{z}$, then we can write:

$$\begin{aligned}\hat{H}_A^{(1)} + \hat{H}_A^{(2)} &= \frac{A_{hf}^{(1)}}{2} \left(\hat{F}_1^2 - \hat{I}_1^2 - \hat{J}_1^2 \right) - \mu_B \left(g_s \hat{S}_{1,z} + g_i \hat{I}_{1,z} \right) B_z \\ &+ \frac{A_{hf}^{(2)}}{2} \left(\hat{F}_2^2 - \hat{I}_2^2 - \hat{J}_2^2 \right) - \mu_B \left(g_s \hat{S}_{2,z} + g_i \hat{I}_{2,z} \right) B_z\end{aligned}\quad (4.23)$$

The basis for this is going to be super messy if we include all the quantum numbers, but we realize that states with different $M_f = m_f^{(1)} + m_f^{(2)}$ do not interact (effectively) and are thus conserved. This grants us a block diagonal matrix representation. The 2 atom spinor (state) can then be written as:

$$|\alpha\rangle \equiv |\alpha_1\rangle \otimes |\alpha_2\rangle \quad (4.24)$$

$$\Rightarrow \left[\hat{H}_A^{(1)} + \hat{H}_A^{(2)} \right] |\alpha\rangle = [\varepsilon_{\alpha,1} + \varepsilon_{\alpha,2}] |\alpha\rangle \quad (4.25)$$

where the eigenvalues $\varepsilon_{\alpha,j}$ are exactly the pseudospin eigenvalues we have seen before during the start of our multi-channel analysis.

Note: for both parts of the Hamiltonian (molecular and atomic), we have used 2 different basis $\{|s, m_s\rangle \otimes |i, m_i\rangle\}$ and $\{|\alpha\rangle = |\alpha_1\rangle \otimes |\alpha_2\rangle\}$ respectively. It turns out that the $\{|s, m_s\rangle \otimes |i, m_i\rangle\}$ is good for deeply bound molecular states at short-ranges, but bad for scattering states where the $\{|\alpha\rangle = |\alpha_1\rangle \otimes |\alpha_2\rangle\}$ basis would then be a better choice. Each of these bases ensure that the matrix representation of their respective Hamiltonian terms are diagonal.

§4.2.1 Spin Character in Molecular States

Now to compare the short-range and long-range regimes, one could do this experimentally by applying an external magnetic field and observing the *spin character* (energies in particular spin states) as the magnetic field is varied (plot energy vs B -field). If the energy curve of a the molecular state runs parallel to energy curves of the separated atoms for some given spin state, we can say that the molecule has the same spin character as an atom in that spin state.

Another way to determine the spin-character is to consider the *channel fraction* f_α of the channel α defined as:

$$f_\alpha = \int_0^\infty \left| u_{E,l}^{(\alpha)}(r) \right|^2 dr \quad (4.26)$$

which grants a measure of the proportion of the wavefunction in a given channel. We then again vary the external magnetic field and observe how the channel fractions vary. This is another indication of the spin character in the molecular state.

§4.3 Atoms in Harmonic Traps

We are now going to look at the simple treatment of atoms under harmonic confinement. These can be implemented in many ways such as counter propagating laser fields. These confinements add a term \hat{H}_{ho} into our single atom Hamiltonian:

$$\hat{H} = \hat{H}_A + \hat{H}_{ho} = \hat{H}_A + \frac{1}{2}m\omega^2 r^2 \quad (4.27)$$

where ω is the confinement frequency. What this would do, is split each of the original energy levels of the initial atomic Hamiltonian \hat{H}_A into an infinite ladder of energy levels with even spacing ($\sim \hbar\omega$). This generally creates a huge mess since there would no longer be a clear distinction in the original energy levels (splittings overlap). Now considering 2-bodies, we have:

$$\begin{aligned} \hat{H} &= \hat{H}_M + \hat{H}_A^{(1)} + \hat{H}_A^{(2)} + \frac{1}{2}m\omega^2(r_1^2 + r_2^2) \\ &= \hat{H}_M + \hat{H}_A^{(1)} + \hat{H}_A^{(2)} + \frac{1}{2}\mu\omega^2 r^2 + \frac{1}{2}M\omega^2 R^2 \end{aligned} \quad (4.28)$$

We can add the trapping potential into the molecular Hamiltonian to get some effective molecular Hamiltonian:

$$\begin{aligned} \hat{H}_{\tilde{M}} &= -\frac{\hbar^2}{2\mu} \left(\frac{d^2}{dr^2} + \frac{2}{r} \frac{d}{dr} \right) + \frac{\hat{L}^2}{2\mu r^2} + \hat{V}_{int}(r) + \frac{1}{2}\mu\omega^2 r^2 + \frac{1}{2}M\omega^2 R^2 \\ &\approx -\frac{\hbar^2}{2\mu} \left(\frac{d^2}{dr^2} + \frac{2}{r} \frac{d}{dr} \right) + \frac{\hat{L}^2}{2\mu r^2} + \frac{1}{2}\mu\omega^2 r^2 + \frac{1}{2}M\omega^2 R^2 \end{aligned} \quad (4.29)$$

where we can drop the interaction potential since the Harmonic potential dominates (which is the case in real experiments). A visualization of the spectrum as a function of an externally applied magnetic field is shown in figure 4.3 below.

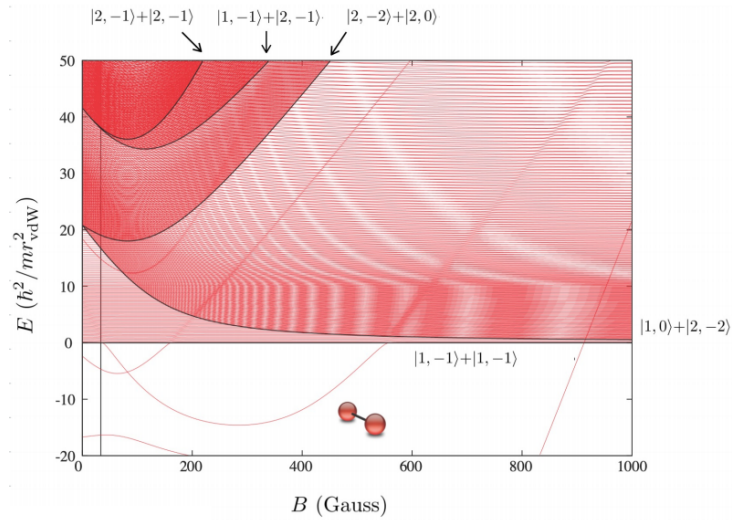


Figure 4.3: Spectrum of a 2 atom system as a function of B (J.P. D'Incao, 2019).

Note: The orientation of the applied magnetic field is in the z -axis, which is orthogonal to the lattice plane.

§4.4 Atoms in Time-Periodic Fields (Floquet Theory)

There are many techniques to approach such systems, such as *Floquet theory*, *time-propagators*, *rotating wave approximations* (for 2-level systems), etc. Here, we will focus on the Floquet approach which has several benefits. Namely, it is 1) non-perturbative and 2) conceptually clear. Supplementary readings for this include [S.I. Chu, D.A. Telnov, Phys Rep, 390,1 \(2004\)](#).

Floquet theory was introduced in 1883 in which a transformation was applied to a time-periodic system of differential equations such that the coefficients of the differential equation becomes time-independent. This is indeed the motivation for Floquet theory, because it allows us to think of a time-dependent system (*bare state picture*) as a stationary system problem (*dressed state picture*). An application of this is to solid-state systems which is in that context referred to as the *Bloch formalism*. The first step to this is defining our Hamiltonian:

$$\hat{H}(\vec{r}, t) = \hat{H}_0(\vec{r}) + \hat{W}(\vec{r}, t) \quad (4.30)$$

where we break up our Hamiltonian into a term that is time-independent (*bare Hamiltonian*) and another that is time-dependent (*dressed Hamiltonian*). We also require that:

$$\hat{W}(\vec{r}, t + \tau) = \hat{W}(\vec{r}, t) \quad (4.31)$$

where τ is the period of the Floquet system. For the purposes of this class, we will only consider pseudo-spin states within \hat{W} , which will be enough for us to gain an understanding of this theory. There are 2 points to take note of here, which are

1. the wavefunction has to have the same periodicity as the Hamiltonian $|\psi(\vec{r}, t + \tau)|^2 = |\psi(\vec{r}, t)|^2$;
2. energy of the system is not conserved since the Hamiltonian is time-dependent which breaks time-translation symmetry.

A powerful concept that is introduced in Floquet theory, is that of *quasi-energy*, which is a quantity that **is** conserved. These are quantities that show up in the *dressed state picture*, which is a combined energy of the energy in the *bare state picture* and some field terms. This can be thought of as a time-averaged energy of the compound system. To get into the meat of things, we of course have to write out the Schrödinger's equation:

$$i\hbar \frac{\partial}{\partial t} \psi(\vec{r}, t) = \hat{H}(\vec{r}, t) \psi(\vec{r}, t) \quad (4.32)$$

We then perform a trick in which we define a “*Floquet Hamiltonian*” $\hat{\mathcal{H}}_F$ as:

$$\boxed{\hat{\mathcal{H}}_F \equiv \hat{H}(\vec{r}, t) - i\hbar \frac{\partial}{\partial t}} \quad (4.33)$$

such that $\hat{\mathcal{H}}_F \psi(\vec{r}, t) = 0$

This admits solutions of the form:

$$\boxed{\psi(\vec{r}, t) \equiv e^{-i\varepsilon t/\hbar} \psi_F(\vec{r}, t)} \quad (4.34)$$

where we have defined the *Floquet wavefunction* $\psi_F(\vec{r}, t)$ which is also periodic in τ . This solution is not immediately obvious and is an ansatz from the Floquet theorem. Using the Floquet wavefunction ansatz, we plug this back into the Floquet Hamiltonian equation to get:

$$\begin{aligned} & \left[\hat{H}(\vec{r}, t) - i\hbar \frac{\partial}{\partial t} \right] e^{-i\varepsilon t/\hbar} \psi_F(\vec{r}, t) = 0 \\ \Rightarrow & \boxed{\hat{\mathcal{H}}_F(t) \psi_F(t) = \varepsilon \psi_F(t)} \end{aligned} \quad (4.35)$$

which is known as the Floquet Schrödinger's equation. The interesting thing about this result is that we are now allowed to treat time just like a spatial degree of freedom which will reduce a lot of complexities that come along with time-dependence. How do we solve this equation then? First, we need to consider the treatment of the Floquet wavefunction. The first assumption, is that we know how to solve eigenstates of the bare Hamiltonian:

$$\hat{H}_0(\vec{r}) \phi_\alpha(\vec{r}) = E_\alpha^{(0)} \phi_\alpha(\vec{r}) \quad (4.36)$$

Working in this basis of $\phi_\alpha(\vec{r})$, we get a diagonal matrix representation of the bare Hamiltonian. We then assert that we can write the Floquet wavefunctions as follows:

$$\psi_F(\vec{r}, t) = \sum_{n=-\infty}^{\infty} \sum_{\alpha} c_{n,\alpha} \phi_\alpha(\vec{r}) e^{in\omega t} \quad (4.37)$$

$$\text{where } \langle n | n' \rangle = \frac{1}{\tau} \int_0^\tau e^{in\omega t} e^{in'\omega t} dt = \delta_{n,n'} \quad (4.38)$$

where $\omega = 2\pi/\tau$. For simplicity, we often write these Floquet states as:

$$|\psi_F\rangle = \sum_{n,\alpha} c_{n,\alpha} |n, \phi_\alpha\rangle \quad (4.39)$$

Plugging in these states into the Floquet Schrödinger's equation, we end up with:

$$\boxed{\sum_{n,\alpha} \left[\langle n', \phi'_\alpha | \hat{H}(t) | n, \phi_\alpha \rangle + (n\hbar\omega - \varepsilon) \delta_{n,n'} \delta_{\alpha,\alpha'} \right] c_{n,\alpha} = 0} \quad (4.40)$$

which is just an eigenvalue problem.

Example:

Consider a 2-level system where the bare Hamiltonian is written as:

$$\hat{H}_0 = E_1^{(0)} |1\rangle \langle 1| + E_2^{(0)} |2\rangle \langle 2| \quad (4.41)$$

while the time-dependent portion of the Hamiltonian is written as:

$$\hat{W}(t) = \left(|1\rangle \langle 2| + |2\rangle \langle 1| \right) \hbar \Omega \cos(\omega t) \quad (4.42)$$

Then using the Floquet wavefunction:

$$\psi_F = \sum_{n,\alpha} c_{n,\alpha} \phi_\alpha e^{in\omega t} \quad (4.43)$$

We get the matrix elements of the time-dependent Hamiltonian as:

$$\left[\hat{W} \right]_{n,\alpha}^{n',\alpha'} = \quad (4.44)$$

Appendices

Appendix A

Scattering Ansatz

When looking for ansatz to scattering problems, we can decompose the ansatz into 3 parts, namely the 1) *incident wave*, 2) *reflected wave* and 3) *transmitted wave* where the reflected and transmitted waves can be grouped together as the *scattered wave*.

1. Incoming Wave:

Because we are looking at finite range potentials, these can take the form:

$$\varphi(\vec{r}) = e^{ikz} \quad (\text{A.1})$$

where we pick our z axis to be the axis of incident wave propagation. k is the wave-number and directly relates to the energy of the incident wave as:

$$E = \frac{\hbar^2 k^2}{2m} \quad (\text{A.2})$$

2. Scattered Wave

Working in spherical coordinates, we first look at the r dependence. We know that the scattered wave is going to propagate radially outward, but also needs to diminish in amplitude to conserve probability current density. As such, we propose the ansatz:

$$\psi(\vec{r}) = \frac{e^{ikr}}{r} \quad (\text{A.3})$$

which does satisfy the free-particle Schrödinger equation. However we cannot impose spherical symmetry and must account for this by adding angular dependence:

$$\psi_s(\vec{r}) = f_k(\theta, \phi) \frac{e^{ikr}}{r} \quad (\text{A.4})$$

where we expect $f_k(\theta, \phi)$ to be determined by $V(\vec{r})$ and hence is called the *scattering amplitude*.

Our current ansatz under the assumptions above would then be:

$$\boxed{\psi(\vec{r}) = e^{ikz} + f_k(\theta, \phi) \frac{e^{ikr}}{r}} \quad (\text{A.5})$$

provided that we are sufficiently far from the scattering center ($r \gg a$ where a is the range of the potential).

§A.1 Scattering Cross Section

To see how $f_k(\theta, \phi)$ translates into the scattered wave, we look at the *scattering cross section* σ . In particular, we perform differential analysis by considering:

$$d\sigma = \frac{\# \text{ of particles scattered into } d\Omega \text{ per unit time}}{\text{Flux of incident particles}} \quad (\text{A.6})$$

where $d\Omega$ is the solid angle about (θ, ϕ) and the incident particle flux is simply the number of incident particles per area per unit time. In words, *the differential cross section is the area that removes from the incident beam the particles to be scattered into solid angle $d\Omega$* . We shall now compute the denominator and numerator terms:

1. Incident Flux (Denominator):

This quantity is actually familiar to us and is known as the *probability current / flux* \vec{J} .

$$\vec{J}_{e^{ikz}} = \frac{\hbar}{m} \text{Im} \{ \psi^* \nabla \psi \} = \frac{\hbar k}{m} \hat{z} \quad (\text{A.7})$$

This result makes sense because it is actually just the velocity ($\frac{p}{m} = \frac{\hbar k}{m}$) of the probability density ($|e^{ikz}|^2 = 1$).

2. Rate of Scattering into $d\Omega$ (Numerator):

We first look at the number of particles scattered into a differential volume $r^2 dr d\Omega$, dn :

$$\begin{aligned} dn &= |\psi(\vec{r})|^2 d^3\vec{r} \\ &= \left| f_k(\theta, \phi) \frac{e^{ikr}}{r} \right|^2 r^2 dr d\Omega \\ &= |f_k(\theta, \phi)|^2 dr d\Omega \end{aligned} \quad (\text{A.8})$$

Previously, we saw that the velocity $\frac{dr}{dt} = \frac{p}{m} = \frac{\hbar k}{m}$, hence:

$$\begin{aligned} \frac{dn}{dt} &= |f_k(\theta, \phi)|^2 \frac{dr d\Omega}{dr/(p/m)} \\ &= \frac{\hbar k}{m} |f_k(\theta, \phi)|^2 d\Omega \end{aligned} \quad (\text{A.9})$$

Putting these 2 results together, we see that the $\frac{\hbar k}{m}$ factors appear in both the denominator and numerator, which cancel to give us:

$$\boxed{d\sigma = |f_k(\theta, \phi)|^2 d\Omega} \Rightarrow \boxed{\sigma = \int |f_k(\theta, \phi)|^2 d\Omega} \quad (\text{A.10})$$

§A.2 Phase Shifts

We will now see that scattering amplitudes can actually be computed in terms of *phase shifts*. We start but first drawing intuition from scattering in 1D.

1D Scattering and Phase Shifts:

Consider the finite-range potential with a hard wall as illustrated below.

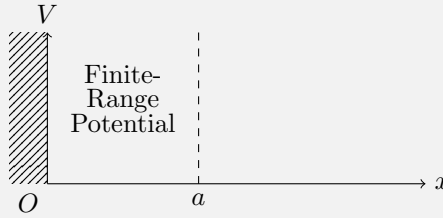


Figure A.1: 1D Finite-Range Potential with a Hard-Wall

Recall that for the potential above, we required an odd function which vanishes at the origin O . The ansatz for the wavefunction for $r > a$ would thus be:

$$\varphi(x) = N \sin(kx) = \frac{N}{2i} (e^{ikx} - e^{-ikx}) \quad (\text{A.11})$$

with N being the normalization factor, e^{ikx} the outgoing wave and e^{-ikx} the ingoing wave. This would be fine if there were just a hard-wall potential, but because of the non-trivial finite-range potential in $0 < r < a$, it must be modified. 2 considerations for this:

1. The outgoing term is required to be modified since it scatters off the finite-range potential.
2. Probability must be conserved upon modification of the ansatz.

This leads us to modify the outgoing wave with just a phase shift:

$$\psi(x) = \frac{N}{2i} (e^{ikx} e^{2i\delta_k} - e^{-ikx}) \quad (\text{A.12})$$

Remember this result as we now look at scattering in 3D. This will be an invaluable tool for us.

To approach scattering in 3D, we further assert that we are dealing with a **central potential** (spherically symmetric potential) $V(\vec{r}) = V(r)$.

§A.2.1 Analysis of a Spherically Symmetric Potential

As a refresher, derivations of the *radial solution* $R_{E\ell}$ and *spherical harmonics* $Y_{m\ell}$ are provided below.

Central Potentials:

In spherical coordinates, the Laplacian on an arbitrary wavefunction ψ is given as:

$$\nabla^2 \psi = \frac{1}{r} \frac{\partial^2}{\partial r^2} (r\psi) + \frac{1}{r^2} \left(\frac{1}{\sin \theta} \frac{\partial}{\partial \theta} \sin \theta \frac{\partial}{\partial \theta} + \frac{1}{\sin^2 \theta} \frac{\partial^2}{\partial \phi^2} \right) \psi \quad (\text{A.13})$$

As such, the full Schrödinger equation with a central potential in spherical coordinates is given by:

$$-\frac{\hbar^2}{2m} \left[\frac{1}{r} \frac{\partial^2}{\partial r^2} r + \frac{1}{r^2} \left(\frac{1}{\sin \theta} \frac{\partial}{\partial \theta} \sin \theta \frac{\partial}{\partial \theta} + \frac{1}{\sin^2 \theta} \frac{\partial^2}{\partial \phi^2} \right) \right] \psi + V(r)\psi = E\psi \quad (\text{A.14})$$

It can be shown that:

$$\hat{L}^2 = -\frac{\hbar^2}{\sin \theta} \frac{\partial}{\partial \theta} \sin \theta \frac{\partial}{\partial \theta} - \frac{\hbar^2}{\sin^2 \theta} \frac{\partial^2}{\partial \phi^2} \quad (\text{A.15})$$

where \hat{L} is the angular momentum operators with their respective eigenfunctions are then:

$$\hat{L} = (\hat{L}_x, \hat{L}_y, \hat{L}_z) \quad (\text{A.16})$$

$$\hat{L}_x \equiv \hat{y}\hat{p}_z - \hat{z}\hat{p}_y, \quad \hat{L}_y \equiv \hat{z}\hat{p}_x - \hat{x}\hat{p}_z, \quad \hat{L}_z \equiv \hat{x}\hat{p}_y - \hat{y}\hat{p}_x \quad (\text{A.17})$$

$$\hat{L}_z \psi_{\ell m} = \hbar m \psi_{\ell m}, \quad m \in \mathbb{R} \quad (\text{A.18})$$

$$\boxed{\hat{L}^2 \psi_{\ell m} = \hbar^2 \ell(\ell+1) \psi_{\ell m}}, \quad \ell \in \mathbb{R} \quad (\text{A.19})$$

As such, the Schrödinger equation reduces to:

$$-\frac{\hbar^2}{2m} \frac{1}{r} \frac{\partial^2}{\partial r^2} (r\psi) + \frac{\mathbf{L}^2}{2mr^2} \psi + V(r)\psi = E\psi \quad (\text{A.20})$$

for which if we choose a separable ansatz $\psi(r, \theta, \phi) = R_{E\ell}(r)Y_{\ell m}(\theta, \phi)$ with $Y_{\ell m}(\theta, \phi)$ being eigenstates of \hat{L}^2 , we get:

$$-\frac{\hbar^2}{2m} \frac{1}{r} \frac{d^2}{dr^2} (rR_{E\ell}) Y_{\ell m} + \frac{\hbar^2 \ell(\ell+1)}{2mr^2} R_{E\ell} Y_{\ell m} + V(r) R_{E\ell} Y_{\ell m} = E R_{E\ell} Y_{\ell m} \quad (\text{A.21})$$

From here, we see that all the spherical harmonics $Y_{\ell m}$ cancel out to give:

$$-\frac{\hbar^2}{2m} \frac{d^2}{dr^2} (rR_{E\ell}) + \frac{\hbar^2 \ell(\ell+1)}{2mr^2} (rR_{E\ell}) + V(r) (rR_{E\ell}) = E (rR_{E\ell}) \quad (\text{A.22})$$

And if we define $u_{E\ell}(r) \equiv rR_{E\ell}(r)$, we get:

$$\boxed{-\frac{\hbar^2}{2m} \frac{d^2 u_{E\ell}(r)}{dr^2} + \left[V(r) + \frac{\hbar^2 \ell(\ell+1)}{2mr^2} \right] u_{E\ell}(r) = E \cdot u_{E\ell}(r)} \quad (\text{A.23})$$

The 2 boxed results constitute the radial and angular equations for a general central potential.

§A.3 Central Potential Scattering

Going back to scattering, remember again that we are looking for solutions where $r \ll a$. In this regime, we can look for solutions where $V(r) = 0$ and $E = \frac{\hbar^2 k^2}{2m}$:

$$\begin{aligned} & -\frac{\hbar^2}{2m} \frac{d^2 u_{E\ell}(r)}{dr^2} + \frac{\hbar^2 \ell(\ell+1)}{2mr^2} u_{E\ell}(r) = \frac{\hbar^2 k^2}{2m} u_{E\ell}(r) \\ \Rightarrow & \left[-\frac{d^2}{dr^2} + \frac{l(l+1)}{r^2} \right] u_{E\ell}(r) = k^2 u_{E\ell}(r) \\ \Rightarrow & \boxed{\left[-\frac{d^2}{d\rho^2} + \frac{l(l+1)}{\rho^2} \right] u_{E\ell}(\rho) = u_{E\ell}(\rho)}, \quad \rho \equiv kr \end{aligned} \quad (\text{A.24})$$

Since we can do a change of variable to eliminate k^2 , the energy for this system is **not** quantized. It works out that solutions to the boxed equation (A.24) above are linear combinations of spherical Bessel functions:

$$u_{E\ell}(\rho) = A_\ell \rho j_\ell(\rho) + B_\ell \rho n_\ell(\rho) \quad (\text{A.25})$$

remembering that ρ is already a function of k which directly related to the energy E , hence the subscripts in $u_{E\ell}$.

Spherical Bessel Functions:

Spherical Bessel functions are canonical solutions to solving the radial portion of the *Helmholtz equation*, $(\nabla^2 + k^2) A = 0$:

$$\begin{aligned} & r^2 \frac{d^2 f(r)}{dr^2} + 2r \frac{df(r)}{dr} + [r^2 - l(l+1)] f(r) = 0 \\ \Rightarrow & \left[-\frac{d^2}{dr^2} - \frac{2}{r} \frac{d}{dr} + \frac{l(l+1)}{r^2} \right] f(r) = f(r) \end{aligned} \quad (\text{A.26})$$

These solutions have the form:

$$\begin{aligned} j_l(r) &= (-r)^l \left(\frac{1}{r} \frac{d}{dr} \right)^l \frac{\sin(r)}{r}, \quad \text{“Spherical Bessel Functions”} \\ n_l(r) &= -(-r)^l \left(\frac{1}{r} \frac{d}{dr} \right)^l \frac{\cos(r)}{r}, \quad \text{“Spherical Neumann Functions”} \end{aligned} \quad (\text{A.27})$$

and are related to the ordinary Bessel functions of the first kind by the relations:

$$\begin{aligned} j_l(r) &= \sqrt{\frac{\pi}{2r}} J_{l+\frac{1}{2}}(r) \\ n_l(r) &= (-1)^{l+1} \sqrt{\frac{\pi}{2r}} J_{-l-\frac{1}{2}}(r) \end{aligned} \quad (\text{A.28})$$

Note that $n_l(r)$ diverges / is *singular* at the origin ($r = 0$) while $j_l(r)$ does not / is

non-singular. The large radius limit ($r \rightarrow \infty$) of these functions go like:

$$\begin{aligned} j_l(r) &\rightarrow \frac{1}{r} \sin\left(r - \frac{l\pi}{2}\right) \\ n_l(r) &\rightarrow -\frac{1}{r} \cos\left(r - \frac{l\pi}{2}\right) \end{aligned} \quad (\text{A.29})$$

Knowing that the plane wave $e^{ikz} = e^{ikr \cos \theta}$ is a solution to equation (A.24), it must then be constituted of linear combinations of spherical Bessel functions:

$$e^{ikr \cos \theta} = \sum_{\ell=0}^{\infty} a_{\ell m} [A_{\ell} j_{\ell}(kr) + B_{\ell} n_{\ell}(kr)] Y_{\ell m}(\theta, \phi) \quad (\text{A.30})$$

A few things to notice before we proceed.

- Remembering that we are working with a spherically symmetric potential, and since we have chosen an axis for the incoming wave to propagate (z -axis), we can deduce that the ϕ (azimuthal) dependence is irrelevant ($z = r \cos \theta$ is independent of $\phi \Rightarrow m = 0$).
- Plane wave solutions have no divergences at the origin, so we cannot include the spherical Neumann functions in the solution for e^{ikz} .

With these in mind, our expansion simplifies to:

$$e^{ikr \cos \theta} = \sum_{\ell=0}^{\infty} a_{\ell 0} A_{\ell} j_{\ell}(kr) Y_{\ell 0}(\theta) \quad (\text{A.31})$$

It then works out that the $a_{\ell 0} A_{\ell}$ coefficients work out to give:

$$e^{ikr \cos \theta} = \sqrt{4\pi} \sum_{\ell=0}^{\infty} (i)^{\ell} \sqrt{2\ell+1} Y_{\ell 0}(\theta) j_{\ell}(kr) \quad (\text{A.32})$$

So we see that a plane wave can be built as an infinite sum of *partial waves* (Each term in ℓ) where each partial wave is an exact solution to (A.24). Applying the approximation when $r \ll a$:

$$\begin{aligned} e^{ikr \cos \theta} &\approx \frac{\sqrt{4\pi}}{k} \sum_{\ell=0}^{\infty} (i)^{\ell} \sqrt{2\ell+1} Y_{\ell 0}(\theta) \frac{\sin\left(kr - \frac{\ell\pi}{2}\right)}{r} \\ &= \frac{\sqrt{4\pi}}{k} \sum_{\ell=0}^{\infty} (i)^{\ell} \sqrt{2\ell+1} Y_{\ell 0}(\theta) \frac{1}{2i} \left[\frac{e^{i\left(kr - \frac{\ell\pi}{2}\right)}}{r} - \frac{e^{-i\left(kr - \frac{\ell\pi}{2}\right)}}{r} \right] \end{aligned} \quad (\text{A.33})$$

This effectively splits the plane wave into outgoing ($e^{i\left(kr - \frac{\ell\pi}{2}\right)}$) and incoming ($e^{-i\left(kr - \frac{\ell\pi}{2}\right)}$) terms which we can now apply our intuition from the 1-dimensional case to get the full solution:

$$\psi(\vec{r}) = \frac{\sqrt{4\pi}}{k} \sum_{\ell=0}^{\infty} (i)^{\ell} \sqrt{2\ell+1} Y_{\ell 0}(\theta) \frac{1}{2i} \left[\frac{e^{i\left(kr - \frac{\ell\pi}{2}\right)} e^{2i\delta_{\ell}}}{r} - \frac{e^{-i\left(kr - \frac{\ell\pi}{2}\right)}}{r} \right] \quad (\text{A.34})$$

If we equate this result to our original elastic scattering ansatz:

$$\begin{aligned}
e^{ikz} + f_k(\theta) \frac{e^{ikr}}{r} &= \frac{\sqrt{4\pi}}{k} \sum_{\ell=0}^{\infty} (i)^\ell \sqrt{2\ell+1} Y_{\ell 0}(\theta) \frac{1}{2i} \left[\frac{e^{i(kr - \frac{\ell\pi}{2})} e^{2i\delta_\ell}}{r} - \frac{e^{-i(kr - \frac{\ell\pi}{2})}}{r} \right] \\
\Rightarrow f_k(\theta) \frac{e^{ikr}}{r} &= \frac{\sqrt{4\pi}}{k} \sum_{\ell=0}^{\infty} (i)^\ell \sqrt{2\ell+1} Y_{\ell 0}(\theta) \frac{1}{2i} (e^{2i\delta_\ell} - 1) \frac{e^{i(kr - \frac{\ell\pi}{2})}}{r} \\
\Rightarrow f_k(\theta) \frac{e^{ikr}}{r} &= \frac{\sqrt{4\pi}}{k} \sum_{\ell=0}^{\infty} \left[\sqrt{2\ell+1} Y_{\ell 0}(\theta) e^{i\delta_\ell} \sin \delta_\ell \right] \frac{e^{ikr}}{r} \\
\Rightarrow \boxed{f_k(\theta) = \frac{\sqrt{4\pi}}{k} \sum_{\ell=0}^{\infty} \sqrt{2\ell+1} Y_{\ell 0}(\theta) e^{i\delta_\ell} \sin \delta_\ell} & \tag{A.35}
\end{aligned}$$

where we used the identity $e^{-i\ell\pi/2} = (-i)^\ell$, so that $(i)^\ell \cdot e^{-i\ell\pi/2} = 1$ and we have also dropped the ϕ dependence of f from spherical symmetry arguments. This indeed grants us an expression for the scattering amplitudes in terms of phase shifts. Recalling result A.10, we then see that:

$$\begin{aligned}
\sigma &= \int |f_k(\theta)|^2 d\Omega \\
&= \int \frac{4\pi}{k^2} \sum_{\ell=0}^{\infty} \sum_{\ell'=0}^{\infty} \sqrt{2\ell+1} \sqrt{2\ell'+1} Y_{\ell 0}(\theta) e^{-i\delta_\ell} \sin \delta_\ell Y_{\ell' 0}(\theta) e^{i\delta_{\ell'}} \sin \delta_{\ell'} d\Omega \\
&= \frac{4\pi}{k^2} \sum_{\ell=0}^{\infty} \sum_{\ell'=0}^{\infty} \sqrt{2\ell+1} \sqrt{2\ell'+1} e^{-i\delta_\ell} e^{i\delta_{\ell'}} \sin \delta_\ell \sin \delta_{\ell'} \int Y_{\ell 0}(\theta) Y_{\ell' 0}(\theta) d\Omega
\end{aligned} \tag{A.36}$$

We know from our analysis of central potentials that spherical harmonics are orthogonal functions. That is to say:

$$\begin{aligned}
&\int Y_{\ell 0}(\theta) Y_{\ell' 0}(\theta) d\Omega = \delta_{\ell, \ell'} \\
\Rightarrow \boxed{\sigma = \frac{4\pi}{k^2} \sum_{\ell=0}^{\infty} (2\ell+1) \sin^2 \delta_\ell} & \tag{A.37}
\end{aligned}$$

Noting that above, $\delta_{\ell, \ell'}$ is the Kronecker delta function, **not** a phase shift.