Phys 852, Quantum mechanics II, Spring 2008

Introduction to Scattering Theory

Statement of the problem:

Scattering theory is essentially time-independent perturbation theory applied to the case of a continuous spectrum. That means that we know there is an eigenstate of the full Hamiltonian for every possible energy, E. Thus the job of finding the full eigenvalues, which was a major part of TIPR, is not necessary here. In scattering theory, we just pick any E, and then try to find the 'perturbed' eigenstate, $|\psi(E)\rangle$. On the other hand, remember that there are usually multiple degenerate eigenstates for any given energy. So the question becomes; which of the presumably infinitely many degenerate full-eigenstates are we trying to compute? The answer comes from causality; we want to be able to completely specify the probability current amplitude coming *in* from $\vec{r} = \infty$, and then we want the theory to give us the corresponding outgoing current amplitude. The way we do this is to pick an 'unperturbed' eigenstate which has the desired incoming current amplitude (we don't need to worry what the outgoing current amplitude of the unperturbed state is). The second step is to make sure that our perturbation theory generates no additional incoming currents, which we accomplish by putting this condition in by hand, under the mantra of 'causality'. As we will see, this means that the resulting 'full eigenstate' will have the desired incoming current amplitude. Now if you go back to what you know, you will recall that 'solving' a partial differential equation requires first specifying the desired boundary conditions, which is exactly what the standard scattering theory formalism is designed to do.

Typically, the scattering formalism is described in the following way: an incident particle in state $|\psi_0\rangle$ is scattered by the potential V, resulting in a scattered state $|\psi_s\rangle$. The incident state $|\psi_0\rangle$ is assumed to be an eigenstate of the 'background' hamiltonian H_0, with eigenvalue E. This is expressed mathematically as

$$(E - H_0)|\psi_0\rangle = 0. \tag{1}$$

Unless otherwise specified, the background Hamiltonian should be taken as that of a free-particle,

$$H_0 = \frac{P^2}{2M}, \tag{2}$$

and the incident state taken as a plane wave

$$\langle\vec{r}|\psi_0\rangle = \psi_0(\vec{r}) = e^{i\vec{k}\cdot\vec{r}}. \tag{3}$$

As with one-dimensional scattering, we do not need to worry about the normalization of the incident state. Furthermore, the potential $V(\vec{R})$ is assumed to be 'localized', so that

$$\lim_{r\to\infty} V(\vec{r}) = 0. \tag{4}$$

The goal of scattering theory is then to solve the full energy-eigenstate problem

$$(E - H_0 - V)|\psi\rangle = 0, \tag{5}$$

where $E > 0$ (unless otherwise specified), and $|\psi\rangle$ is the eigenstate of the full Hamiltonian $H = H_0 + V$ with energy E. It should be clear that there is a different $|\psi_0\rangle$ and correspondingly, a different $|\psi\rangle$ for each energy E, even though our notation does not indicate this explicitly.

1 Green's function method

1.1 The Lippman-Schwinger Eq.

We start by defining the scattered state, $|\psi_s\rangle$ via

$$|\psi_s\rangle = |\psi\rangle - |\psi_0\rangle. \tag{6}$$

The full Scrödinger equation (5) can be written as

$$(E - H_0)|\psi\rangle = V|\psi\rangle, \tag{7}$$

which after substituting $|\psi\rangle = |\psi_0\rangle + |\psi_s\rangle$, and making use of (1) gives

$$(E - H_0)|\psi_s\rangle = V|\psi\rangle. \tag{8}$$

Operating on both sides with $(E - H_0)^{-1}$ leads to

$$|\psi_s\rangle = (E - H_0)^{-1}V|\psi\rangle, \tag{9}$$

which, by adding $|\psi_0\rangle$ to both sides, becomes

$$|\psi\rangle = |\psi_0\rangle + (E - H_0)^{-1}V|\psi\rangle. \tag{10}$$

This is known as the Lippman-Schwinger equation.

1.2 The Green's function

It is often expressed in a slightly more compact notation by introducing the concept of a 'Green's function', defined as

$$G_H(E) = \lim_{\epsilon \to 0}(E - H_0 + i\epsilon)^{-1}. \tag{11}$$

The $i\epsilon$ term is is added 'by hand' to enforce 'causality' by making sure that $|\psi_s\rangle$ has no incoming probability current associated with it. It makes sense that scattered waves propagate away from the source, and not the other way around. For simplicity, we can use the symbol G_0 for the unperturbed Green's function, defined as

$$G_0 = G_{H_0}(E) = \lim_{\epsilon \to 0}(E - H_0 + i\epsilon)^{-1}. \tag{12}$$

Using this definition, the Lippman-Schwinger equation assumes its standard form:

$$|\psi\rangle = |\psi_0\rangle + G_0 V|\psi\rangle. \tag{13}$$

Solving the Lippman-Schwinger equation for $|\psi\rangle$ is formally very simple, giving

$$|\psi\rangle = (1 - G_0 V)^{-1}\,|\psi_0\rangle. \tag{14}$$

We will look at the meaning of this solution in the next section.

1.3 The Born Series

Another way to solve the Lippman-Schwinger equation is by the iteration method. To solve (13) by iteration, we first rewrite the equation as

$$|\psi_{new}\rangle = |\psi_0\rangle + G_0 V|\psi_{old}\rangle. \tag{15}$$

We then start with the zeroth order approximation, $|\psi_{old}\rangle = |\psi_0\rangle$, and use (15) to generate a better approximation, $|\psi_{new}\rangle = (1+G_0V)|\psi_0\rangle$. Using this as $|\psi_{old}\rangle$ then leads to a better approximation, $|\psi_{new}\rangle = (1 + G_0V + G_0VG_0V)|\psi_0\rangle$. After an infinite number of iterations, this procedure leads to

$$|\psi\rangle = (1 + G_0V + G_0VGV + G_0VG_0VG_0V + \ldots)\,|\psi_0\rangle, \tag{16}$$

which is known as the Born series. Written as an integral equation, the Born-series for the wavefunction, $\psi(\vec{r}) = \langle\vec{r}|\psi\rangle$, looks like

$$\psi(\vec{r}) = \psi_0(\vec{r}) + \int dV' G_0(\vec{r},\vec{r}\,')V(\vec{r}\,')\psi_0(\vec{r}\,') + \int dV'\,dV'' G_0(\vec{r},\vec{r}\,')V(\vec{r}\,')G_0(\vec{r}\,',\vec{r}\,'')V(\vec{r}\,'')\psi_0(\vec{r}\,'') + \ldots, \tag{17}$$

where we have defined $\psi_0(\vec{r}) = \langle\vec{r}|\psi_0\rangle$ and $G_0(\vec{r},\vec{r}') = \langle\vec{r}|G_0|\vec{r}'\rangle$. We can interpret this result by 'reading' each term from right-to-left, as follows: If we put a detector at position $\vec{r}$, then the probability that the detector would fire after the collision is over is proportional to $|\psi(\vec{r})|^2$. The first term on the r.h.s. is thus the probability amplitude that the particle made it to the detector without scattering (what it would be if $V = 0$). The second terms describes the particle scattering once, at a point $\vec{r}\,'$, where its amplitude is increased/decreased by a factor $V(\vec{r}')$, and then propagating as a free-spherical wave centered at $\vec{r}\,'$ to the detector. The integral over all $\vec{r}\,'$ then sums over all possible collision locations. The next terms describes the particle scattering twice, summing over both collision locations. The third term would include all possible paths with three collisions, and so-on. Thus we see that the total amplitude is the sum over all possible trajectories by which the particle could have made it to the detector, assuming straight-line propagation between point-contact collisions. From this interpretation, we can guess that the Green's function would have the form:

$$G_0(\vec{r},\vec{r}') = \frac{e^{ik|\vec{r}-\vec{r}'|}}{|\vec{r}-\vec{r}|'}, \tag{18}$$

as the $e^{ik|\vec{r}-\vec{r}'|}$ factor just adjusts the phase of the state to reflect propagation with wavelength $\lambda = 2\pi/k$, over a distance $d = |\vec{r}-\vec{r}'|$, while the $1/|\vec{r}-\vec{r}'|$ factor lead to a probability density which decreases as $1/d^2$, consistent with conservation of probability on an expanding spherical phase front. As we will see, aside from an overall constant, this is the correct three-dimensional Green's function.

The quantum picture of scattering, as suggested by the Born series, is of free propagation (described by G_0) punctuated by instantaneous "collisions", described by V. This picture is at odds with the classical picture of a smooth continuous motion on the 'potential surface'. Indeed, in high-energy physics, we learn that all interactions are due to the exchange of 'virtual' (non-energy conserving) gauge bosons, e.g. photons or gluons. The notion of an inter-particle "potential" is therefore an approximation that neglects the retardation effect due to the finite propagation velocity of the mediating particle. This the quantum picture suggested by the Born series is more accurate than the classical view, as we can think of each "collision" as the exchange of a virtual particle, which is indeed a discrete event.

1.3.1 Does the Born-series always converge?

The iteration method we used to derive the Born-series is just a more compact equivalent formulation of standard perturbation theory. In other words, you would get the same result if you let $V \to \lambda V$, and expanded $|\psi\rangle = |\psi_0\rangle + \lambda|\psi_1\rangle + \lambda^2|\psi_2\rangle + \ldots$, and so on. Historically, the scattering problem was solved perturbatively, where it was soon found that the series did not always converge. Instead the sum would diverge towards infinity as more and more terms were included. This was the famous 'renormalization' problem. It was then proposed that a particular infinity could be subtracted, leading to the correct physical result.

To goal of the renormalization program is to add a small correction to each term in the Born series, so that when summing the whole series, the sum of the corrections gives an infinity that exactly cancels the infinity in the pure Born series. To see how this works, we can start by defining the eigenstates of $(1 - G_0V)^{-1}$ according to

$$G_0V|z_n\rangle = z_n|z_n\rangle, \tag{19}$$

where z_n is the n^{th} complex eigenvalue. We assume a discrete spectrum for convenience, as the argument will also hold for a continuous spectrum. In this basis, we can express the operator G_0V as

$$G_0V = \sum_n \frac{|z_n\rangle\langle z_n|}{1 - z_n}. \tag{20}$$

Note that the series expansion $(1 - z)^{-1}$ only converges for $|z| < 1$. This is because a series expansion converges only as far from the expansion point as the nearest singularity in the function being expanded. Here the expansion point is $z = 0$ and the singularity is at $z = 1$. We can perform a valid series expansion of $(1 - G_0V)^{-1}$ via

$$(1 - G_0V)^{-1} = \sum_n u(1 - |z_n|)\,|z_n\rangle\langle z_n|\left(1 + z_n + z_n^2 + \ldots\right) + \sum_n u(|z_n| - 1)\frac{|z_n\rangle\langle z_n|}{1 - z_n}, \tag{21}$$

where $u(x)$ is the unit step function. For the case $|z_n| > 1$, we can expand in powers of $1/z_n$, as

$$\begin{aligned} \frac{1}{1 - z_n} &= -\frac{1}{z_n}\frac{1}{1 - \frac{1}{z_n}} \\ &= -\frac{1}{z_n}\left(1 + z_n^{-1} + z_n^{-2} + \ldots\right). \end{aligned} \tag{22}$$

These two series can be combined to give

$$\begin{aligned} (1 - G_0V)^{-1} &= \sum_n |z_n\rangle\langle z_n| \sum_{m=0}^{\infty}\left(z_n^m + u(|z_n| - 1)\left[-z_n^m + \left(-z_n^{-m-1}\right)\right]\right) \\ &= \sum_{m=0}^{\infty}\sum_n |z_n\rangle\langle z_n|\left[z_n^m - u(|z_n| - 1)\left(z_n^m + z_n^{-m-1}\right)\right] \\ &= \sum_{m=0}^{\infty}\left[(G_0V)^m - R_m\right] \end{aligned} \tag{23}$$

where the m^{th} renormalization term is

$$R_m = \sum_n u(|z_n| - 1)\,|z_n\rangle\langle z_n|\,\left(z_n^m + z_n^{-m-1}\right). \tag{24}$$

The idea is then that the renormalized series will converge normally, so you can take only as many terms as required for precision. Of course this renormalization is difficult in practice because the eigenvalues and eigenvectors of G_0V are not usually known, but it establishes the proof-of-principle of the 'renormalized' Born series.

1.4 The T-Matrix

From the Born-series, we see that the scattered wave $|\psi_s\rangle = |\psi\rangle - |\psi_0\rangle$ is given by

$$|\psi_s\rangle = (G_0V + G_0VG_0 + G_0VG_0VG_0V + \ldots)|\psi_0\rangle. \tag{25}$$

Based on our path-integral interpretation, we see that each term contains at least one 'scattering event'. For each term, the scattered wave then propagated freely from the last scattering point to the detector. This final free-propagation can be factored out giving

$$|\psi_s\rangle = G_0(V + VG_0V + VG_0VG_0V + \ldots)|\psi_0\rangle. \tag{26}$$

Then the sum inside parentheses is just the story of all the possible ways the particle could have made it to the location of the final scattering event. If we put all of this story in a 'black box', and call it a T-matrix, we get

$$|\psi_s\rangle = G_0T|\psi_0\rangle, \tag{27}$$

which defines the T-matrix. Comparison with (9) and (14) shows that

$$|\psi_s\rangle = G_0V(1 - G_0V)^{-1}|\psi_0\rangle \tag{28}$$

from which we see immediately that

$$T = V(1 - G_0V)^{-1}, \tag{29}$$

or equivalently

$$T = (1 - VG_0)^{-1}\,V. \tag{30}$$

This equivalence can be proven by hitting both equations from the left with $(1 - VG_0)$ and from the right with $(1 - G_0V)$, which gives $V + VG_0V = V + VG_0V$.

Ignoring the issue of convergence for a moment, the series expansion $(1-A)^{-1} = 1 + A + A^2 + \ldots$, gives

$$T = V + VG_0V + VG_0VG_0V + VG_0VG_0VG_0V + \ldots. \tag{31}$$

Projecting this onto position eigenstates results in the position-space matrix elements of the T-matrix:

$$T(\vec{r},\vec{r}\,') = V(\vec{r})\delta(\vec{r} - \vec{r}\,') + V(\vec{r})G(\vec{r},\vec{r}\,')V(\vec{r}\,') + \int dV''\, V(\vec{r})G(\vec{r},\vec{r}\,'')V(\vec{r}\,'')G(\vec{r}\,'',\vec{r}\,')V(\vec{r}\,') + \ldots, \tag{32}$$

where $T(\vec{r},\vec{r}\,') = \langle\vec{r}|T|\vec{r}\,'\rangle$ and $G_0(\vec{r},\vec{r}\,') = \langle\vec{r}|G_0|\vec{r}\,'\rangle$.

1.5 Computing the Green's Function via the Calculus of Residues

Because $G_0 = (E - H_0 + i\epsilon)$, it follows that the eigenstates of G_0 are the eigenstates of H_0. Thus, the Green's function can be expressed in the basis of eigenstates of H_0, giving

$$G_0 = \sum_m \int_{E_c}^{\infty} dE'\, \frac{|E',m\rangle\langle E',m|}{E - E' + i\epsilon} + \sum_{n,m} \frac{|n,m\rangle\langle n,m|}{E - E_n + i\epsilon}, \tag{33}$$

where E_c is the continuum threshold energy, the summation over m accounts for any degeneracies, and the summation over n includes any bound-states which lie below the continuum threshold, i.e. $E_n < E_c$. Simplifying to the case with no degeneracies, no bound-states, and $E_c = 0$ gives

$$G_0 = \int_0^{\infty} dE'\, \frac{|E'\rangle\langle E'|}{(E - E' + i\epsilon)}. \tag{34}$$

We can project onto position eigenstates to give

$$\langle \vec{r}|G_0|\vec{r}\,'\rangle = \int_0^\infty dE' \frac{\langle \vec{r}|E'\rangle\langle R'|\vec{r}\,'\rangle}{E - E' + i\epsilon}, \tag{35}$$

or equivalently

$$G(\vec{r},\vec{r}\,') \int_0^\infty dE' \, \frac{\psi^*_{E'}(\vec{r})\psi_{E'}(\vec{r}\,')}{E - E' + i\epsilon}, \tag{36}$$

which, if the energy eigenstate wavefunctions are known, can often be solved by changing integration variables from energy to wave-vector, and then using contour integration to obtain an analytic expression.

1.5.1 Free particle in 1-dimension

For a free particle in one-dimension we have $E = \frac{\hbar^2 k^2}{2M}$, and $\langle x|E\rangle = (2\pi)^{-1/2}e^{ikx}$. With these substitutions, equation (36) becomes

$$\begin{aligned} G(x,x') &= \frac{1}{2\pi}\int_{-\infty}^{\infty} dk' \, \frac{e^{ik'(x-x')}}{E - \frac{\hbar^2 k'^2}{2M} + i\epsilon} \\ &= -\frac{2M}{2\pi\hbar^2}\int_{-\infty}^{\infty} dk' \, \frac{e^{ik'(x-x')}}{k'^2 - k^2 - i\epsilon}. \end{aligned} \tag{37}$$

With $k'^2 - k^2 - i\epsilon = (k' + \sqrt{k^2 + i\epsilon})(k' - \sqrt{k^2 + i\epsilon})$ and $\sqrt{k^2 + i\epsilon} = k + \frac{i\epsilon}{2k} = k + i\epsilon$, this becomes[1]

$$G(x,x') = -\frac{2M}{2\pi\hbar^2}\int_{-\infty}^{\infty} dk' \, \frac{e^{ik'(x-x')}}{(k' + k + i\epsilon)(k' - k - i\epsilon)}. \tag{38}$$

This can be solved by the method of contour integration, which means we extend k' onto the complex plane via $k \to k_R + ik_I$, which leads to $e^{ik(x-x')} \to e^{ik'_R(x-x') - k'_I(x-x')}$. Because we want the function to vanish at $|k| \to \infty$, we see that for $x > x'$ we must close on the upper half-plane, so that the contour includes only the pole at $k' = k + i\epsilon$. For $x < x'$, we must instead close the contour on the lower half-plane, so only the pole at $k' = -k - i\epsilon$ is enclosed. Using the residue theorem, $\oint dz \frac{f(z)}{z - z_0} = \pm 2\pi i f(z_0)$, where the '+' is used for counter-clockwise path integration, and the '$-$' for clockwise, leads directly to

$$G(x,x') = \begin{cases} -\frac{2M}{2\pi\hbar^2} 2\pi i \frac{e^{ik(x-x')}}{2k}; & x > x' \\ -\frac{2M}{2\pi\hbar^2}(-2\pi i)\frac{e^{-ik(x-x')}}{-2k}; & x < x' \end{cases}. \tag{39}$$

These results can be combined into a single expression:

$$\langle x|G_0|x'\rangle = -\frac{iM}{\hbar^2 k} e^{ik|x-x'|}. \tag{40}$$

This clearly shows that the current is flowing in the direction from x' to x. This shows that the choice $-i\epsilon$ has led to a purely outgoing current with respect to the point x'. With $-i\epsilon \to +i\epsilon$, we would have obtained a purely incoming current.

[1] Since ϵ is real-positive and infinitesimal, it satisfies $c\,\epsilon = \arg(c)\epsilon$ for any constant c.

1.5.2 Free particle in 3-dimensions

This result can also be derived via contour integration, starting from

$$G_0 = \int d^3k \frac{|\vec{k}\rangle\langle\vec{k}|}{E - \frac{\hbar^2 k^2}{2M} + i\epsilon}. \tag{41}$$

Projecting onto position eigenstates, and factorizing the denominator gives

$$\langle\vec{r}|G_0|\vec{r}\,'\rangle = -\frac{2M}{(2\pi)^3\hbar^2}\int d^3k' \frac{e^{i\vec{k}'\cdot(\vec{r}-\vec{r}\,')}}{(k'+k+i\epsilon)(k'-k-i\epsilon)}, \tag{42}$$

where $k = \sqrt{2ME}/\hbar$. Choosing the z-axis along $\vec{r} - \vec{r}\,'$ gives

$$\langle\vec{r}|G_0|\vec{r}\,'\rangle = -\frac{2M}{(2\pi)^2\hbar^2}\int_{-1}^{1} du \int_0^\infty k'^2 dk' \frac{e^{ik'|\vec{r}-\vec{r}\,'|u}}{(k'+k+i\epsilon)(k'-k-i\epsilon)} \tag{43}$$

Performing the u-integration gives

$$\langle\vec{r}|G_0|\vec{r}\,'\rangle = -\frac{2M}{(2\pi)^2\hbar^2}\int_0^\infty k'^2 dk' \frac{e^{ik'|\vec{r}-\vec{r}\,'|} - e^{-ik'|\vec{r}-\vec{r}\,'|}}{(k'+k+i\epsilon)(k'-k-i\epsilon)ik'|\vec{r}-\vec{r}\,'|} \tag{44}$$

The two-terms in the integrand can then be combined to extend the integral to $-\infty$, so that

$$\langle\vec{r}|G_0|\vec{r}\,'\rangle = -\frac{2M}{(2\pi)^2\hbar^2}\int_{-\infty}^\infty k'^2 dk' \frac{e^{ik'|\vec{r}-\vec{r}\,'|}}{(k'+k+i\epsilon)(k'-k-i\epsilon)ik'|\vec{r}-\vec{r}\,'|} \tag{45}$$

Since $|\vec{r} - \vec{r}\,'| > 0$, we can close on the upper half-plane, so that the Residue theorem gives

$$\langle\vec{r}|G_0|\vec{r}\,'\rangle = -\frac{2M}{(2\pi)^2\hbar^2}(2\pi i)k^2 \frac{e^{ik|\vec{r}-\vec{r}\,'|}}{2ik^2|\vec{r}-\vec{r}\,'|}. \tag{46}$$

Thus the final expression for the 3-d Green's function becomes

$$G(|\vec{r}-\vec{r}\,'|) = -\frac{M}{2\pi\hbar^2}\frac{e^{ik|\vec{r}-\vec{r}\,'|}}{|\vec{r}-\vec{r}\,'|}, \tag{47}$$

which agrees with our previous guess (18).

1.6 Example: 1-d delta-function scattering

1.6.1 The T-matrix of a 1-d delta-function

Consider a free particle in one dimension incident on a delta-function potential $V(x) = g\delta(x)$. We want to solve the scattering problem and find the reflection and transmission probabilities T and R. We first compute the T-matrix via Eqs. (32) and (40), giving

$$\begin{aligned}
T(x,x') &= g\delta(x)\delta(x') + g\delta(x)\left(-\frac{iM}{\hbar^2 k}\right)e^{ik|x-x'|}g\delta(x') \\
&+ g\delta(x)\int dx'' \left(-\frac{iM}{\hbar^2 k}\right)e^{ik|x-x''|}g\delta(x'')\left(-\frac{iM}{\hbar^2 k}\right)e^{ik|x''-x'|}g\delta(x') + \dots \\
&= g\delta(x)\delta(x')\left[1 + \left(-i\frac{gM}{\hbar^2 k}\right) + \left(-\frac{igM}{\hbar^2 k}\right)^2 + \dots\right] \\
&= \frac{g\delta(x)\delta(x')}{1 + i\frac{gM}{\hbar^2 k}}
\end{aligned} \tag{48}$$

We can now compute the scattered wave via Eq. (27). Taking $\psi_0(x) = e^{ikx}$ then gives

$$\begin{aligned}
\psi_s(x) &= \int dx'\, dx'' G(x,x')T(x',x'')\psi_0(x'') \\
&= \int dx'\, dx'' \left(-\frac{iM}{\hbar^2 k}\right) e^{ik|x-x'|} \frac{g\delta('x)\delta(x'')}{1+i\frac{gM}{\hbar^2 k}} e^{ikx''} \\
&= -\frac{e^{ik|x|}}{1-i\frac{\hbar^2 k}{Mg}}.
\end{aligned} \tag{49}$$

Introducing the scattering length

$$a = \frac{\hbar^2}{Mg}, \tag{50}$$

we arrive at the full solution

$$\psi(x) = e^{ikx} - \frac{e^{ik|x|}}{1-ika}. \tag{51}$$

For $x < 0$ this gives

$$\psi(x) = e^{ikx} - \frac{e^{-ikx}}{1-ika}, \tag{52}$$

from which we can identify the reflection amplitude

$$r = -\frac{1}{1-ika}. \tag{53}$$

The reflection probability, $R = |r|^2$ is therefore

$$R = |r|^2 = \frac{1}{1+(ka)^2}. \tag{54}$$

Turning off the potential requires $g \to 0$, corresponding to $a \to \infty$, in which case we have $R = 0$ as expected. For $x > 0$ we find

$$\begin{aligned}
\psi(x) &= e^{ikx} - \frac{e^{ikx}}{1-ika} \\
&= \frac{ika}{1-ika} e^{ikx},
\end{aligned} \tag{55}$$

from which we can identify the transmission amplitude as

$$t = \frac{ika}{1-ika}. \tag{56}$$

This leads to a transmission probability of

$$T = |t|^2 = \frac{(ka)^2}{1+(ka)^2}, \tag{57}$$

which goes to 1 as $g \to 0$, as required. We note also that $R + T = 1$, satisfying conservation of probability.

1.6.2 Direct solution of the Lippman-Schwinger equation

The previous example was to illustrate the T-matrix formalism. For 1-d scatters made up entirely of delta-functions, by far the easiest approach is to solve the Lippman-Schwinger equation (LSE) directly. Hitting the LSE from the left with $\langle x|$ gives

$$\langle x|\psi\rangle = \langle x|\psi_0\rangle + \langle x G_0 V|\psi\rangle. \tag{58}$$

Inserting the projector between the G_0 and the V, and making use of the diagonality of V leads to

$$\psi(x) = \psi_0(x) + \int dx'\, G_0(x,x')V(x')\psi(x'), \tag{59}$$

which is an integral equation for $\psi(x)$. For the case where $V(x) = g\delta(x - x_0)$, we can perform the integral, giving

$$\psi(x) = \psi_0(x) + gG_0(x,x_0)\psi(x_0). \tag{60}$$

The unknown quantity, $\psi(x_0)$ can be found by setting $x = x_0$,

$$\psi(x_0) = \psi_0(x_0) + gG_0(x_0,x_0)\psi(x_0), \tag{61}$$

which has the solution

$$\psi(x_0) = \frac{\psi_0(x_0)}{1 - gG_0(x_0,x_0)}, \tag{62}$$

which gives the solution to the LSE as

$$\psi(x) = \psi_0(x) + \frac{gG_0(x,x_0)\psi_0(x_0)}{1 - gG(x_0,x_0)}. \tag{63}$$

With $\psi_0(x) = e^{ikx}$ and $G_0(x,x') = -i\frac{M}{\hbar^2 k}e^{ik|x-x'|}$, this becomes

$$\begin{aligned} \psi(x) &= e^{ikx} - i\frac{Mg}{\hbar^2 k}\frac{e^{ik|x|}}{1 + i\frac{Mg}{\hbar^2 k}} \\ &= e^{ikx} - \frac{e^{ik|x|}}{1 - ika}, \end{aligned} \tag{64}$$

where we have again introduced $a = \frac{\hbar^2}{Mg}$.

2 Scattering probabiilities

2.1 The scattering amplitude

In general, we want to find the probability to detect the particle at position $\vec{r}$ after it has left the scattering region. If we choose the center of the scattering potential as the origin, and if the detector is sufficiently far from the scatterer, then we can compute the probability amplitude at the detector from the large-r limit of the full wavefunction,

$$\lim_{r\to\infty} \psi(\vec{r}) = \psi_0(\vec{r}) + \lim_{r\to\infty} \int d^3r'\, d^3r''\, G(\vec{r},\vec{r}\,')T(\vec{r}\,',\vec{r}\,'')\psi_0(\vec{r}\,''). \tag{65}$$

Taking a plane wave for the incident state,

$$\psi_0(\vec{r}) = e^{i\vec{k}\cdot\vec{r}}, \tag{66}$$

and putting in the 3-d Greens function (47), we find

$$\lim_{r\to\infty} \psi(\vec{r}) = e^{i\vec{k}\cdot\vec{r}} - \frac{M}{2\pi\hbar^2} \lim_{r\to\infty} \int d^3r'\, d^3r''\, \frac{e^{ik|\vec{r}-\vec{r}\,'|}}{|\vec{r}-\vec{r}\,'|} T(\vec{r}\,',\vec{r}\,'') e^{i\vec{k}\cdot\vec{r}\,''}. \tag{67}$$

Now with $\vec{r} = r\,\vec{e}_r(\theta,\phi) = r(\cos\theta\vec{e}_z z + \sin\theta\cos\phi\vec{e}_x + \sin\theta\sin\phi\vec{e}_y)$ we find

$$\begin{aligned}
\lim_{r\to\infty} |\vec{r}-\vec{r}\,'| &= \sqrt{(\vec{r}-\vec{r}\,')^2} \\
&= \sqrt{r^2 - 2r\vec{e}_r\cdot\vec{r}\,' + r\,'^2} \\
&\approx r\sqrt{1 - 2\frac{\vec{e}_r\cdot\vec{r}\,'}{r} + \frac{r\,'^2}{r^2}} \\
&\approx r\left(1 - \frac{\vec{e}_r\cdot\vec{r}}{r}\right) \\
&\approx r - \vec{e}_r\cdot\vec{r}\,',
\end{aligned} \tag{68}$$

For convenience we choose $\vec{e}_z$ along $\vec{k}$, so that $\theta = 0$ corresponds to the forward-scattering direction. Similarly we find

$$\lim_{r\to\infty} \frac{1}{|\vec{r}-\vec{r}\,'|} \approx \frac{1}{r}. \tag{69}$$

This gives

$$\lim_{r\to\infty} G(\vec{r},\vec{r}\,') = -\frac{M}{2\pi\hbar^2}\frac{e^{ikr}}{r} e^{-ik\vec{e}_r(\theta,\phi)\cdot\vec{r}\,'}, \tag{70}$$

which leads to

$$\lim_{r\to\infty} \psi(\vec{r}) = e^{ikz} - \frac{M}{2\pi\hbar^2}\frac{e^{ikr}}{r} \int d^3r'\, d^3r''\, e^{-ik\vec{e}_r(\theta,\phi)\cdot\vec{r}\,'} T(\vec{r}\,',\vec{r}\,'') e^{ikz''}. \tag{71}$$

It is conventional to define the scattering amplitude, $f(\theta,\phi|k\rangle$, via

$$\lim_{r\to\infty} \psi(\vec{r}) = e^{ikz} + f(\theta,\phi|k)\frac{e^{ikr}}{r}, \tag{72}$$

so we see immediately that

$$f(\theta,\phi|k) = -\frac{M}{2\pi\hbar^2} \int d^3r'\, d^3r''\, e^{-ik\vec{e}_r(\theta,\phi)\cdot\vec{r}\,'}\, T(\vec{r}\,',\vec{r}\,'')\, e^{ik\vec{e}_z\cdot\vec{r}\,''}. \tag{73}$$

With the substitutions

$$k\,\vec{e}_r(\theta,\phi) \rightarrow \vec{k}', \tag{74}$$

and

$$k\vec{e_z} \rightarrow \vec{k}, \tag{75}$$

the scattering amplitude generalizes to

$$\begin{aligned} f(\vec{k}',\vec{k}) &= -\frac{M}{2\pi\hbar^2}\int d^3r'\,d^3r\,e^{-i\vec{k}'\cdot\vec{r}'}\,T(\vec{r}',\vec{r})e^{i\vec{k}\cdot\vec{r}} \\ &= -\frac{(2\pi)^2 M}{\hbar^2}\int d^3r' d^3r\,\langle\vec{k}'|\vec{r}'\rangle\langle\vec{r}'|T|\vec{r}\rangle\langle\vec{r}|\vec{k}\rangle \\ &= -\frac{(2\pi)^2 M}{\hbar^2}\langle\vec{k}'|T|\vec{k}\rangle, \end{aligned} \tag{76}$$

which should be interpreted as the probability amplitude to scatter in the direction $\vec{k}'$, given an incident wave-vector $\vec{k}$. The function $f(\theta,\phi|k)$ is valid only for the case of elastic scattering, $|\vec{k}'| = |\vec{k}|$, whereas the function $f(\vec{k}',\vec{k})$ is completely general (however we won't be considering inelastic scattering at present).

Eq. 76 shows that the scattering amplitude is the Fourier transform of the T-matrix. In optics it is well known that the image in the far-field is the Fourier transform of the near-field image. This is because propagation over a large distance allows the Fourier components of the field to spatially separate. This is exactly what we are seeing here. The T-matrix describes the exact scattered field over all space, including inside the interaction region. The Fourier transform of the T-matrix therefore describes the same scattered field in momentum space. The scattering amplitude, on the other hand, describes the scattered field only in the far-field region ($r \rightarrow \infty$), hence it follows that the different momentum components would spatially separate, with the result that the scattering amplitude should reflect the Fourier transform of the scattered field. In other words, only the component of total amplitude corresponding to a particular $\vec{k}$-value will make it to a detector located in the $\vec{k}$ direction.

2.2 The Scattering Cross-Section

Up to now we have taken the incident wave to be a plane-wave $|\psi_0\rangle = |\vec{k}\rangle$, where

$$\langle\vec{r}|\vec{k}\rangle = e^{i\vec{k}\cdot\vec{r}}. \tag{77}$$

This state is delta-normalized so that $\langle\vec{k}|\vec{k}'\rangle = (2\pi)^3\delta^3(\vec{k}-\vec{k}')$. We note that this choice of normalization has the drawback that that $|\psi_0(\vec{r})|^2$ does not have the right units to be a probability density. The units of a probability density are $1/[volume]$, while Eq. (77) shows that $|\psi_0(r)|^2 = |\langle\vec{r}|\vec{k}\rangle|^2$ is clearly dimensionless. One possible way to give a probabilistic interpretation to $|\psi_0(\vec{r})|^2$ would be to assume a finite quantization volume V, so that the probability density would be defined as $\rho(\vec{r}) = |\psi_0(\vec{r})|^2\frac{1}{V}$, so that $\int_V d^3r\rho(\vec{r}) = 1$.

A plane wave corresponds to a uniform probability flow at speed $v = \hbar k/M$, so that the current density is $\vec{j}(\vec{r}) = \rho(\vec{r})\vec{v}(\vec{r})$, so that for a plane wave, $|j| = v/V$. The probability current through a surface (perpendicular to $\vec{k}$) of area A_0 is then given by

$$J = jA_0 = \frac{A_0}{V}\frac{\hbar k}{M} \equiv J_{in}. \tag{78}$$

In defining this as the incident current, we should interpret A_0 as the cross-sectional area of the incident particle 'beam'. The infinitesimal scattered current through an infinitesimal area element dA at distance

r_0 in the θ, ϕ direction is then given by

$$dJ(r_0, \theta, \phi) = \frac{|\psi_s(r, \theta, \phi)|^2}{V} v\, dA = \frac{|f(\theta, \phi|k)|^2}{r_0^2} \frac{1}{V} \frac{\hbar k}{m} dA. \tag{79}$$

With the surface area element begin given by $dA = r_0^2 d\Omega = r^2 \sin\theta d\theta d\phi$, this simplifies to

$$dJ_S(\theta, \phi) = \frac{|f(\theta, \phi|k)|^2}{V} \frac{\hbar k}{M} d\Omega \tag{80}$$

The scattered probability current into the solid angle region Ω_0 would then be given by

$$J_S(\Omega_0) = \int_{\Omega_0} dJ(\theta, \phi) = \frac{\hbar k}{MV} \int_{\Omega_0} d\Omega\, |f(\theta, \phi|k)|^2, \tag{81}$$

which shows that the scattering probabilities are independent of the choice of quantization volume, V. In analogy with the way we defined reflection and transmission probabilities in 1-d, the probability to scatter into solid angle Ω_0 would be the ratio $J_S(\Omega_0)/J_{in}$, giving

$$P_S(\Omega_0) = \frac{1}{A_0} \int_{\Omega_0} d\Omega |f(\theta, \phi|k)|^2. \tag{82}$$

That the scattering probability would decrease as the incident 'beam' area increases has the 'classical' interpretation that with a wider beam, one would be more likely to miss a target with a fixed cross-sectional area σ, assuming $A_0 \gg \sigma$. This leads to the total scattering probability

$$P_S = \frac{1}{A_0} \oint d\Omega\, |f(\theta, \phi|k)|^2, \tag{83}$$

where the integration is over the entire 4π solid angle. We note that only $|\psi_s\rangle$ contributes to the scatter. This is done deliberately to account for the finite cross-sectional area of the incident beam. For pure plane wave, there would be an interference between $|\psi_0\rangle$ and $|\psi_s\rangle$ at every point in space, but in reality, this interference only occurs inside the beam volume, whereas P_S calculated above applies only to a detector located outside of the beam volume.

We can define the effective cross-sectional area of the scatterer based on an analogy with classical scattering of particles from a simple solid-object. Consider a target of cross-sectional area σ, which we are trying to hit with particles that travel in a straight line along $\vec{e}_z$, but whose transverse position is random within the cross-sectional area A_0. The probability to hit the target is therefore the ratio of the two areas $P_{hit} = \sigma/A_0$. This leads us to define the effective cross-section of a generalized scatterer via

$$\sigma_{tot} = P_S \cdot A_0. \tag{84}$$

For quantum-mechanical scattering, this leads to

$$\sigma_{tot} = \oint d\Omega\, |f(\theta, \phi|k)|^2. \tag{85}$$

Likewise we can define the fraction of the effective cross-section due to scattering into a solid angle Ω_0 as

$$\sigma(\Omega_0) = P_S(\Omega_0) \cdot A_0 = \int_{\Omega_0} d\Omega |f(\theta, \phi|k)|^2. \tag{86}$$

Hence the infinitesimal element of the cross-sectional area due to scattering in the direction indicated by θ, ϕ must be

$$d\sigma(\theta, \phi) = d\Omega\, |f(\theta, \phi|k)|^2. \tag{87}$$

Based on this it is common to define the 'differential cross-section', denoted by $\frac{\partial\sigma}{\partial\Omega}$, according to

$$\frac{\partial\sigma}{\partial\Omega} \equiv \frac{d\sigma(\theta,\phi)}{d\Omega} = |f(\theta,\phi|k)|^2. \tag{88}$$

Thus the differential cross-section is the square modulus of the scattering amplitude. It may be helpful to think of "$\frac{d\sigma}{d\Omega}$" as simply a symbol, rather than as some sort of derivative.

A given detector located at angular position θ_d, ϕ_d, can be characterized by its solid-angle of acceptance Ω_d, as well as its detection efficiency $\mathcal{E}$ (i.e. the fraction of particles entering the detector which are actually detected), and its dark-count rate $\mathcal{D}$ (i.e. the probability that the detector fired but no particle actually entered the detector). If a particle is incident on the scatterer with momentum $\hbar\vec{k}$ and beam area A_0, the probability that the detector will fire is given by

$$\begin{aligned} P_{detect} &= \mathcal{E}P_S(\Omega_d) + \mathcal{D}(1 - P_S(\Omega_d)) \\ &= \mathcal{E} - \mathcal{D}\frac{\sigma_{tot}}{A_0} + \mathcal{D} \\ &= \frac{\mathcal{E} - \mathcal{D}}{A_0}\int_{\Omega_0} d\Omega \frac{d\sigma(\theta,\phi)}{d\Omega} + \mathcal{D}, \end{aligned} \tag{89}$$

. If the solid angle subtended by the detector is sufficiently small, than we can pull the differential cross-section outside of the integral, and evaluate it at the angular location of the detector, giving

$$P_{detect} = (\mathcal{E} - \mathcal{D})\Omega_d \frac{|f(\theta_d,\phi_d|k)|^2}{A_0} + \mathcal{D}. \tag{90}$$

2.3 Example: The Yukawa potential in the first Born-Approximation

The Yukawa potential is given by

$$V(r) = \frac{V_0}{r}\frac{e^{-\mu r}}{\mu}. \tag{91}$$

It is essentially a Coulomb potential with an exponential drop-off as $r \to \infty$. In the limit $\mu \to 0$ and $V_0 \to 0$ with V_0/μ held fixed, we recover the Coulomb potential. Consider a metallic conductor, on a coarse scale it is electrically neutral, since there are an equal number of electrons and protons. At short ranges the conduction electrons would see each other, as well as neighboring crystal ions, but at long range it really sees nothing, due to the overall neutrality. Thus if this range were known, the the electron-electron and electron-ion interactions could be replaced by Yukawa potentials, with the effective 'screening length', without changing the physics. The Yukawa potential has the advantage, relative to the Coulomb potential, that certain important classes of integrals then converge to finite numbers. It is often assumed that the pure Coulomb physics can be then obtained simply by taking the $\mu \to 0$ limit only at the very end of the calculation, i.e. after the integrals have converged to finite values.

In this example we will solve the problem of scattering from the Yukawa potential approximately, by keeping only the first-order term in the Born series. This means we replace $T = V + VGV + VGVGV + VGVGVGV + \ldots$ with $T \approx V$. This leads to

$$T(\vec{r}', \vec{r}'') \approx V(\vec{r}')\delta^3(\vec{r}' - \vec{r}''). \tag{92}$$

From Eq. (76) we see that this leads to

$$f(\vec{k}'|\vec{k}) = -\frac{M}{2\pi\hbar^2}\int d^3r'\, e^{i(\vec{k}-\vec{k}')\cdot\vec{r}'}V(\vec{r}'). \tag{93}$$

If we choose $\vec{e}'_z$ to lie along the $\vec{k}-\vec{k}'$ direction, then expanding $\vec{r}'$ in spherical coordinates gives

$$\begin{aligned} f(\vec{k}'|\vec{k}) &= -\frac{MV_0}{2\pi\hbar^2\mu}\int_0^{2\pi} d\phi' \int_0^{\pi} d\theta' \sin\theta' \int_0^{\infty} dr' r^2 e^{i|\vec{k}-\vec{k}'|r'\cos\theta'} \frac{e^{-\mu r'}}{r'} \\ &= -\frac{MV_0}{\hbar^2\mu}\int_{-1}^{1} du \int_0^{\infty} dr'\, r' e^{i|\vec{k}-\vec{k}'|ur'-\mu r'} \end{aligned} \tag{94}$$

Using

$$\int_{-1}^{1} du\, e^{iau} = \frac{2\sin a}{a} \tag{95}$$

gives

$$\begin{aligned} f(\vec{k}'|\vec{k}) &= -\frac{2MV_0}{\hbar^2|\vec{k}-\vec{k}'|}\int_0^{\infty} dr'\, r' \frac{\sin(|\vec{k}-\vec{k}'|r')}{r'} e^{-\mu r'} \\ &= -\frac{2MV_0}{\hbar^2\mu}\frac{1}{\mu^2+|\vec{k}-\vec{k}'|^2}. \end{aligned} \tag{96}$$

Since $|\vec{k}'| = |\vec{k}| = k$, we can write

$$\begin{aligned} |\vec{k}-\vec{k}'|^2 &= 2k^2 - 2k^2\cos\theta \\ &= 2k^2(1-\cos\theta), \end{aligned} \tag{97}$$

which gives

$$f(\theta,\phi|k) = -\frac{2MV_0}{\hbar^2\mu}\frac{1}{\mu^2+2k^2(1-\cos\theta)}. \tag{98}$$

This leads to the differential cross-section

$$\frac{d\sigma}{d\Omega} = \left(\frac{2MV_0}{\hbar^2\mu}\right)^2 \frac{1}{|\mu^2+2k^2(1-\cos\theta)|^2}, \tag{99}$$

which describes the angular distribution of the scattered probability.

If we let $\mu \to 0$ and $V_0 \to 0$, with

$$\frac{V_0}{\mu} = \frac{ZZ'e^2}{4\pi\epsilon_0} \tag{100}$$

we recover the Coulomb potential. This leads to the partial scattering amplitude

$$\frac{d\sigma}{d\Omega} = \left(\frac{2MZZ'e^2}{4\pi\epsilon_0\hbar^2}\right)^2 \frac{1}{4k^4(1-\cos\theta)^2}, \tag{101}$$

which famously recovers the classical Rutherford scattering. That the first-Born approximation would give the classical result is not surprising, since the first-Born result is valid in the high-energy limit, for which classical and quantum results typically agree.

Returning the the Yukawa potential, we can compute the total cross-section via

$$\sigma_{tot} = 2\pi\left(\frac{2MV_0}{\hbar^2\mu}\right)^2 \int_{-1}^{1} du \frac{1}{(\mu^2+2k^2-2k^2u)^2}. \tag{102}$$

With $y = \mu^2 + 2k^2 - 2k^2 u$, this becomes

$$\begin{aligned} \sigma_{tot} &= 2\pi \left(\frac{2MV_0}{\hbar^2 \mu} \right)^2 \int_{\mu^2}^{\mu^2+4k^2} dy \frac{1}{y^2} \\ &= \left(\frac{2MV_0}{\hbar^2 \mu} \right)^2 \frac{4\pi}{\mu^2(\mu^2+4k^2)}. \end{aligned} \tag{103}$$

For Coulomb scattering this gives $\sigma_{tot} = \infty$. This means all incident probability current will be scattered, no matter how large A_0 is. For this reason we say that the Coulomb interaction is an infinite range interaction. For finite μ, on the other hand, the Yukawa potential is effectively a finite range interaction.

3 Conservation of angular momentum

3.1 Scattering from spherically symmetric potentials

We now focus on the case where the scattering potential $V(\vec{r})$ is spherically symmetric. This is typical of two-body collisions in the absence of external fields. As we know, the main consequence of this symmetry is that angular momentum will be conserved. Quantum mechanically, this means that L^2 and L_z will be constants of motion. It is most convenient to chose the z-axis along along the incident wave propagation direction, so that $\vec{k} = k\vec{e}_z$ With this choice, the incident wave is azimuthally symmetric, and thus contains only $m = 0$ components. Due to the spherical symmetry, no $m \neq 0$ states can be created by the scatter, so that the complete scattering problem can be treated in the $m = 0$ subspace, which will simplify our calculations somewhat.

Up to now we have considered only the case where the incident (unperturbed) state is a plane wave, which is a state with well-defined kinetic energy. Because we are going to expand this state onto angular momentum eigenstates, it is interesting to consider first the angular momentum of a classical particle moving with constant velocity along the z-direction. The classical angular momentum is $\vec{L} = \vec{r} \times \vec{p}$, for the case $\vec{p} = \hbar k\vec{e}_z$, we find

$$\vec{L} = \det \begin{vmatrix} \vec{e}_x & \vec{e}_y & \vec{e}_z \\ x & y & z \\ 0 & 0 & \hbar k \end{vmatrix} = \hbar k(y\vec{e}_x - x\vec{e}_y). \tag{104}$$

Thus we see that classical the classical angular momentum vanishes only if $x = y = 0$, and otherwise, it can have arbitrarily large $|\vec{L}|$, depending on its x and y coordinates.

Quantum mechanically, x and y are delocalized, so based on the classical free-particle, we should expect to find that the incident plane wave will have a non-zero projection onto each ℓ state. Since the scatterer conserves ℓ and m, this means that the incoming and outgoing probability currents associated with each ℓ-value will be independently conserved. In this section, we will break the incident plane wave into its ℓ-components, and then solve the scattering problem separately within each ℓ-manifold. This will lead to the definition of the 'partial-wave' scattering amplitude, $f_\ell(k)$, associated with each angular momentum quantum number, ℓ.

3.2 Partial waves

Scattering Theory requires that $|\psi_0\rangle$ be an eigenstate of the free-space Hamiltonian:

$$H_0 = \frac{P^2}{2M} = \frac{p_r^2}{2M} + \frac{L^2}{2MR^2}. \tag{105}$$

The plane wave states , $|\vec{k}\rangle$, defined by $\vec{P}|\vec{k}\rangle = \hbar k|\vec{k}\rangle$, are simultaneous eigenstates of H_0, P_x, P_y and P_z, and are not eigenstates of L^2 or L_z. However, since $[H_0, L^2] = 0$ and $[H_0, L_z] = 0$ it follows that simultaneous eigenstates of H_0, L^2 and L_z must exist. We can label these states $|k, \ell, m^{(0)}\rangle$, and define them via

$$H_0|k,\ell,m^{(0)}\rangle = \frac{\hbar^2 k^2}{2M}|k,\ell,m^{(0)}\rangle \tag{106}$$

$$L^2|k,\ell,m^{(0)}\rangle = \hbar^2\ell(\ell+1)|k,\ell,m^{(0)}\rangle \tag{107}$$

$$L_z|k,\ell,m^{(0)}\rangle = \hbar m|k,\ell,m^{(0)}\rangle. \tag{108}$$

If we like, we can separate these states into a tensor-product of a radial state times an angular state, according to $|k,\ell,m^{(0)}\rangle = |k,\ell^{(0)}\rangle \otimes |\ell,m\rangle$, where $\langle r|k,\ell^{(0)}\rangle = R_\ell^{(0)}(r|k)$ and $\langle\theta,\phi|\ell,m\rangle = Y_\ell^m(\theta,\phi)$. Here the $Y_\ell^m(\theta,\phi)$ are the usual spherical harmonics. From the theory of central potentials, we know that the radial eigenfunctions, $R_\ell^{(0)}(r|k)$, satisfy the radial wave equation

$$\left[\frac{\hbar^2k^2}{2M} + \frac{\hbar^2}{2M}\frac{1}{r^2}\frac{\partial}{\partial r}r^2\frac{\partial}{\partial r} - \frac{\hbar^2\ell(\ell+1)}{2Mr^2}\right]R_\ell^{(0)}(r|k) = 0. \tag{109}$$

The solutions to this equation are well-known special functions called *spherical Bessel functions of the first kind*, denoted by $j_\ell(kr)$. Thus the free-particle angular momentum eigenstates, called 'partial waves' are given by

$$\langle r,\theta,\phi|k,\ell,m^{(0)}\rangle = \sqrt{\frac{2k^2}{\pi}}j_\ell(kr)Y_\ell^m(\theta,\phi), \tag{110}$$

which are normalized as

$$\int d^3r\,\left[\langle k,\ell,m^{(0)}|r,\theta,\phi\rangle\langle r,\theta,\phi|k',\ell',m'^{(0)}\rangle\right] = \delta(k-k')\delta_{\ell,\ell'}\delta_{m,m'}. \tag{111}$$

The projector onto the basis of partial waves is then

$$I = \sum_{\ell=0}^{\infty}\sum_{m=-\ell}^{\ell}\int_0^\infty dk\,|k,\ell,m^{(0)}\rangle\langle k,\ell,m^{(0)}|. \tag{112}$$

3.2.1 Threshold behavior

It is interesting to examine the behavior of these functions near the origin, i.e. inside the (finite) scattering region. Their behavior as $r \to 0$ is given by

$$\lim_{r\to 0} j_\ell(kr) = \frac{(kr)^\ell}{(2\ell+1)!}. \tag{113}$$

This means that as $k \to 0$, all the partial waves go rapidly to zero except for the $\ell = 0$ wave. For each ℓ, there is an energy scale below which the ℓ^{th} partial wave is effectively zero inside the scattering region. This means that the ℓ^{th} component of the incident wave no longer 'sees' the scatterer, and so its contrubution to the scattering cross-section is effectively zero. This effect is known as 'Threshold behavior'. This leads to the well known result that for most potentials, there will be a critical k-value, below which only S-wave scattering makes a significant contribution to the scattering amplitude, known as the S-wave regime.

3.3 The scattering phase-shift

The spherical Bessel functions, $j_\ell(kr)$, in addition to being solutions of the free particle radial wave equation, also satisfy the free-particle boundary condition at $r = 0$, which is derivable from the requirement that $\psi(\vec{r})$ should be everywhere continuous and smooth. If this boundary condition is relaxed, then there is a second linearly independent solutions, called the *spherical Bessel function of the second kind*, denoted as $y_\ell(kr)$, that are singular at $r = 0$. These spherical Bessel functions can be defined by the Rayleigh formulas,

$$j_\ell(\rho) = \rho^\ell \left(-\frac{1}{\rho}\frac{d}{d\rho}\right)^\ell \frac{\sin\rho}{\rho}, \tag{114}$$

$$y_\ell(\rho) = -\rho^\ell \left(-\frac{1}{\rho}\frac{d}{d\rho}\right)^\ell \frac{\cos\rho}{\rho}. \tag{115}$$

If we wish, instead, to find solutions with a well-defined direction of probability flow (inwards or outwards), we can use *spherical Bessel functions of the third kind*. The first of these two spherical Bessel functions is defined by

$$h_\ell(\rho) = j_\ell(\rho) + i y_\ell(\rho), \tag{116}$$

while the second linearly independent solutions is simply $h_\ell^*(\rho) = j_\ell(\rho) - i y_\ell(\rho)$. Rayleigh's formula for $h_\ell(kr)$ is

$$h_\ell(\rho) = -i\rho^\ell \left(-\frac{1}{\rho}\frac{d}{d\rho}\right)^\ell \frac{e^{i\rho}}{\rho}. \tag{117}$$

From the sign of the exponent, we see that $h_\ell(\rho)$ has a purely outgoing probability current, so that $h_\ell^*(\rho)$ has a purely incoming current. Thus $h_\ell(kr)$ and $h_\ell^*(kr)$ are the spherical 'running waves' whereas $j_\ell(kr)$ and $y_\ell(kr)$ are spherical 'standing waves'. The inverse relationships are

$$j_\ell(kr) = \frac{1}{2}\left[h_\ell(kr) + h_\ell^*(kr)\right], \tag{118}$$

and

$$y_\ell(kr) = \frac{1}{2i}\left[h_\ell(kr) - h_\ell^*(kr)\right]. \tag{119}$$

In the limit $r \to \infty$, the spherical Bessel functions have the asymptotic forms,

$$\lim_{r\to\infty} j_\ell(kr) = \frac{\sin(kr - \pi\ell/2)}{kr}, \tag{120}$$

$$\lim_{r\to\infty} y_\ell(kr) = -\frac{\cos(kr - \pi\ell/2)}{kr}, \tag{121}$$

$$\lim_{r\to\infty} h_\ell(kr) = -ie^{i(kr-\pi\ell/2)}. \tag{122}$$

If we like we can consider the case where, instead of a plane wave for $|\psi_0\rangle$, we have a pure incoming partial wave, having well defined energy, $E = \frac{\hbar^2 k^2}{2M}$, and angular momentum, so that $\psi_0(\vec{r}) = h_\ell^*(kr)Y_\ell(\theta)$. If we then let the ket $|k, \ell\rangle$ represent the full scattering solution, conservation of angular momentum requires it to have the limiting form

$$\lim_{r\to\infty} \langle r, \theta|k, \ell\rangle = a_\ell h_\ell^*(kr) + b_\ell(k) h_\ell(kr), \tag{123}$$

which says that the incoming and outgoing currents have the same angular momentum, ℓ. The incoming probability current will be proportional to $|a_\ell|^2$. Conservation of probability then requires that the incoming and outgoing current be equal, i.e. $|b_\ell| = |a_\ell|$. Thus a_ℓ and b_ℓ can differ only by a pure phase-factor. We can therefore choose the following form for the limiting behavior

$$\lim_{r\to\infty} \langle r, \theta | k, \ell \rangle = \frac{a_\ell}{i} \left(h_\ell^*(kr) + e^{i2\delta_\ell(k)} h_\ell(kr) \right). \tag{124}$$

where we have introduced the 'partial-wave scattering phase-shift', $\delta_\ell(k)$. If there is no scatterer, then we must recover the free-space result, $j_\ell(kr)$, so that $\delta_\ell(k) = 0$. **The effect of a scatter is then limited only to introducing a non-zero scattering phase-shift.**

By inserting the $r \to \infty$ limit for $h_\ell(r)$, via (122), we find that the limiting form of the full eigenfunction, including the effects of the scatterer, must then be

$$\lim_{r\to\infty} \psi(r, \theta) = a_\ell \left[\frac{e^{-i(kr - \pi\ell/2)}}{kr} - e^{i2\delta_\ell(k)} \frac{e^{i(kr-\pi\ell/2)}}{kr} \right] Y_\ell(\theta), \tag{125}$$

or equivalently,

$$\lim_{r\to\infty} \psi(r, \theta) = -2ia_\ell e^{i\delta_\ell(k)} \frac{\sin(kr - \pi\ell/2 + \delta_\ell(k))}{kr}, \tag{126}$$

The complete information about a scatterer, at least to the extent that can be obtained by measurements at $r \to \infty$, is therefore contained in the set of partial-wave phase-shifts, $\{\delta_0(k), \delta_1(k), \delta_2(k), \ldots\}$.

3.4 Relationship between the scattering amplitude and the scattering phase-shifts

We now return to our initial assumption of an incident plane-wave, $\psi_0(\vec{r}) = e^{ikz}$, rather than an incoming partial wave. The incident plane wave is given in spherical coordinates by

$$\langle r,\theta,\phi|\psi_0\rangle = e^{ikr\cos\theta}. \tag{127}$$

Because there is no ϕ-dependence, its expansion onto partial waves can contain only azimuthally-symmetric $m = 0$ states. It must still, however, be a superposition of different ℓ states, and due to angular momentum conservation, we know that a spherically symmetrjic scatterer will *not* mix states with different ℓ. It is not necessary to work through the details of how to compute the expansion coefficients, rather we just need the result

$$\begin{aligned}
\psi_0(\vec{r}) &= e^{ikr\cos\theta} \\
&= \sum_\ell \langle r,\theta,\phi|k,\ell,0^{(0)}\rangle \langle k,\ell,0|\psi_0\rangle \\
&= \sum_{\ell=0}^{\infty} i^\ell \sqrt{4\pi(2\ell+1)}\, j_\ell(kr) Y_\ell^0(\theta) \\
&= \sum_{\ell=0}^{\infty} \frac{i^\ell}{2}\sqrt{4\pi(2\ell+1)}\left(h_\ell^*(kr) + h_\ell(kr)\right),
\end{aligned} \tag{128}$$

which we see consists of equal contributions from incoming, $h_\ell^*(kr)$, and outgoing, $h_\ell(kr)$, waves. This is good, because probability conservation still applies if there is no scatterer, $V(r) = 0$, even for an incident plane-wave

We now turn to the eigenstates of the full-problem, $|\psi\rangle$, which must satisfy

$$[H_0 + V]\,|\psi\rangle = \frac{\hbar^2 k^2}{2M}|\psi\rangle. \tag{129}$$

As long as $V(\vec{R}) = V(R)$, the solutions still have eigenvalues k, and ℓ, hence we will again assign them the ket $|k\ell\rangle$. These eigenstates decompose into radial and angular parts, with the angular part given by a spherical harmonic, $\langle r,\theta,\phi|k,\ell,m\rangle = R_\ell(r|k)Y_\ell^m(\theta,\phi)$. The radial wave equation is now given by

$$\left[\frac{\hbar^2k^2}{2M} + \frac{\hbar^2}{2M}\frac{1}{r^2}\frac{\partial}{\partial r}r^2\frac{\partial}{\partial r} - \frac{\hbar^2\ell(\ell+1)}{2Mr^2} + V(r)\right]R_\ell(r|k) = 0. \tag{130}$$

From equation (124), we know already that, as a result of conservation laws, the solution must take the limiting form

$$\begin{aligned}
\lim_{r\to\infty} R_\ell(r|k) &= \frac{a_\ell(k)}{i}\left(h_\ell^*(kr) + e^{i2\delta_\ell(k)}h_\ell(kr)\right) \\
&= a_\ell\left(\frac{e^{-i(kr-\pi\ell/2)}}{kr} - e^{i2\delta_\ell(k)}\frac{e^{i(kr-\pi\ell/2)}}{kr}\right)
\end{aligned}$$

In the spherically-symmetric case, the scattering amplitude, $f(\theta,\phi|k)$, depends only on θ and k, and was defined via

$$\lim_{r\to\infty}\psi(\vec{r}) = e^{i\vec{k}\cdot\vec{r}} + f(\theta|k)\frac{e^{ikr}}{r}. \tag{131}$$

We can expand the incident plane-wave onto partial waves, giving

$$\lim_{r\to\infty}\psi(r)=\sum_{\ell=0}^{\infty}\frac{e^{i\pi\ell/2}}{2}\sqrt{4\pi(2\ell+1)}\left(h_\ell^*(kr)+h_\ell(kr)\right)Y_\ell^0(\theta)+f(\theta|k)\frac{e^{ikr}}{r}. \tag{132}$$

We can also expand the scattering amplitude onto spherical harmonics as

$$f(\theta|k)=\sum_{\ell=0}^{\infty}c_\ell(k)Y_\ell^0(\theta)=\sum_{\ell=0}^{\infty}\sqrt{4\pi(2\ell+1)}f_\ell(k)Y_\ell(\theta), \tag{133}$$

where $f_\ell(k)$ is the 'partial wave scattering amplitude'. In terms of $f(\theta|k)$, the partial amplitudes are given by

$$f_\ell(k)=\frac{1}{\sqrt{4\pi(2\ell+1)}}\int d\Omega Y_\ell^*(\theta)f(\theta|k). \tag{134}$$

This definition leads to the result

$$\lim_{r\to\infty}\psi(r,\theta)=\sum_{\ell=0}^{\infty}\sqrt{4\pi(2\ell+1)}\left[\frac{e^{i\pi\ell/2}}{2}(h_\ell^*(kr)+h_\ell(kr))+f_\ell(k)\frac{e^{ikr}}{r}\right]Y_\ell(\theta) \tag{135}$$

Replacing $h_\ell(kr)$ with its limiting form (122), then gives

$$\begin{aligned}\lim_{r\to\infty}\psi(r) &= \sum_{\ell=0}^{\infty}\sqrt{4\pi(2\ell+1)}\frac{i^{\ell+1}}{2}\left[\frac{e^{-i(kr-\pi\ell/2)}}{kr}-\frac{e^{i(kr-\pi\ell/2)}}{kr}-2ikf_\ell(k)\frac{e^{i(kr-\pi\ell/2)}}{r}\right]Y_\ell^0(\theta)\\ &= -\sum_{\ell=0}^{\infty}\sqrt{4\pi(2\ell+1)}\frac{(i)^\ell}{2}\left[\frac{e^{-i(kr-\pi\ell/2)}}{kr}-(1+2ikf_\ell(k))\frac{e^{i(kr-\pi\ell/2)}}{r}\right]Y_\ell^0(\theta).\end{aligned} \tag{136}$$

By comparison with (125) we then see that the relationship between the partial amplitude and the partial phase-shift is

$$1+2ikf_\ell(k)=e^{i2\delta_\ell(k)}. \tag{137}$$

Inverting this formula gives

$$f_\ell(k)=\frac{e^{i\delta_\ell(k)}\sin(\delta_\ell(k))}{k}. \tag{138}$$

Plugging this into (133) then gives the scattering amplitude in terms of the partial phase-shifts,

$$f(\theta|k)=\sum_{\ell=0}^{\infty}\sqrt{4\pi(2\ell+1)}\frac{e^{i\delta_\ell(k)}\sin(\delta_\ell(k))}{k}Y_\ell(\theta). \tag{139}$$

3.5 The partial-wave scattering cross-section

For spherically symmetric potentials, the total scattering cross-section (85) becomes

$$\sigma_{tot} = 2\pi \int_0^\pi d\theta \, \sin\theta \, |f(\theta|k)|^2. \tag{140}$$

Based on the result (139), this can be written in terms of the partial phase-shifts as

$$\begin{aligned}
\sigma_{tot} &= \frac{4\pi}{k^2} \sum_{\substack{\ell=0 \\ \ell'=0}}^{\infty} \sqrt{(2\ell+1)(2\ell'+1)} \sin(\delta_\ell(k)) \sin(\delta_{\ell'}(k)) e^{i(\delta_\ell - \delta_{\ell'})} \int d\Omega \, \sin\theta \, Y_\ell^*(\theta) Y_{\ell'}(\theta), \\
&= \frac{4\pi}{k^2} \sum_{\ell=0}^{\infty} (2\ell+1) \sin^2(\delta_\ell(k)),
\end{aligned}$$

where we have made use of the orthogonality relation for the spherical harmonics. From this expression, we can identify the ℓ^{th} partial cross-section as

$$\begin{aligned}
\sigma_\ell &= 4\pi(2\ell+1) \frac{\sin^2(\delta_\ell(k))}{k^2} \\
&= 4\pi(2\ell+1) |f_\ell(k)|^2.
\end{aligned}$$

The partial cross-section, σ_ℓ, gives the probability that that a plane wave with energy $\hbar^2 k^2/(2M)$, will scatter into a state with total angular momentum ℓ.

3.6 The Optical Theorem

The optical theorem states

$$\sigma_{tot} = \frac{4\pi}{k}\text{Im}\{f(\theta = 0|k)\}. \tag{141}$$

This is useful because it allows us to calculate the total cross-section, which contains contributions from scattering into all possible angles, by only evaluating the scattering amplitude at $\theta = 0$, which indicates the forward-scattering direction. Using the results we have derived so far, the proof of the optical theorem is straightforward. From Eq. (139) we find

$$f(\theta = 0|k) = \sum_{\ell=0}^{\infty} \sqrt{4\pi}\sqrt{2\ell+1}\,(\cos\delta_\ell(k) + i\sin\delta_\ell(k))\,\frac{\sin\delta_\ell(k)}{k}\mathrm{Y}_\ell^0(0). \tag{142}$$

Since

$$\mathrm{Y}_\ell^0(0) = \frac{\sqrt{2\ell+1}}{\sqrt{4\pi}}, \tag{143}$$

we see that

$$f(\theta = 0|k) = \sum_\ell (2\ell+1)\,(\cos\delta_\ell(k) + i\sin\delta_\ell(k))\,\frac{\sin\delta_\ell(k)}{k}, \tag{144}$$

so that

$$\text{Im}\{f(\theta = 0|k)\} = \frac{1}{k}\sum_\ell (2\ell+1)\sin^2\delta_\ell(k). \tag{145}$$

Comparing this with (141) we see that

$$\sigma_{tot} = \frac{4\pi}{k}\text{Im}\{f(\theta = 0|k)\}. \tag{146}$$

The reason this works, is because the probability to scatter is just the incident probability current minus the forward-scattering probability current, divided by the incident current. Since the incident current is presumably known, it is no surprise that the total cross section is directly related to the forward-scattering amplitude.

3.7 The s-wave scattering length

The s-wave scattering length iand effective range are defined by the equation

$$k\cot(\delta_0(k)) = -\frac{1}{a} + \frac{1}{2}r_e k^2 + \dots. \tag{147}$$

If we assume that $\delta_0(k)$ is a small angle, then this can be approximated by

$$\delta_0(k) = -ak\left(1 + \frac{1}{2}ar_e k^2 + \dots\right). \tag{148}$$

In the case where $r_e k \ll 1/(ak)$ we can make the approximation $\delta_0(k) \approx -ak$, which leads to $f_0(k) \approx e^{-i2ka}$ for the case $ak \ll 1$ this can be approximated to second order by

$$(1 + 2ikf_0(k)) = e^{i2\delta_0(k)} = \frac{e^{i\delta_0(k)}}{e^{-i\delta_0(k)}} \approx \frac{1 - iak}{1 + iak} + O((ak)^3). \tag{149}$$

For the zero-range pseudo-potential we found in HW7.5, that $T(\vec{r}, \vec{r}') = \frac{g\delta^3(\vec{r})\delta^3(\vec{r}')}{1+i\frac{Mg}{2\pi\hbar^2}k}\frac{\partial}{\partial r}r$. Applying Eq. (76) and taking $g = 2\pi\hbar^2 a/M$ gives for the pseudo-potential,

$$(1 + 2ikf_0(k)) = \frac{1 - iak}{1 + iak}. \tag{150}$$

Thus, under the condition that k is small enough to satisfy $ak \ll 1$ and $r_e k \ll 1/(ak)$, we can replace the true potential with the pseudo-potential

$$V(\vec{r}) = \frac{2\pi\hbar^2 a}{M}\delta^3(\vec{r})\frac{\partial}{\partial r}r, \tag{151}$$

and compute the scattering physics correctly to second order in k. In many cases, particularly with cold-atoms, this allows us to find analytic solutions to many-body problems which agree quantitatively with experiment. This shows that a is the parameter which governs low energy scattering, while r_e is the parameter which tells when the energy is low enough to be governed only by a.

3.8 Identical particles and scattering

If the spin-state of a pair of identical particles is known, then the symmetry of the wavefunction is fully determined by the requirement that Bosons have totally symmetric states and Fermions have totally antisymmetric states under exchange of particle labels. For a pair of Fermions with a symmetric (triplet for spin-1/2) spin state require an antisymmetric wavefunction $\psi(-r) = -\psi(r)$ where $r = r_1 - r_2$ is the relative coordinate. For a a pair of Fermions an in anti-symmetric (singlet for spin-1/2) state, a symmetric wavefunction is required. The situation is reversed for Bosons. The primary result from partial wave analysis is that the exchange transformation is $\theta \to \pi - \theta$ and $\phi \to \phi - \pi$., so that the exchange properties of the partial waves are governed strictly by the properties of the spherical harmonics $Y_\ell^0(\theta)$. For even ℓ, these spherical harmonics are symmetric, while for odd ℓ, they are antisymmetric under $\theta \to \pi - \theta$. This means that a totally symmetric wavefunction can be expanded onto $\ell = even$ partial waves only, while anti-symmmetric wavefunctions contain only odd ℓ components.

This means, e.g. that spin-polarized fermions are non-interacting as $k \to 0$. This is because each particle has the same spin direction, so the pair-wise spin-states must be symmetric. This requires anti-symmetric wavefunctions, which contain only $\ell = 1, 3, 5, \ldots$. Since at low enough k all waves other than $\ell = 0$ are 'frozen out' by the threshold behavior, and the S-wave amplitude is identically zero by symmetry, than there will be no scattering at all. As the energy is increased, the interaction will then initially consist only of P-wave scattering, which can be approximated using a P-wave pseudopotential if desired. Spin-polarized bosons, on the other hand, do interact at low k, but for small enough k, the interaction is governed only by the S-wave scattering length a. This approximation will break down only when the energy is high-enough to excite D-waves, since the P-wave amplitude is exactly zero due to exchange symmetry. This means that replacing the scattering potential by the S-wave pseudopotential can lead to highly accurate results at low energy.

3.9 Example: soft-sphere s-wave scattering

Now let us try to compute the s-wave phase-shift for a soft sphere scatterer, defined by

$$V(r) = V_0 u(R - r), \tag{152}$$

where $u(r)$ is the unit step function. The hard-sphere scatterer is recovered in the limit $V_0 \to \infty$. For s-waves, there can be no θ-dependence, so that the problem reduces to a one-dimensional problem. The easiest wave to proceed is then via the method of boundary conditions. This method is closely analogous to the methods used in 1-d scattering, and is likewise well suited for potentials made from combinations of spherical step-potentials, and spherical delta-shell potentials.

3.9.1 Ansatz for outermost region

The boundary condition at $r \to \infty$ is given by (124). Using the Rayleigh (117) formula to obtain the exact form of $h_0(k)$, gives

$$\lim_{r\to\infty} \psi_0(r) = \frac{e^{-ikr}}{kr} - e^{i2\delta_0(k)}\frac{e^{ikr}}{kr}. \tag{153}$$

Since this is an exact eigenstate of H_0, we should take it as the state for all $r > R$. Using the usual definition $R_\ell(r|k) = \frac{u(r)}{r}$, and dropping any overall constant factors, we let

$$u_I(r) = e^{-ikr} - e^{i2\delta_0(k)}e^{ikr}, \tag{154}$$

for $r > R$, which we can call region I.

3.10 Anzatz for innermost region

For region II, $r < R$, we also need a free-space s-wave state, but with $k \to K = \sqrt{k^2 - 2MV_0/\hbar^2}$. Thus we start with two arbitrary constants, by taking

$$u_{II}(r) = ae^{-ikr} - be^{ikr}. \tag{155}$$

The point $r = 0$ needs to be handled carefully. The primary requirement is the $\psi(\vec{r})$ must be smooth and continuous at $r = 0$. If we expand u in this region as

$$u(r) = u_0 + u_1 r + u_2 r^2 + \ldots, \tag{156}$$

then the requirement that $\psi(r) = \frac{u(r)}{r}$ be continuous is simply $u_0 = 0$, so that there is no $1/r$ singularity. The condition of smoothness is that $\frac{\partial}{\partial r}\psi(r) = 0$, which gives

$$\frac{\partial}{\partial r}\frac{u(r)}{r}\Big|_{r=0} = \left(\frac{u'(r)}{r} - \frac{u(r)}{r^2}\right)\Big|_{r=0} = 0. \tag{157}$$

Plugging in the series expansion gives

$$(u_1 r^{-1} + 2u_2 + 3u_3 r + \ldots)\Big|_{r=0} - (u_0 r^{-2} + u_1 r^{-1} + u_2 + u_3 r + \ldots)\Big|_{r=0} = 0. \tag{158}$$

With $u_0 = 0$ from continuity, and by eliminating terms which vanish for $r = 0$, this becomes

$$u_1 r^{-1} + 2u_2 - u_1 r^{-1} - u_2 = u_2 = 0. \tag{159}$$

In fact these conditions are always satisfied if a and b are chosen so that

$$u_{II}(r) = A\sin(Kr). \tag{160}$$

3.10.1 Boundary condition at interface

At the point $r = R$ we again require continuity and smoothness for $\psi(r)$. The continuity condition $\psi_I(R) = \psi_{II}(R)$ requires

$$u_I(R) = u_{II}(R), \tag{161}$$

or

$$A\sin(KR) = e^{-ikR} - e^{i2\delta_0(k)}e^{ikR} \tag{162}$$

Smoothness at $r = R$ requires $\frac{\partial}{\partial R}\psi_I(R) = \frac{\partial}{\partial R}\psi_I I(R)$ leads to

$$\frac{u_I'(R)}{R} - \frac{u_I(R)}{R^2} = \frac{u_{II}'(R)}{R} - \frac{u_{II}(R)}{R^2}. \tag{163}$$

Since we already have $u_I(R) = u_{II}(R)$, this just requires

$$u_I'(R) = u_{II}'(R), \tag{164}$$

which gives

$$AK\cos(KR) = -ik(e^{-ikR} + e^{i2\delta_0(k)}e^{ikR}). \tag{165}$$

We can clearly eliminate A just by dividing (162) by (165), giving

$$k\tan(KR) = iK\frac{e^{-ikR} - e^{i2\delta_0(k)}e^{ikR}}{e^{-ikR} + e^{i2\delta_0(k)}e^{ikR}}. \tag{166}$$

Multiplying through by $e^{-ikR} + e^{i2\delta_0(k)}e^{ikR}$ then gives

$$k\tan(KR)(e^{-ikR} + e^{i2\delta_0(k)}e^{ikR}) = iK(e^{-ikR} - e^{i2\delta_0(k)}e^{ikR}). \tag{167}$$

Solving for $e^{i2\delta_0(k)}$ gives

$$e^{i2\delta_0(k)} = \frac{K + ik\tan(KR)}{K - ik\tan(KR)}e^{-i2kR}. \tag{168}$$

Note that in general

$$\frac{z}{z^*} = \frac{re^{i\theta}}{re^{-i\theta}} = e^{i2\theta}, \tag{169}$$

where

$$\theta = \tan^{-1}\left(\frac{y}{x}\right). \tag{170}$$

this gives us

$$\delta_0(k) = -kR + \tan^{-1}\left(\frac{k\tan(KR)}{K}\right). \tag{171}$$

If we wish to, we can use Eq. (147), which states

$$k\cot(\delta_0(k)) = -\frac{1}{a} + \frac{1}{2}r_e k^2 + \ldots, \tag{172}$$

to determine the s-wave scattering length. Expanding $k\cot(\delta_0(k))$ in powers of k, with $K = \sqrt{k^2 - v^2}$, so that $v = \sqrt{2MV_0}/\hbar$, gives

$$k\cot(\delta_0(k)) = -\frac{v}{Rv - \tanh(Rv)} + \frac{1}{6}\left(3R - \frac{R^3v^2}{(Rv - \tanh(Rv))^2} + \frac{3}{v(Rv - \tanh(Rv))}\right)k^2 + \ldots. \tag{173}$$

From this we can see immediately that the scattering length is given by

$$a = R - \frac{1}{v}\tanh(Rv), \tag{174}$$

and the effective range is

$$r_e = \frac{1}{3}\left(3R - \frac{R^3v^2}{(Rv - \tanh(Rv))^2} + \frac{3}{v(Rv - \tanh(Rv))}\right). \tag{175}$$

It is good to see that we recover the hard sphere scattering length $a \to R$ and effective range $r_e \to 2R/3$ in the limit $v \to \infty$.