PartI

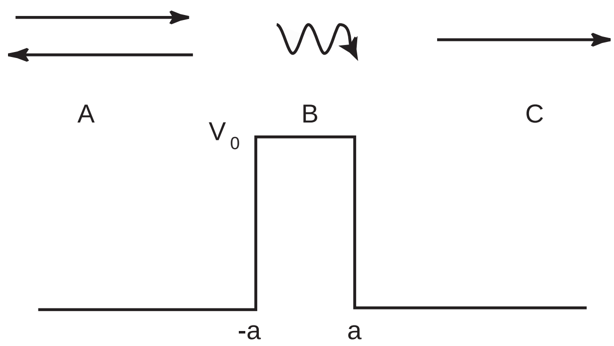
Scattering Theory

1 Scattering Theory in One Dimention

In this section, we present the basics of scattering theory as we demonstrate some examples of scattering in one-dimensional systems shown in the figure below, describing a left-moving incident particle on a potential barrier.

$$\begin{aligned} i\hbar \frac{\partial}{\partial t}\Psi(x,t) &= H\Psi(x,t) \\ H &= -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V(x) \end{aligned}$$

$$V(x) = \begin{cases} V_0 & x \in [-a,a] \\ 0 & \text{otherwise} \end{cases}$$



We assume that the time dependent variable in the wavefunction is separable (stationary state).

$$\begin{aligned} \Psi(x,t) &= e^{-i\omega t}\Psi(x) \\ H\Psi(x) &= E\Psi(x), \quad E = \hbar\omega \end{aligned}$$

1.1 Transfer Matrix Method

1.1.1 Transfer Matrix for Scattering State and Bound State

Let us divide the system shown in the figure above into three regions: A: $(-\infty, -a)$, B: $[-a, a]$, C: (a, ∞). For the solutions int the regions (r =A, B, C), we can write with the wave number k_r for which the potential is constant.

$$\Psi_r(x) = \xi^+ e^{ik_r x} + \xi^- e^{-ik_r x}, \quad \frac{\hbar^2 k_r^2}{2m} = E - V_r$$

We define the former wavefunction as Ψ_1 and the latter as Ψ_2, and the junction conditions for the wavefunction when $x = \xi$ can be $\Psi_1(\xi) = \Psi_2(\xi)$ and $\Psi_1'(\xi) = \Psi_2'(\xi)$, which we can further write down as:

$$\begin{aligned} \xi_1^+ e^{ik_1\xi} + \xi_1^- e^{-ik_1\xi} &= \xi_2^+ e^{ik_2\xi} + \xi_2^- e^{-ik_2\xi} \\ k_1(\xi_1^+ e^{ik_1\xi} - \xi_1^- e^{-ik_1\xi}) &= k_2(\xi_2^+ e^{ik_2\xi} - \xi_2^- e^{-ik_2\xi}) \end{aligned}$$

In matrix representation, we can write

$$\boldsymbol{M}_\xi(k_1) \begin{pmatrix} \xi_1^+ \\ \xi_1^- \end{pmatrix} = \boldsymbol{M}_\xi(k_2) \begin{pmatrix} \xi_2^+ \\ \xi_2^- \end{pmatrix}$$

$$\boldsymbol{M}_\xi(k) = \begin{pmatrix} e^{ik\xi} & e^{-ik\xi} \\ ke^{ik\xi} & ke^{-ik\xi} \end{pmatrix}, \quad \boldsymbol{M}_\xi^{-1}(k) = \begin{pmatrix} \frac{1}{2}e^{-ik\xi} & \frac{1}{2k}e^{-ik\xi} \\ \frac{1}{2}e^{ik\xi} & -\frac{1}{2k}e^{ik\xi} \end{pmatrix}$$

Thus, we rewrite the equations to give

$$\begin{pmatrix} \xi_1^+ \\ \xi_1^- \end{pmatrix} = \boldsymbol{T}_\xi(k_1, k_2) \begin{pmatrix} \xi_2^+ \\ \xi_2^- \end{pmatrix} \qquad \boldsymbol{T}_\xi(k_1, k_2) = \boldsymbol{M}_\xi^{-1}(k_1)\boldsymbol{M}_\xi(k_2)$$

We repeatedly use the above equation particularly in our present case to yield

$$\begin{pmatrix} \xi_A^+ \\ \xi_A^- \end{pmatrix} = \boldsymbol{T} \begin{pmatrix} \xi_C^+ \\ \xi_C^- \end{pmatrix}, \quad \boldsymbol{T} = \boldsymbol{T}_{-a}(k_{out}, k_{in})\boldsymbol{T}_a(k_{in}, k_{out})$$

Thus,

$$\frac{\hbar^2 k_{out}^2}{2m} = E, \quad \frac{\hbar^2 k_{in}^2}{2m} + V_0 = E$$

We can solve the scattering problems for more complicated scatterer in the same way we showed above. Let us now consider two different boundary conditions.

- Boundary condition I: $\Psi(x) \sim e^{ikx}, \quad x \to \infty$ Recall that an asymptotic form of the time-dependent wavefunction where $x \to +\infty$ is $e^{i(kx-\omega t)}$, so the waves (i.e., only the scattering waves) traveling toward the positive direction on x axis are what required in the limit $x \to +\infty$. Such states are called the scattering states, and require the conditions $\xi_C^- = 0, \ (\xi_C^+ = 1)$. The scattering states always exist whenever energy E is positive (E ¿ 0). For the reflection coefficient $\mathcal{R}$ and the transmission coefficient $\mathcal{T}$,

$$\begin{pmatrix} \xi_A^+ \\ \xi_A^- \end{pmatrix} = \boldsymbol{T} \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \begin{pmatrix} T_{11} \\ T_{21} \end{pmatrix}$$

giving ξ_A^+, $and \xi_A^-$ thus, we obtain

$$\begin{aligned} \mathcal{R} &= \frac{\xi_A^-}{\xi_A^+} = \frac{T_{21}}{T_{11}} \\ \mathcal{T} &= \frac{1}{\xi_A^+} = \frac{1}{T_{11}} \end{aligned}$$

.

(Note that the reflection rate is $|\mathcal{R}|^2$ and the transmission rate is $|\mathcal{T}|^2$.) Furthermore, there is a relation between the transmission coefficient and the reflection coefficient, which can be written

$$|\mathcal{T}|^2 + |\mathcal{R}|^2 = 1$$

We may generally explain the above relation by studying the Wronskians of the differential equation. Suppose we have the potential V that is real and whose solution is $\Psi(x)$ then, its complex conjugate $\Psi^*(x)$ can also be the solution. The Schroedinger equation does not contain the first-order derivatives; thereby Wronskians $W(x) = W(\Psi(x), \Psi^*(x))$ is independent of x.

[1] Asymptotically we can write

$$\psi(x) = e^{ikx} + \mathcal{R}e^{-ikx} \quad x \approx \mathcal{T}e^{ikx} \quad x \approx \infty$$

from which we evaluate the Wronskians to give $W() = W(\infty)$, revealing indeed that we have $|\mathcal{T}|^2 + |\mathcal{R}|^2 = 1$. As another way to express the above,

[1]Consider the solutions for the differential equation of $f(x)$

$$f'' + p(x)f' + q(x)f = 0$$

from which we write the Wronskians for the two solutions f_1 and f_2,

$$W(x) = W(f_1, f_2) = \det \begin{pmatrix} f_1 & f_2 \\ f_1' & f_2' \end{pmatrix}$$

Thus,

$$W' = \det \begin{pmatrix} f_1 & f_2 \\ f_1'' & f_2'' \end{pmatrix} = \det \begin{pmatrix} f_1 & f_2 \\ -pf_1' - qf_1 & -pf_2' - qf_2 \end{pmatrix} = -pW$$

which leads to

$$W(x) = W(y)e^{-\int_y^x dt p(t)}$$

we define the current J_x in x direction to have

$$\begin{aligned} J_x &= \frac{\hbar}{2mi} W(\psi^*, \psi) \\ &= \frac{\hbar}{2mi}\left(\psi^* \frac{d\psi}{dx} - \frac{d\psi^*}{dx}\psi\right) \end{aligned}$$

and write out the conservation law of J_x to be

$$\frac{dJ_x}{dx} = 0.$$

.

[2]

- Boundary condition II: To satisfy the condition $\int_{-\infty}^{\infty} |\Psi(x)| dx < +\infty$, we will need the pure imaginary wave number; i.e., the energy E is negative. ($E < 0$) Which we may write

$$k_{out} = i\kappa, \;\; \kappa = \frac{\sqrt{2m|E|}}{\hbar}$$

Furthermore, to avoid the exponential divergence of the wavefunction when we define k_{out}, we will need both $\xi_A^+ = 0$ and $\xi_C^- = 0$. So, we write

$$\begin{pmatrix} 0 \\ 1 \end{pmatrix} = \boldsymbol{T} \begin{pmatrix} \xi_C^+ \\ 0 \end{pmatrix}$$

whose first equation

$$T_{11} = 0$$

gives restriction to the wave number k. This is called the **bound state** in contrast with the scattering state. In our earlier discussion of the scattering

[2] Where $x \approx$,

$$\begin{aligned} W(-\infty) &= \det \begin{pmatrix} e^{ikx} + \mathcal{R}e^{-ikx} & e^{-ikx} + \mathcal{R}^* e^{ikx} \\ ike^{ikx} - ik\mathcal{R}e^{-ikx} & -ike^{-ikx} + ik\mathcal{R}^* e^{ikx} \end{pmatrix} \\ &= \det \begin{pmatrix} e^{ikx} + \mathcal{R}e^{-ikx} & e^{-ikx} + \mathcal{R}^* e^{ikx} \\ 2ike^{ikx} & 2ik\mathcal{R}^* e^{ikx} \end{pmatrix} = \det \begin{pmatrix} e^{ikx} + \mathcal{R}e^{-ikx} & (1 - |\mathcal{R}|^2)e^{-ikx} \\ 2ike^{ikx} & 0 \end{pmatrix} \\ &= 2ik(|\mathcal{R}|^2 - 1) \end{aligned}$$

, while at $x \approx \infty$ we have

$$\begin{aligned} W(\infty) &= \det \begin{pmatrix} \mathcal{T}e^{ikx} & \mathcal{T}^* e^{-ikx} \\ ik\mathcal{T}e^{ikx} & -ik\mathcal{T}^* e^{-ikx} \end{pmatrix} = \det \begin{pmatrix} \mathcal{T}e^{ikx} & \mathcal{T}^* e^{-ikx} \\ 0 & -2ik\mathcal{T}^* e^{-ikx} \end{pmatrix} \\ &= -2ik|\mathcal{T}|^2 \end{aligned}$$

states, we defined the transmission coefficient $\mathcal{T}$ and the reflection coefficient $\mathcal{R}$, from which we understand that the energy and the wave number in the bound states are defined as the

polars in the upper-half of the complex plane k of

the transmission and the reflection coefficient.

The Transfer-matrix Approach to the Scattering Problem in One-dimensional Square-well Potential

Here we discuss specific calculations for the scattering problem in a simple square-well potential. To begin with, we write the transfer matrix for a single boundary [3]

$$\boldsymbol{T}_\xi(k_1,k_2)=\frac{1}{2k_1}\begin{pmatrix}(k_1+k_2)e^{-i(k_1-k_2)\xi} & (k_1-k_2)e^{-i(k_1+k_2)\xi}\\ (k_1-k_2)e^{i(k_1+k_2)\xi} & (k_1+k_2)e^{i(k_1-k_2)\xi}\end{pmatrix}$$

$$\begin{aligned}
\boldsymbol{T} &= \boldsymbol{T}_{-a}(k_o,k_i)\boldsymbol{T}_a(k_i,k_o)\\
&= \frac{1}{4k_ik_o}\begin{pmatrix}(k_o+k_i)e^{i(k_o-k_i)a} & (k_o-k_i)e^{i(k_o+k_i)a}\\ (k_o-k_i)e^{-i(k_o+k_i)a} & (k_o+k_i)e^{-i(k_o-k_i)a}\end{pmatrix}\\
&\quad\times\begin{pmatrix}(k_i+k_o)e^{-i(k_i-k_o)a} & (k_i-k_o)e^{-i(k_i+k_o)a}\\ (k_i-k_o)e^{i(k_i+k_o)a} & (k_i+k_o)e^{i(k_i-k_o)a}\end{pmatrix}\\
T_{11} &= \frac{e^{i2k_oa}}{4k_ik_o}\left[(k_i+k_o)^2e^{-2ik_ia}-(k_i-k_o)^2e^{2ik_ia}\right]\\
T_{21} &= -\frac{1}{4k_ik_o}(k_i^2-k_o^2)(e^{-2ik_ia}-e^{2ik_ia})\\
T_{12} &= \frac{1}{4k_ik_o}(k_i^2-k_o^2)(e^{-2ik_ia}-e^{2ik_ia})\\
T_{22} &= \frac{e^{-i2k_oa}}{4k_ik_o}\left[(k_i+k_o)^2e^{2ik_ia}-(k_i-k_o)^2e^{-2ik_ia}\right]
\end{aligned}$$

Therefore, int the following case:

[3]

$$\begin{aligned}
\boldsymbol{T}_\xi(k_1,k_2) &= \boldsymbol{M}_\xi^{-1}(k_1)\boldsymbol{M}_\xi(k_2)\\
&= \frac{1}{2}\begin{pmatrix}e^{-ik_1\xi} & \frac{1}{k_1}e^{-ik_1\xi}\\ e^{ik_1\xi} & -\frac{1}{k_1}e^{ik_1\xi}\end{pmatrix}\begin{pmatrix}e^{ik_2\xi} & e^{-ik_2\xi}\\ k_2e^{ik_2\xi} & -k_2e^{-ik_2\xi}\end{pmatrix}\\
&= \frac{1}{2k_1}\begin{pmatrix}k_1e^{-ik_1\xi} & e^{-ik_1\xi}\\ k_1e^{ik_1\xi} & -e^{ik_1\xi}\end{pmatrix}\begin{pmatrix}e^{ik_2\xi} & e^{-ik_2\xi}\\ k_2e^{ik_2\xi} & -k_2e^{-ik_2\xi}\end{pmatrix}\\
&= \frac{1}{2k_1}\begin{pmatrix}(k_1+k_2)e^{-i(k_1-k_2)\xi} & (k_1-k_2)e^{-i(k_1+k_2)\xi}\\ (k_1-k_2)e^{i(k_1+k_2)\xi} & (k_1+k_2)e^{i(k_1-k_2)\xi}\end{pmatrix}
\end{aligned}$$

- Complete transmission

$$T_{21} = 0$$

that is where we have

$$\sin 2k_i a = \sin \frac{2a\sqrt{2m(E-V_0)}}{\hbar} = 0$$

there will be no reflection $\mathcal{R} = 0$ so, we will have a complete transmission $|\mathcal{T}| = 1$.

- Bound state

$Where E \leq 0$, that is $k_o = i\kappa$ (where κ is real, ($\frac{\hbar^2 k_o^2}{2m} = E$) We look for the solutions for

$$T_{11} = 0$$

, which we find the bound states when

$$\left(\frac{k_i + i\kappa}{k_i - i\kappa}\right)^2 = e^{i4k_i a}$$

- Tunneling

The classical particles cannot pass through a barrier where

$$E < V_0$$

, but if we calculate the transmission rate having considered

$$\begin{aligned} k_i &= i\kappa_i \\ \kappa_i &= \frac{\sqrt{2m(V_0 - E)}}{\hbar} \end{aligned}$$

generally we can obtain $|T| > 0$, meaning that the quantum effect allowed the particles to be passed through the barrier. This is called the tunneling effect. In the case where we have energy of the incident particles that is much smaller in contrast to the potential ($|k_o| << |k_i| = \kappa$) , we can write [4]

$$|\mathcal{T}|^2 \approx \frac{16k_o^2}{\kappa^2}\left(\frac{1}{1-e^{-4\kappa a}}\right)^2 e^{-4\kappa a}$$

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$$\begin{aligned} |T_{11}| &= \frac{\kappa}{4k_o}\left[\left(1+\frac{k_o}{i\kappa}\right)^2 e^{2\kappa a} - \left(1-\frac{k_o}{i\kappa}\right)^2 e^{-2\kappa a}\right] \\ &= \frac{\kappa}{4k_o}(e^{2\kappa a} - e^{-2\kappa a}) \\ |\mathcal{T}|^2 &= \frac{1}{|T_{11}|^2} = \frac{16k_o^2}{\kappa^2}\frac{1}{(1-e^{-4\kappa a})^2}e^{-4\kappa a} \end{aligned}$$

thus, lowers the transmission rate of the thickness of the potential barrier by remarkably high speed.

- Delta-function potential

  Where

$$V(x) = g\delta(x)$$

, [5] we consider the limit of

$$V_0 2a \to g, \quad (|V_0| \to \infty, \quad a \to 0)$$

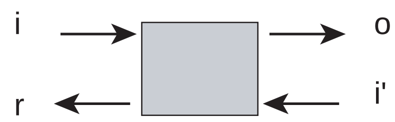
[6] (Note that $\frac{2m}{\hbar^2} g \equiv \tilde{g}$)we obtain

$$\begin{aligned} T_{11} &= 1 + i\frac{\tilde{g}}{2k_o}, \quad T_{21} = -i\frac{\tilde{g}}{2k_o}, \\ T_{22} &= 1 - i\frac{\tilde{g}}{2k_o}, \quad T_{12} = i\frac{\tilde{g}}{2k_o} \end{aligned}$$

Thus, giving

$$|\mathcal{T}|^2 = \frac{1}{1 + \left(\frac{\tilde{g}}{2k_o}\right)^2}, \quad |\mathcal{R}|^2 = \frac{\left(\frac{\tilde{g}}{2k_o}\right)^2}{1 + \left(\frac{\tilde{g}}{2k_o}\right)^2}$$

1.1.2 The Transfer Matrix and the Scattering Matrix



[5]

$$\begin{aligned} V_0 2a &\to g, \quad (|V_0| \to \infty, \quad a \to 0) \\ -k_i^2 2a &\to \frac{2m}{\hbar^2} g \equiv \tilde{g} \quad (-\frac{\hbar k_i^2}{2m} \to V_0) \\ |k_i| &\to \infty, \quad a \to 0, \quad (|k_i| a \to 0) \end{aligned}$$

[6]

$$\begin{aligned} T_{11} &= \frac{1}{4k_i k_o}\left((k_i + k_o)^2 - (k_i - k_o)^2 e^{i4k_i a}\right) \\ &\approx \frac{1}{4k_i k_o}\left(4k_i k_o - (k_i - 0)^2 i4k_i a\right) \\ &= 1 - i\frac{k_i^2 a}{k_o} = 1 + i\frac{\tilde{g}}{2k_o} \\ T_{21} &= -\frac{1}{4k_i k_o}(k_i^2 - 0)(-i4k_i a) \\ &= i\frac{k_i^2 a}{k_o} = -i\frac{\tilde{g}}{2k_o} \end{aligned}$$

Let us suppose the wavefunction with the incidence and reflection from free-space to an arbitrary region shows in the figure above. When we have the wavefunction of the left side $\psi_i e^{ikx} + \psi_r e^{-ikx}$ and the light side $\psi_o e^{ikx} + \psi_{i'} e^{-ikx}$, the consetvation of probability yields an equation. [7]

$$|\psi_i|^2 - |\psi_r|^2 = |\psi_o|^2 - |\psi_{i'}|^2$$

Now we define the one-dimensional scattering matrix S

$$\begin{pmatrix} \psi_r \\ \psi_o \end{pmatrix} = \boldsymbol{S} \begin{pmatrix} \psi_i \\ \psi_{i'} \end{pmatrix}$$

At which $\boldsymbol{S}$ becomes the unitary matrix
[8]

$$\boldsymbol{S}\boldsymbol{S}^\dagger = \boldsymbol{S}^\dagger \boldsymbol{S} = \boldsymbol{I}$$

We further define the transfer matrix $\boldsymbol{T}$ to obtain

$$\begin{pmatrix} \psi_o \\ \psi_{i'} \end{pmatrix} = \boldsymbol{T} \begin{pmatrix} \psi_i \\ \psi_r \end{pmatrix}$$

$$\boldsymbol{T}^\dagger \boldsymbol{J} \boldsymbol{T} = \boldsymbol{J}$$

$$\boldsymbol{J} = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

[9]

To provide more details, we define the scattering matrix $\boldsymbol{S}$ (including the multichannel cases)

$$\boldsymbol{S} = \begin{pmatrix} r & t' \\ t & r' \end{pmatrix}$$

[7] Calculation of the Wronskians.

[8] The conservation law

$$|\psi_r|^2 + |\psi_o|^2 = (\psi_r^*, \psi_o^*) \begin{pmatrix} \psi_r \\ \psi_o \end{pmatrix} = (\psi_i^*, \psi_{i'}^*) \boldsymbol{S}^\dagger \boldsymbol{S} \begin{pmatrix} \psi_i \\ \psi_{i'} \end{pmatrix} = (\psi_i^*, \psi_{i'}^*) \begin{pmatrix} \psi_i \\ \psi_{i'} \end{pmatrix}$$

is valid for arbitrary $\psi_i, \psi_{i'}$ thus, $\boldsymbol{S}^\dagger \boldsymbol{S} = \boldsymbol{I}$.

[9] The conservation law is written

$$|\psi_o|^2 - |\psi_{i'}|^2 = (\psi_o^*, \psi_{i'}^*) \boldsymbol{J} \begin{pmatrix} \psi_o \\ \psi_{i'} \end{pmatrix} = (\psi_i^*, \psi_r^*) \boldsymbol{T}^\dagger \boldsymbol{J} \boldsymbol{T} \begin{pmatrix} \psi_i \\ \psi_r \end{pmatrix} = (\psi_i^*, \psi_r^*) \boldsymbol{J} \begin{pmatrix} \psi_i \\ \psi_r \end{pmatrix}$$

,giving

$$\boldsymbol{T}^\dagger \boldsymbol{J} \boldsymbol{T} = \boldsymbol{J}$$

so that we can write

$$\boldsymbol{T} = \begin{pmatrix} t^{\dagger -1} & r' t'^{-1} \\ -t'^{-1} r & t'^{-1} \end{pmatrix}$$

[10] Here we can write

$$\begin{aligned} \boldsymbol{T}^{-1} =& \boldsymbol{J}\boldsymbol{T}^{\dagger}\boldsymbol{J} \\ (\boldsymbol{T}\boldsymbol{T}^{\dagger})^{-1} =& (\boldsymbol{T}^{-1})^{\dagger}\boldsymbol{T}^{-1} = \boldsymbol{J}\boldsymbol{T}\boldsymbol{T}^{\dagger}\boldsymbol{J} \end{aligned}$$

GIven that each pair becomes idential with the non-negative eigenvalues of $\boldsymbol{T}\boldsymbol{T}^{\dagger}$ and $(\boldsymbol{T}\boldsymbol{T}^{\dagger})^{-1}$, all eigenvalues can be written

$$e^{\pm 2x_n}, x_n \geq 0$$

[10]The unitarity can bu expressed in the relation equaitons

$$\boldsymbol{S}^{\dagger}\boldsymbol{S} = \begin{pmatrix} r^{\dagger} & t^{\dagger} \\ t'^{\dagger} & r'^{\dagger} \end{pmatrix} \begin{pmatrix} r & t' \\ t & r' \end{pmatrix} = \begin{pmatrix} r^{\dagger} r + t^{\dagger} t & r^{\dagger} t' + t^{\dagger} r' \\ t'^{\dagger} r + r'^{\dagger} t & t'^{\dagger} t' + r'^{\dagger} r' \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \quad (*1)$$

$$\boldsymbol{S}\boldsymbol{S}^{\dagger} = \begin{pmatrix} r & t' \\ t & r' \end{pmatrix} \begin{pmatrix} r^{\dagger} & t^{\dagger} \\ t'^{\dagger} & r'^{\dagger} \end{pmatrix} = \begin{pmatrix} r r^{\dagger} + t' t'^{\dagger} & r t^{\dagger} + t' r'^{\dagger} \\ t r^{\dagger} + r' t'^{\dagger} & t t^{\dagger} + r' r'^{\dagger} \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \quad (*2)$$

with the definition of the S matrix we obtain

$$\begin{aligned} \psi_r =& r\psi_i + t'\psi_{i'} \\ \psi_o =& t\psi_i + r'\psi_{i'} \end{aligned}$$

It is clear that if the boundary condition $\psi_{i'} = 0$ is required, t will represent the transmission rate, and$r$, the reflection rate. To obtain the transfer matrix through solving $\psi_o, \psi i'$, we rewrite the first equation

$$\psi_{i'} = - t'^{-1} r\psi_i + t'^{-1}\psi_r$$

and the second equation,

$$\psi_o = t\psi_i - r' t'^{-1} r\psi_i + r' t'^{-1}\psi_r = (t - r' t'^{-1} r)\psi_i + r' t'^{-1}\psi_r$$

The unitarity may give

$$\begin{aligned} 1 =& t t^{\dagger} + r' r'^{\dagger} = t t^{\dagger} + r'(t'^{-1} t') r'^{\dagger} = t t^{\dagger} + r' t'^{-1}(-r t^{\dagger}) \\ =& (t - r' t'^{-1} r) t^{\dagger} \end{aligned}$$

which leads to obtain

$$\psi_o = = t^{\dagger -1}\psi_i + r' t'^{-1}\psi_r$$

$$\begin{pmatrix} \psi_o \\ \psi_{i'} \end{pmatrix} = \begin{pmatrix} t^{\dagger -1} & r' t'^{-1} \\ -t'^{-1} r & t'^{-1} \end{pmatrix} \begin{pmatrix} \psi_i \\ \psi_r \end{pmatrix}$$

$$\boldsymbol{T} = \begin{pmatrix} t^{\dagger -1} & r' t'^{-1} \\ -t'^{-1} r & t'^{-1} \end{pmatrix}$$

The further calculations may yield [11]

$$\left(\boldsymbol{T}\boldsymbol{T}^\dagger + (\boldsymbol{T}\boldsymbol{T}^\dagger)^{-1} + 2\boldsymbol{I}\right)^{-1} = \frac{1}{4}\begin{pmatrix} tt^\dagger & \\ & t'^\dagger t' \end{pmatrix}$$

Thus, we know that $\frac{1}{\cosh x_n}$ may give the absolute eigenvalues for $t^\dagger t'$ and$t'^\dagger t'$. [12]

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$$\begin{aligned}
\boldsymbol{T}\boldsymbol{T}^\dagger =& \begin{pmatrix} t^{\dagger^{-1}} & r't'^{-1} \\ -t'^{-1}r & t'^{-1} \end{pmatrix}\begin{pmatrix} t^{-1} & -r^\dagger t'^{\dagger^{-1}} \\ t'^{\dagger^{-1}}r'^\dagger & t'^{\dagger^{-1}} \end{pmatrix} \\
=& \begin{pmatrix} t^{\dagger^{-1}}t^{-1} + r't'^{-1}t'^{\dagger^{-1}}r'^\dagger & -t^{\dagger^{-1}}r^\dagger t'^{\dagger^{-1}} + r't'^{-1}t'^{\dagger^{-1}} \\ -t'^{-1}rt^{-1} + t'^{-1}t'^{\dagger^{-1}}r'^\dagger & t'^{-1}rr^\dagger t'^{\dagger^{-1}} + t'^{-1}t'^{\dagger^{-1}} \end{pmatrix} \\
\boldsymbol{T}^{-1} =& \boldsymbol{J}\boldsymbol{T}^\dagger\boldsymbol{J} \\
(\boldsymbol{T}\boldsymbol{T}^\dagger)^{-1} =& (\boldsymbol{T}^{-1})^\dagger\boldsymbol{T}^{-1} = \boldsymbol{J}\boldsymbol{T}\boldsymbol{T}^\dagger\boldsymbol{J} \\
\boldsymbol{T}\boldsymbol{T}^\dagger + (\boldsymbol{T}\boldsymbol{T}^\dagger)^{-1} =& 2\begin{pmatrix} t^{\dagger^{-1}}t^{-1} + r't'^{-1}t'^{\dagger^{-1}}r'^\dagger & \\ & t'^{-1}rr^\dagger t'^{\dagger^{-1}} + t'^{-1}t'^{\dagger^{-1}} \end{pmatrix} \\
=& 2\begin{pmatrix} (tt^\dagger)^{-1} + r'(t'^\dagger t')^{-1}r'^\dagger & \\ & t'^{-1}rr^\dagger t'^{\dagger^{-1}} + (t'^\dagger t')^{-1} \end{pmatrix} \\
=& 2\begin{pmatrix} (tt^\dagger)^{-1} + r'(1 - r'^\dagger r')^{-1}r'^\dagger & \\ & t'^{-1}rr^\dagger t'^{\dagger^{-1}} + (t'^\dagger t')^{-1} \end{pmatrix} \\
=& 2\begin{pmatrix} ((tt^\dagger)^{-1} + (r'^{\dagger^{-1}}r'^{-1} - 1)^{-1} & \\ & t'^{-1}rr^\dagger t'^{\dagger^{-1}} + (t'^\dagger t')^{-1} \end{pmatrix} \\
\boldsymbol{T}\boldsymbol{T}^\dagger + (\boldsymbol{T}\boldsymbol{T}^\dagger)^{-1} + 2\boldsymbol{I} =& 2\begin{pmatrix} (tt^\dagger)^{-1} + r'^{\dagger^{-1}}r'^{-1}(r'^{\dagger^{-1}}r'^{-1} - 1)^{-1} & \\ & t'^{-1}(t't'^\dagger + rr^\dagger)t'^{\dagger^{-1}} + (t'^\dagger t')^{-1} \end{pmatrix} \\
=& 2\begin{pmatrix} (tt^\dagger)^{-1} + (1 - r'r'^\dagger)^{-1} & \\ & 2(t'^\dagger t')^{-1} \end{pmatrix} = 4\begin{pmatrix} (tt^\dagger)^{-1} & \\ & (t'^\dagger t')^{-1} \end{pmatrix}
\end{aligned}$$

given that

$$\left(\boldsymbol{T}\boldsymbol{T}^\dagger + (\boldsymbol{T}\boldsymbol{T}^\dagger)^{-1} + 2\boldsymbol{I}\right)^{-1} = \frac{1}{4}\begin{pmatrix} tt^\dagger & \\ & t'^\dagger t' \end{pmatrix}$$

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$$(2 + e^{2x_n} + e^{-2x_n})^{-1} = ((e^{x_n} + e^{-x_n})^{-1})^2 = \frac{1}{4\cosh x_n} \equiv \frac{1}{4}\begin{pmatrix} tt^\dagger & \\ & t'^\dagger t' \end{pmatrix}$$

1.2 The Green's Function and Scattering Integral Equations

Consider the Schrodinger equation in the form

$$\begin{aligned} (E - H_0(x))\Psi(x) &= V(x)\Psi(x) \\ H_0(x) &= -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} \end{aligned}$$

Suppose we obtained the Green function $G_0(\xi bylletting \delta(x)$ to be the Dirac delta function

$$(E - H_0(\xi))G_0(\xi) = \delta(\xi)$$

With homogeneous solution $\phi(x)$

$$(E - H_0(x))\Phi(x) = 0$$

we write the equation

$$\Psi(x) = \Phi(x) + \int_{-\infty}^{\infty} dy G_0(x-y)V(y)\Psi(y) \quad \text{(LS)}$$

[13] Next, we recast the equations above in the form, which clearly show the energy dependence instead of the x space coordinate dependence

$$\begin{aligned} (E - H_0)\Psi &= V\Psi, \\ (E - H_0)G_0(z) &= 1 \\ G_0(E) &= \frac{1}{E - H_0} \\ (E - H_0)\Phi &= 0 \\ \Psi &= \Phi + \frac{1}{E - H_0}V\Psi \\ &= \Phi + G_0 V\Psi \quad \text{(LS)} \end{aligned}$$

[13] We may simply check by making substitution into the Schrodinger equation

The last line of equation is called the Lippmann-Schwinger equation. [14] [15] [16]

[14]We consider that the inverse number of the operator $(z - H_0)$ uses the eigenstate $|\epsilon\rangle$ of the energy ϵ for H_0 to be defined as

$$G_0(z) = \sum_{\epsilon} \frac{1}{z-\epsilon} |\epsilon\rangle\langle\epsilon|$$

Generally, in contrast to the real energy of $z = E$, $G_0(z)$ cannot be defined for its unique property it has. We will instead have to use the limit $z \to E \pm i\delta$ at the end by calculating for the complex energy z. Throughout the proceeding sections, we need to note this as an important fact. The further details of the calculations can be found in the following.

[15]The relation between the formal solution and the coordinate representation can be considered as

$$\begin{aligned}
(z - H_0)G_0 =& 1 \\
\langle x|(z - H_0)G_0|x'\rangle =& \langle x|x'\rangle \\
\int dx'' \int dpdp' \, \langle x|p\rangle\langle p|(z - H_0)|p'\rangle\langle p'|x''\rangle\langle x''|G_0|x'\rangle =& \langle x|x'\rangle
\end{aligned}$$

On the one hand, $\langle x|x'\rangle = \delta(x - x')$ is the eigenfunction for the eigenvalue x' of the operator$\hat{x}$ such that we may treat it as $\hat{x}|x\rangle = x|x\rangle$.

$$\hat{x}\langle x|x'\rangle = \int dx'' \, x\langle x|x''\rangle\langle x''|x'\rangle = \int dx'' \, x\delta(x - x'')\delta(x'' - x') = x'\delta(x - x') = x'\langle x|x'\rangle$$

For $\langle x|p\rangle = \frac{1}{\sqrt{2\pi\hbar}} e^{ipx/\hbar}$ on the other hand, we may treat it as $\hat{p}|p\rangle = p|p\rangle$ because $\hat{p} = -i\hbar\partial_x$ is the eigenfunction of the eigenvalue p for the operator $\hat{p} = -i\hbar\partial_x$. Th completeness and the orthonormality are given

$$\begin{aligned}
\int dx'' \, \langle x|x''\rangle\langle x'|x''\rangle^* =& \int dx'' \, \delta(x - x'')\delta(x' - x'') = \delta(x' - x') \quad \textit{completeness} \\
\int dx \, \langle x|x'\rangle^*\langle x|x''\rangle =& \int dx \, \delta(x - x')\delta(x - x'') = \delta(x' - x'') \quad \textit{orthonormality} \\
\int dp \, \langle x|p\rangle\langle x'|p\rangle^* =& \frac{1}{2\pi\hbar} \int dp \, e^{ip(x-x')/\hbar} = \frac{1}{\hbar}\delta((x - x')/h) = \delta(x - x') \quad \textit{completeness} \\
\int dx \, \langle x|p\rangle^*\langle x|p'\rangle =& \frac{1}{2\pi\hbar} \int dx \, e^{-i(p-p')x)/\hbar} = \delta(p - p') \quad \textit{orthonormality}
\end{aligned}$$

Thus, we have $\langle x|G_0|x'\rangle = G_0(x, x')$ to write

$$\begin{aligned}
\langle p|(z - H_0)|p'\rangle =& \langle p|(z - \frac{\hat{p}^2}{2m})|p'\rangle = \delta(p - p'))(z - \frac{p^2}{2m}) \\
\int dx'' \int dpdp' \, \langle x|p\rangle\langle p|(z - H_0)|p'\rangle\langle p'|x''G_0(x'', x') =& \frac{1}{2\pi\hbar} \int dx'' \int dp \, e^{ip(x-x''}(z - \frac{p^2}{2m})G_0(x'', x') \\
=& \left(z + \frac{1}{2m}\frac{d^2}{dx^2}\right) \int dx'' \, \delta(x - x'')G_0(x'', x') = \left(z + \frac{1}{2m}\frac{d^2}{dx^2}\right) G_0(x, x')
\end{aligned}$$

Given by the translational symmetry, we have $G_0(x, x') = G_0(x - x')$

We can further write the variation of the Lippmann-Schwinger equation in the

---

[16]Let us summarize different types of normalization for the plane waves.

- L volume $V = L^3$ =boundary condition
  Let us define $\boldsymbol{k}_n = \frac{2\pi}{L}(n_x, n_y, n_z),\ n_i = 0, \pm 1, \pm 2, \cdots$ to write

$$\begin{aligned}
\langle \boldsymbol{r}|\boldsymbol{n}\rangle =& \psi_n(\boldsymbol{r}) = \frac{1}{\sqrt{V}} e^{i\boldsymbol{k}_n\cdot\boldsymbol{r}} \\
\langle n|n'\rangle =& \int_V d\boldsymbol{r}\, \psi_n^*(\boldsymbol{r})\psi_{n'}(\boldsymbol{r}) = \delta_{nn'} : \textit{normalization} \\
\sum_n \langle \boldsymbol{r}|n\rangle\langle n|\boldsymbol{r}'\rangle =& \sum_n \psi_n(\boldsymbol{r})\psi_n^*(\boldsymbol{r}') = \frac{1}{V}\sum_n e^{-i(\boldsymbol{k}_n - \boldsymbol{k}_{n'})\cdot\boldsymbol{r}} \\
=& \frac{1}{(2\pi)^3}(\frac{2\pi}{L})^3 \sum_n e^{-i(\boldsymbol{k}_n - \boldsymbol{k}_{n'})\cdot\boldsymbol{r}} = \frac{1}{(2\pi)^3}\int d\boldsymbol{k}\, e^{-i(\boldsymbol{k}_n - \boldsymbol{k}_{n'})\cdot\boldsymbol{r}} \\
=& \delta(\boldsymbol{r} - \boldsymbol{r}') = \langle \boldsymbol{r}|\boldsymbol{r}'\rangle \\
\sum_n |n\rangle\langle n| =& 1 : \textit{completeness}
\end{aligned}$$

- Take the continuum limit for the wave-number represetation

$$\begin{aligned}
\langle \boldsymbol{r}|\boldsymbol{k}\rangle =& \psi_k(\boldsymbol{r}) = \frac{1}{\sqrt{(2\pi)^3}} e^{i\boldsymbol{k}\cdot\boldsymbol{r}} \\
\textit{means}\ |\boldsymbol{k}\rangle =& \sqrt{\frac{V}{(2\pi)^3}}|\boldsymbol{n}\rangle \\
\langle \boldsymbol{k}|\boldsymbol{k}'\rangle =& \frac{1}{(2\pi)^3}\int d\boldsymbol{r}\, \psi_k^*(\boldsymbol{r})\psi_{k'}(\boldsymbol{r}) = \delta(\boldsymbol{k} - \boldsymbol{k}') : \textit{normalization} \\
\int d\boldsymbol{k}\, \langle \boldsymbol{r}|\boldsymbol{k}\rangle\langle \boldsymbol{k}|\boldsymbol{r}'\rangle =& \int d\boldsymbol{k}\, \psi_k(\boldsymbol{r})\psi_k^*(\boldsymbol{r}') = \frac{1}{(2\pi)^3}\sum_n e^{-i\boldsymbol{k}\cdot(\boldsymbol{r} - \boldsymbol{r}')} \\
=& \delta(\boldsymbol{r} - \boldsymbol{r}') = \langle \boldsymbol{r}|\boldsymbol{r}'\rangle \\
\int d\boldsymbol{k}\, |\boldsymbol{k}\rangle\langle \boldsymbol{k}| =& 1 : \textit{completeness}
\end{aligned}$$

- For the momentum representation

$$\begin{aligned}
\langle \boldsymbol{r}|\boldsymbol{p}\rangle =& \psi_p(\boldsymbol{r}) = \frac{1}{\sqrt{(2\pi\hbar)^3}} e^{i\boldsymbol{p}\cdot\boldsymbol{r}/\hbar} \\
\textit{Thatis},\ |\boldsymbol{p}\rangle =& \frac{1}{\sqrt{\hbar^3}}|\boldsymbol{k}\rangle = \sqrt{\frac{V}{(2\pi\hbar)^3}}|\boldsymbol{n}\rangle \\
\langle \boldsymbol{p}|\boldsymbol{p}'\rangle =& \frac{1}{(2\pi\hbar)^3}\int d\boldsymbol{r}\, \psi_p^*(\boldsymbol{r})\psi_{p'}(\boldsymbol{r}) = \delta(\boldsymbol{p} - \boldsymbol{p}') : \textit{normaliation} \\
\int d\boldsymbol{p}\, \langle \boldsymbol{r}|\boldsymbol{p}\rangle\langle \boldsymbol{p}|\boldsymbol{r}'\rangle =& \int d\boldsymbol{p}\, \psi_p(\boldsymbol{r})\psi_p^*(\boldsymbol{r}') = \frac{1}{(2\pi\hbar)^3}\sum_n e^{-i\boldsymbol{p}\cdot(\boldsymbol{r} - \boldsymbol{r}')/\hbar} \\
=& \delta(\boldsymbol{r} - \boldsymbol{r}') = \langle \boldsymbol{r}|\boldsymbol{r}'\rangle \\
\int d\boldsymbol{p}\, |\boldsymbol{p}\rangle\langle \boldsymbol{p}| =& 1 : \textit{completeness}
\end{aligned}$$

form

$$\begin{aligned}\Psi &= (1 - G_0 V)\Phi = (1 + GV)\Phi \\ G &= \frac{1}{E - H} \\ &= G_0 + G_0 V G = G_0 + G_0(VG_0) + G_0(VG_0)^2 + \cdots\end{aligned}$$

[17] Let us now consider more specified one-dimensional Green's function G_0 via

[17]Here we used the relation

$$\begin{aligned}A(B - A)B &= (AB - 1)B = A - B \\ &= -B(A - B)A = B(B - A)A\end{aligned}$$

The substitution of $A = E - H_0$,and $B = E - H_0 - V$ into the equation above gives

$$-G_0 V G = G_0 - G = -G V G_0$$

hence, we have $(1 - G_0 V)G = G_0$. That is

$$(1 - G_0 V) = G G_0 = (G_0 + G V G_0) G_0 = 1 + GV$$

We also obtain a useful reration

$$G = G_0 + G_0 V G = G_0 + G_0(VG_0) + G_0(VG_0)^2 + \cdots$$

Fourier analysis [18] [19] [20]

[18]Clariy the space coordinate to express

$$G_0(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dk e^{ikx} \hat{G}_0(k)$$

so, we can write $\delta(x) = \frac{1}{2\pi} \int dk e^{ikx}$ to give

$$E = \frac{\hbar^2 K^2}{2m}$$

which leads to $(E - H_0)G_0(x) = \delta(x)$ thus $\hat{G}_0(k) = \frac{1}{\sqrt{2\pi}} \left(\frac{2m}{\hbar^2}\right) \frac{1}{K^2 - k^2}$

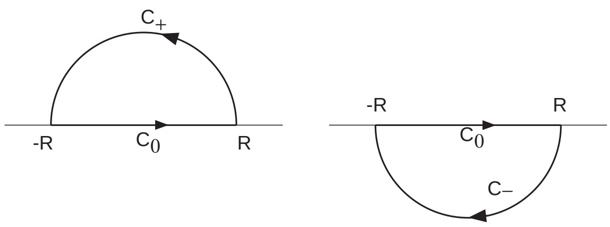
$$G_0(x) = \frac{1}{2\pi} \left(\frac{2m}{\hbar^2}\right) \int_{\infty} dk \frac{1}{K^2 - k^2} e^{ikx}$$

In the following, we consider E of the positive and ngative energies.

[19]Where $E \geq 0$, the integral remains indefinite for the unique characteristic observed along the real axis. We now consider expanding the energy E into the complex energy $E \to E \pm i0$. This in fact corresponds to having $K \to K \pm i0$ thus gives

$$\begin{aligned} G_0^{\pm}(x) &= \frac{1}{2\pi} \left(\frac{2m}{\hbar^2}\right) \int_{\infty} dk \frac{1}{2K} \left(\frac{1}{k + K \pm i0} - \frac{1}{k - K \mp i0}\right) e^{ikx} \\ &= \left(\frac{2m}{\hbar^2}\right) i \frac{1}{2K} \times \mp e^{\pm iKx} \quad (x > 0) \mp e^{\mp iKx} \quad (x < 0) \\ &= \left(\frac{2m}{\hbar^2}\right) \frac{\mp i}{2K} e^{\pm iK|x|} \end{aligned}$$

The evaluation of the integral is done via the complex integration along the paaths $C_0 + C_+$ or $C_0 + C_-$ shows in the figure below. Further, we proceed by use of the Jordan's lemma.



When $|f(z)|$ is uniformly 0 on the upper-half/lower-half plane at $|z| \to \infty$, we can write

$$\int_{C_\pm} dz f(z) e^{\pm iaz} \to 0, \quad (R \to \infty, a > 0)$$

[20]Where $E < 0$, we write

$$K = i\kappa = i\frac{\sqrt{2m|E|}}{\hbar}, \quad \kappa > 0$$

which we can use directly to evaluate the integral. Applying a clear case such as $K \to K + i0$ ($E \to$

$$G_0(E) = \begin{cases} \left(\frac{2m}{\hbar^2}\right)\frac{\mp i}{2K}e^{\pm iK|x|}, & K \to K \pm i0 = \frac{\sqrt{2mE}}{\hbar} \pm i0, \quad E \to E \pm i0, E > 0 \\ \left(\frac{2m}{\hbar^2}\right)\frac{-1}{2\kappa}e^{-\kappa|x|}, & \kappa = \frac{\sqrt{2m|E|}}{\hbar}, \qquad E < 0 \end{cases}$$

[21] Where the energy $E > 0$, the Green's function and its homogeneous solution take the traveling waves $\Phi(x) = \frac{1}{\sqrt{2\pi}}e^{ikx}$ of $+x$ direction. the substitution into the Lippmann-Schwinger equation may give

$$\Psi^{\pm}(x) = \frac{1}{\sqrt{2\pi}}e^{ikx} + \left(\frac{2m}{\hbar^2}\right)\frac{(\mp i)}{2k}\int_{-\infty}^{\infty} dyV(y)e^{\pm ik|x-y|}\Psi^{\pm}(y)$$

form which the solutions that satisfy the boundary condition I we discussed in the prior section can be clarilfied to be $\Psi^+(x)$. For this $\Psi^+(x)$ where $x << -a$, we can write

$$\begin{aligned} \Psi^+(x) \approx & \quad \frac{1}{\sqrt{2\pi}}\left(e^{ikx} + e^{-ikx}f(k,)\right) \\ f(k,) \quad = & \quad \left(\frac{2m}{\hbar^2}\right)\frac{-i\sqrt{2\pi}}{2k}\int_{-\infty}^{\infty} dyV(y)e^{iky}\Psi^+(y) \end{aligned}$$

While in $a << x$, we can write

$$\begin{aligned} \Psi^+(x) \approx & \quad \frac{1}{\sqrt{2\pi}}\left(e^{ikx}(1 + f(k,\infty)\right) \\ f(k,\infty) \quad = & \quad \left(\frac{2m}{\hbar^2}\right)\frac{-i\sqrt{2\pi}}{2k}\int_{-\infty}^{\infty} dyV(y)e^{-iky}\Psi^+(y) \end{aligned}$$

which giving the reflection coefficient ($\mathcal{R}$) and the transmission coefficient ($\mathcal{T}$) to be

$$\mathcal{R} = f(k,), \qquad \mathcal{T} = 1 + f(k,\infty)$$

. To obtain more specific form of the equation, we need a specific form of Ψ^+. The approximation of taking $\Psi^+(x) \approx \Phi(x)$ in the right term of the equation is called the Born approximation.

$E + i0$) may give

$$\begin{aligned} G_0^+(x) &= \left(\frac{2m}{\hbar^2}\right)\frac{-i}{2K}e^{iK|x|} \\ &= \left(\frac{2m}{\hbar^2}\right)\frac{-1}{2\kappa}e^{-\kappa|x|} \end{aligned}$$

[21]Note that this solution remains indefinite as we have the linear combination of the homogeneous solution $e^{\pm ikx}$. This indefinition rests on how to take the formal solution as we are discussing in the next section.

The Scattering Problems in One-dimentional Delta-function Potential via Integral Equation

Here we discuss how to solve the scattering problem in the delta-function potential $V(x) = g\delta(x)$ in detail. The scattering integral equation is written

$$\Psi(x) = \frac{1}{\sqrt{2\pi}} e^{ikx} + \left(\frac{2m}{\hbar^2}\right) \frac{(-i)}{2k} \int_{-\infty}^{\infty} dy V(y) e^{ik|x-y|} \Psi(y)$$

$$\Psi(x) = \frac{1}{\sqrt{2\pi}} e^{ikx} - i\tilde{g}\frac{1}{2k} e^{-ikx}\Psi(0), \quad x < 0 \frac{1}{\sqrt{2\pi}} e^{ikx} - i\tilde{g}\frac{1}{2k} e^{ikx}\Psi(0), \quad x > 0$$

Let us have $x = 0$ to give

$$\Psi(0) = \frac{1}{\sqrt{2\pi}} \frac{1}{1 + i\tilde{g}\frac{1}{2k}}$$

thus

$$\mathcal{T} = 1 - \frac{i}{2k}\tilde{g}\frac{1}{1 + i\tilde{g}\dfrac{1}{2k}} = \frac{1}{1 + \dfrac{i\tilde{g}}{2k}}, \qquad \mathcal{R} = -\frac{\dfrac{i\tilde{g}}{2k}}{1 + \dfrac{i\tilde{g}}{2k}}$$

1.3 Levinson's Theorem in One Dimension

Now we discuss the Levinson 's theorem, which relates to connecting the number of bound sates to the scattering states. We consider the solutions and the new boundary conditions for the Schroedinger equation

$$-\frac{\hbar^2}{2m}\frac{d^2 f_{\pm\infty}}{dx^2} + V(x) f_{\pm\infty} = E f_{\pm\infty} = \frac{\hbar^2 k^2}{2m} f_{\pm\infty}$$

- $f_{\infty}(k, x) \to e^{ikx}$, $x \to \infty$
- $f_{-\infty}(k, x) \to e^{-ikx}$, $x \to -\infty$

The integral equations for the solutions above can be obtained via taking the Green's function

$$\begin{aligned} G_{\infty} = G_1 &= -\frac{2m}{\hbar^2}\theta(x' - x)\frac{\sin k(x - x')}{k} \\ G_{-\infty} = G_2 &= \frac{2m}{\hbar^2}\theta(x - x')\frac{\sin k(x - x')}{k} \end{aligned}$$

22 23

[22]Let us consider another way to obtain the Green 's function. Generally, we consider the Green 's function in the second-order differential equation for $y = y(x)$

$$G''(x,x') + p(x)G'(x,x') + q(x)G(x,x') = \delta(x-x'),\ \text{' is the } x \text{ differentials}$$

Suppose we already obtained the independent homogeneous solutions $y_+(x)$, and $y_-(x)$ so we write

$$y_i'' + p(x)y_i' + q(x)y_i = 0, \quad i = +,-$$

Based on the variation of parameter we have

$$G = C_+y_+ + C_-y_-$$

whichleads to

$$G' = (C_+'y_+ + C_-'y_-) + (C_+y_+' + C_-y_-')$$

Now requires

$$(C_+'y_+ + C_-'y_-) = 0$$

which yields

$$G'' = (C_+y_+' + C_-y_-')' = (C_+'y_+' + C_-'y_-') + (C_+y_+'' + C_-y_-'')$$

so we can write

$$\begin{aligned} G'' + pG' + qG &= C_+(y_+'' + py_+' + qy_+) + C_-(y_-'' + py_-' + qy_-) \\ &\quad + C_+'y_+' + C_-'y_-' = C_+'y_+' + C_-'y_-' = \delta(x-x') \end{aligned}$$

which giving

$$\begin{aligned} \begin{pmatrix} y_+ & y_- \\ y_+' & y_-' \end{pmatrix} \begin{pmatrix} C_+' \\ C_-' \end{pmatrix} &= \begin{pmatrix} 0 \\ \delta(x-x') \end{pmatrix} \\ \begin{pmatrix} C_+' \\ C_-' \end{pmatrix} &= \frac{1}{W} \begin{pmatrix} y_-' & -y_- \\ -y_+' & y_+ \end{pmatrix} \begin{pmatrix} 0 \\ \delta(x-x') \end{pmatrix} = \frac{1}{W} \begin{pmatrix} -y_-\delta(x-x') \\ y_+\delta(x-x') \end{pmatrix} \end{aligned}$$

hence,

$$G(x,x') = \int_{b_-}^{x} dt \frac{-y_+(x)y_-(t)}{W(t)} \delta(t-x') + \int_{b_+}^{x} dt \frac{y_-(x)y_+(t)}{W(t)} \delta(t-x')$$

Note that b_+, and b_- may impose differnt boundary conditions for the integral constants.

[23]We consider some examples for such cases.

Where$b_- = b_+ = x' - 0$

$$G_2(x,x') = \theta(x-x') \frac{-y_+(x)y_-(x') + y_-(x)y_+(x')}{W(x')}$$

Where $b_- = b_+ = x' + 0$

$$G_1(x,x') = \theta(x'-x) \frac{y_+(x)y_-(x') - y_-(x)y_+(x')}{W(x')}$$

For these Green 's function written above, we add each formal solution to determine the integral equations

$$\begin{aligned} f_\infty(k,x) &= e^{+ikx} - \frac{2m}{\hbar^2}\frac{1}{k}\int_x^\infty dx' \, \sin k(x-x')V(x')f_\infty(k,x') \\ f_{-\infty}(k,x) &= e^{-ikx} + \frac{2m}{\hbar^2}\frac{1}{k}\int_{-\infty}^x dx' \, \sin k(x-x')V(x')f_{-\infty}(k,x') \end{aligned}$$

It is clear that each solution satisfies the boundary conditions.

We now regard the functions $f_{\pm\infty}(k,x)$ as functions of the complex number k to investigate the analyticity. First, given the integral equations we should have the complex number k where

$$\mathrm{Im}\, k > 0$$

which clearly indicates that there are the convergence conditions of the integrals for each term by successive approximation of $f_{\pm\infty}(k,x)$. In fact, the series itself is said to converge while $f_{\pm\infty}(k,x)$ beocmes the regular function of k on the complex plane k and on the upper-half plane.

We make evaluations for the Wronslians in $f_\infty(k,x)$, $f_\infty(-k,x)$, $f_{-\infty}(k,x)$ and $f_{-\infty}(-k,x)$ where $x \to \infty$,

$$\begin{aligned} W(f_\infty(k,x), f_\infty(-k,x)) &= -2ik \\ W(f_{-\infty}(k,x), f_{-\infty}(-k,x)) &= 2ik \end{aligned}$$

Where$b_- = \infty, \; b_+ = -\infty$

$$\begin{aligned} G(x,x') &= \int_x^\infty dt \frac{y_+(x)y_-(t)}{W(t)}\delta(t-x') + \int_{-\infty}^x dt \frac{by_-(x)y_+(t)}{W(t)}\delta(t-x') \\ &= \frac{y_+(\xi_<)y_-(\xi_>)}{W(x')} \\ \xi_> &= \max(x,x'), \quad \xi_< = \min(x,x') \end{aligned}$$

specially

$$\begin{aligned} (E-H_0)G_0 &= \frac{\hbar^2}{2m}(k^2 + \frac{d^2}{dx^2})G_0'' = \delta(x-x') \\ E = \frac{\hbar^2 k^2}{2m} \end{aligned}$$

as $y_\pm(x) = e^{i\pm x}$ $W(y_+,y_-) = \det \begin{pmatrix} e^{ikx} & e^{-ikx} \\ ike^{ikx} & -ike^{-ikx} \end{pmatrix} = -2ik$

- $$\frac{\hbar^2}{2m}G_2(x,x') = \theta(x-x')\frac{\sin k(x-x')}{k}$$
- $$\frac{\hbar^2}{2m}G_1(x,x') = -\theta(x'-x)\frac{\sin k(x-x')}{k}$$

Thus, the solutions are independent where $k \neq 0$. This allows us to expand the equations [24]

$$\begin{aligned} f_{-\infty}(k,x) &= c_{11}(k) f_{\infty}(k,x) + c_{12}(k) f_{\infty}(-k,x) \\ f_{\infty}(k,x) &= c_{21}(k) f_{-\infty}(-k,x) + c_{22}(k) f_{-\infty}(k,x) \end{aligned}$$

We now consider $x \to \pm\infty$ for tha latter equation above to write in the form

$$c_{21} e^{ikx} + c_{22} e^{-ikx} \quad (x \to -\infty), \qquad e^{ikx} \quad (x \to \infty)$$

These are the solutions that satisfy the boundary conditions for the scattering thus, the relation between the transmission coefficient and the reflection coefficient are expressed as

$$\begin{aligned} \mathcal{R} &= \frac{c_{22}}{c_{21}} \\ \mathcal{T} &= \frac{1}{c_{21}} = \frac{1}{T_{11}} : Referthetransfermatrix \end{aligned}$$

Here we consider the Wronskians for each form of $f_{\mp\infty}(k,x)$ and $f_{\pm\infty}(\pm k,x)$ to derive

$$\begin{aligned} c_{11}(k) &= -\frac{1}{2ik} W(f_{-\infty}(k,x), f_{\infty}(-k,x)) \\ c_{12}(k) &= \frac{1}{2ik} W(f_{-\infty}(k,x), f_{\infty}(k,x)) \\ c_{21}(k) &= -\frac{1}{2ik} W(f_{\infty}(k,x), f_{-\infty}(k,x)) \\ c_{22}(k) &= \frac{1}{2ik} W(f_{\infty}(k,x), f_{-\infty}(-k,x)) \end{aligned}$$

---

[24]b The successive substitution may give

$$\begin{aligned} f_{-\infty}(k) &= c_{11}(k)\big(c_{21}(k) f_{-\infty}(-k) + c_{22}(k) f_{-\infty}(k)\big) + c_{12}(k)\big(c_{21}(-k) f_{-\infty}(k) + c_{22}(-k) f_{-\infty}(-k)\big) \\ &= \big(c_{11}(k)c_{22}(k) + c_{12}(k)c_{21}(-k)\big) f_{-\infty}(k) + \big(c_{11}(k)c_{21}(k) + c_{12}(k)c_{22}(-k)\big) f_{-\infty}(-k) \end{aligned}$$

Where $k \neq 0$

$$c_{11}(k)c_{22}(k) + c_{12}(k)c_{21}(-k) = 1, \quad c_{11}(k)c_{21}(k) + c_{12}(k)c_{22}(-k) = 0$$

Likewise

$$\begin{aligned} f_{\infty}(k) &= c_{21}(k)\big(c_{11}(-k) f_{\infty}(-k) + c_{12}(-k) f_{\infty}(k)\big) + c_{22}(k)\big(c_{11}(k) f_{\infty}(k) + c_{12}(k) f_{\infty}(-k)\big) \\ &= \big(c_{12}(-k)c_{21}(k) + c_{11}(k)c_{22}(k)\big) f_{\infty}(k) + \big(c_{11}(-k)c_{21}(k) + c_{12}(k)c_{22}(k)\big) f_{\infty}(-k) \end{aligned}$$

thus,

$$c_{12}(-k)c_{21}(k) + c_{11}(k)c_{22}(k) = 1, \quad c_{11}(-k)c_{21}(k) + c_{12}(k)c_{22}(k) = 0$$

Especially the forms of $c_{21}(k)$, the equations are expressed in regular $f_{\pm\infty}(k, x)$ on the upper-half of the complex k plane, and the zero-point k_B on the upper-half of the plane gives the polar of $\mathcal{T}$; i.e., giving the bound states, because $c_{21}(k)$ is also a regular function.

We may also show some other facts for $c_{21}(k)$.

- Where $|k| \to \infty$,$c_{21}(k) = 1 + \mathcal{O}(\frac{1}{k})$

  In $|k| \to \infty$, where the incident energu is large enough, the effects by the potentials can be ignored, so that we understand from the transmission coefficient to take $\mathcal{T} \to 1$ or from the analyticity property.

- The zero-point $c_{21}(k)$ of k_B exists on the imaginary axis, not on th real axis. [25]

[25] It is clear from the discussion of the transfer matrix.

- All the zero-points k_B for $c_{21}(k)$ are in the first-order.Thus, $\dot{c}_{21}(k_B) \neq 0$. [26]

We can integrate $\frac{d}{dk}\log c_{21}(k)$ along the integral path C where the path is ormed by the real axis and the half circle on the upper-half plane. This integration may completely detached ($\frac{\dot{c}_{21}}{c_{21}} = \mathcal{O}(\frac{1}{k^2})$, $|k| \to \infty$ away from the half-circle. From the

[26] At the wave number k_B, in which the bound states are allowed to exist, $f_{\pm\infty}(k_B, x)$ become linearly dependent to each other.

$$\begin{aligned} c_{21}(k_B) &= 0, \quad c_{11}(k_B)c_{22}(k_B) = 1, \quad c_{11}(k_B) \neq 0, \quad c_{22}(k_B) \neq 0 \\ f_\infty(k_B, x) &= c_{22}(k_B) f_{-\infty}(k_B, x) \\ W(f_\infty(k_B, x), f_{-\infty}(k_B, x)) &= 0 \end{aligned}$$

k differentiation is written by $\dot{}$,

$$\begin{aligned} \dot{c}_{21}(k_B) &= -\frac{1}{2ik_B}\Big(W(\dot{f}_\infty(k_B, x), f_{-\infty}(k_B, x)) + W(f_\infty(k_B, x), \dot{f}_{-\infty}(k_B, x))\Big) \\ &= -\frac{1}{2ik_B}\left(\frac{1}{c_{22}} W(\dot{f}_\infty(k_B, x), f_\infty(k_B, x)) + c_{22} W(f_{-\infty}(k_B, x), \dot{f}_{-\infty}(k_B, x))\right) \end{aligned}$$

To evauate this we diffentiate the Schroedinger equation and equation above with respect to k. Which gives,

$$\begin{aligned} f'' + k^2 f &= \frac{2m}{\hbar^2} V f \\ \dot{f}'' + 2kf + k^2 \dot{f} &= \frac{2m}{\hbar^2} V \dot{f} \end{aligned}$$

With the potential terms being cancelled in the equation, we can rewrite

$$f''\dot{f} - \dot{f}'' f - 2kf^2 = \frac{d}{dx} W(\dot{f}, f) - 2kf^2 = 0$$

This above equation is used for f_∞ to give $\operatorname{Im} k > 0$ $\lim_{x\to\infty} f_\infty(k, x) = 0$ thus

$$W(\dot{f}_\infty, f_\infty) = -2k \int_x^\infty dx' \, [f_\infty(k, x')]^2$$

the same as $\operatorname{Im} k > 0$ のとき $\lim_{x\to-\infty} f_{-\infty}(k, x) = 0$

$$W(\dot{f}_{-\infty}, f_{-\infty}) = 2k \int_{-\infty}^x dx' \, [f_{-\infty}(k, x')]^2$$

hence,

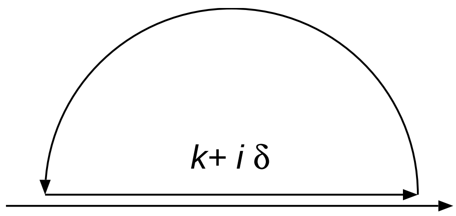
$$\begin{aligned} \dot{c}_{21}(k_B) &= -\frac{1}{2ik_B}\left(-\frac{1}{c_{22}(k_B)} 2k_B \int_x^\infty dx' \, [f_\infty(k_B, x')]^2 + c_{22}(k_B)(-2k_B) \int_{-\infty}^x dx' \, [f_{-\infty}(k_B, x')]^2\right) \\ &= -i \int_{-\infty}^\infty dx' [f_\infty(k_B, x') f_{-\infty}(k_B, x')] \\ &= -i c_{22}(k_B) \int_{-\infty}^\infty dx' [f_{-\infty}(k_B, x')]^2 = -i \frac{1}{c_{22}(k_B)} \int_{-\infty}^\infty dx' [f_\infty(k_B, x')]^2 \end{aligned}$$

Thus, $i\dot{c}_{21}(k_B)c_{22}(k_B)$ is not zero for $f_\infty(k_B, x)$.

argument principle, the number of zero-point N for c_{21} on the upper-half plane can be written

$$\begin{aligned} N &= \frac{1}{2\pi i}\int_C \frac{d}{dk}\log c_{21}(k) = \frac{1}{2\pi i}\log c_{21}(k+i0)\Big|_{k=-\infty}^{\infty} \\ &= \frac{1}{2\pi}\Big(\mathrm{Arg}\, c_{21}(-\infty+i0) - \mathrm{Arg}\, c_{21}(\infty+i0)\Big) \\ &= \frac{1}{2\pi}\Big(\mathrm{Arg}\, T_{11}(-\infty+i0) - \mathrm{Arg}\, T_{11}(\infty+i0)\Big) \\ &= -\frac{1}{2\pi}\Big(\mathrm{Arg}\, \mathcal{T}(-\infty+i0) - \mathrm{Arg}\, \mathcal{T}(\infty+i0)\Big) \end{aligned}$$

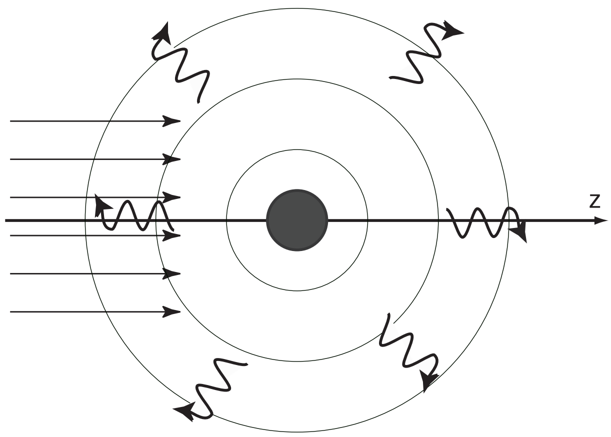
Note that the changes in argument are measured on the straight line in which the argument deviates infinitesimally on the real axis towards the upper-half plane.



The N represents the number of bound states. It is defined by the transmission coefficient $\mathcal{T}$ (more precisely, by what $\mathcal{T}$ is analytic continued to the complex k plane), which provides the scattering information. This is called the Levinson's theorem.

2 The Scattering Theory in Three Dimention

In this section, we discuss the scattering theory in three-dimension by following the methods especially using the integral equation that are introduced in our earlier discussions on one-dimensional scattering theory. More specifically, we consider a spherically-symmetric scatterer at periphery of origin, in which the plane waves incident in z-axis direction.



2.1 The Scattering Amplitude and the Differntial Cross Sections

In such case shown in the figure bove, the boundary condition for the stationary state be

$$\Psi(\vec{r}) \overset{\vec{r}\to\infty}{\longrightarrow} \frac{1}{(2\pi)^{3/2}}\left(e^{ikz} + \frac{f(\theta)}{r}e^{ikr}\right)$$

We can rewrite the above by using $mv = \hbar k\$, and\ \mathrm{V}_0 = (2\pi)^3$ [27] [28]

[27]We can understand from $\int_{-\pi}^{\pi} dx\ \int_{-\pi}^{\pi} dy\ \int_{-\pi}^{\pi} dz\ |\Psi|^2 = 1$ that $\Psi(\vec{r}) = \frac{1}{(2\pi)^{3/2}}e^{i\vec{k}\cdot\vec{r}}$ has a particle for every volume $v_0 = (2\pi)^3$.

[28]Given

$$\vec{\nabla} f = \frac{\partial f}{\partial r}\hat{r} + \frac{1}{r}\frac{\partial f}{\partial \theta}\hat{\theta} + \frac{1}{r\sin\theta}\frac{\partial f}{\partial \phi}\hat{\phi}$$

,

$$\begin{aligned}\Psi_s^*\vec{\nabla}\Psi_s &= \frac{1}{(2\pi)^3}\frac{f^*(\theta)}{r}e^{-ikr}\left(-\frac{f(\theta)}{r^2}e^{ikr}\hat{r} + \frac{f(\theta)}{r}e^{ikr}ik\hat{r} + \frac{1}{r}\frac{\partial f(\theta)}{\partial \theta}\frac{1}{r}e^{ikr}\hat{\theta}\right) \\ &= \frac{1}{(2\pi)^3}\frac{|f|^2}{r^2}ik\hat{r} + \mathcal{O}(\frac{1}{r^2})\end{aligned}$$

$$\begin{aligned}
\Psi_0 &= \frac{1}{(2\pi)^{3/2}} e^{ikz} \\
\vec{j}_0 &= \left(\frac{\hbar}{2mi}\right)\left(\Psi_0^* \vec{\nabla}\Psi_0 - (\vec{\nabla}\Psi_0^*)\Psi_0\right) = \frac{1}{(2\pi)^3}\frac{\hbar k}{m}\hat{z} = \frac{v}{V_0}\hat{z} \\
\Psi_s &= \frac{1}{(2\pi)^{3/2}}\frac{f(\theta)}{r} e^{ikr} \\
\vec{j}_s &= \left(\frac{\hbar}{2mi}\right)\left(\Psi_s^* \vec{\nabla}\Psi_s - (\vec{\nabla}\Psi_s^*)\Psi_s\right) = \frac{1}{(2\pi)^3}\frac{|f(\theta)|^2}{r^2}\frac{\hbar k}{m}\hat{r} + o(\frac{1}{r^2}) \approx \frac{v}{V_0}\frac{|f(\theta)|^2}{r^2}\hat{r}
\end{aligned}$$

The boundary condition at infinite distance away is the superposition of the plane waves and the spherical waves.

Let $f(\theta)$ be the scattering amplitude. We can write the differntial scattering cross section $\sigma(\theta)$ given the ratio between the incidene flux per unit area $\Phi_0 = \vec{j}_z \cdot \hat{z}$ snf the scattering flux $\Phi_s = \vec{j}_s \cdot d\vec{S}$ per surface element $d\vec{S} = r^2 d\vec{\Omega}$ $(d\vec{\Omega} = d\Omega\hat{r})$

$$\Phi_s = \sigma(\theta) d\Omega \cdot \Phi_0$$

This gives

$$\sigma(\theta) = |f(\theta)|^2$$

Now that we call $\sigma_T = \int d\Omega\sigma(\theta)$ a total scattering cross section.

Now we can express the equation of continuity for the waveunction $\Psi(\vec{r}, t)$, which is the solution for the time-dependent Schroedinger equation,

$$\begin{aligned}
\frac{\partial\rho(\vec{r},t)}{\partial t} + \vec{\nabla}\cdot\vec{j}(\vec{r},t) &= 0 \\
\rho(\vec{r},t) &= |\Psi(\vec{r},t)|^2 \\
\vec{j}(\vec{r},t) &= \frac{\hbar}{2mi}\left(\Psi^*(\vec{r},t)\vec{\nabla}\Psi(\vec{r},t) - h.c.\right)
\end{aligned}$$

[29] This gives the wavefunction for the stationary states, the main forcus of our discussion

$$\vec{\nabla}\cdot\vec{j}(\vec{r},t) = 0$$

[29] We use Schroedinger equation in the forms of time resolution $\partial_t N = \partial_t \int_V d\vec{r}|\Psi(\vec{r})|^2$ for the number of particles N in an arbitrary volume V and write

$$\begin{aligned}
\partial_t N &= \int d\vec{r}\left(\dot{\Psi}^*(\vec{r})\Psi(\vec{r}) + \Psi^*(\vec{r})\dot{\Psi}(\vec{r})\right) = \int_V d\vec{r}\frac{1}{i\hbar}\left(- H\Psi^*(\vec{r})\Psi(\vec{r}) + \Psi(\vec{r})H\Psi^*(\vec{r})\right) \\
&= -\left(\frac{\hbar}{2mi}\right)\int_V d\vec{r}\big(- (\nabla^2\Psi^*(\vec{r}))\Psi(\vec{r}) + \Psi^*(\vec{r})\nabla^2\Psi(\vec{r})\big) \\
&= -\left(\frac{\hbar}{2mi}\right)\int_{\partial V} d\vec{S}\big(- (\vec{\nabla}\Psi^*(\vec{r}))\Psi(\vec{r}) + \Psi^*(\vec{r})\vec{\nabla}\Psi(\vec{r})\big) = -\int_{\partial V} d\vec{S}\vec{j}(\vec{r}) \\
\vec{j}(\vec{r}) &= \left(\frac{\hbar}{2mi}\right)\left[\Psi^*(\vec{r})\vec{\nabla}\Psi(\vec{r}) - (\vec{\nabla}\Psi^*(\vec{r}))\Psi(\vec{r})\right]
\end{aligned}$$

which shows that $\vec{j}$ is the current operator so, given that the volume V is the arbitrary volume, Integrate the wquation above over a region bounded by a largy sphere S_R having a radius R with its center located origin. Applying the Gauss theorem to write [30]

---

the equation of continuity

$$\partial_t|\Psi(\vec{r})|^2 + \vec{\nabla}\cdot\vec{j} = 0$$

is obeyed. We can also obtain the above equation directly without using the arbitral characteristics of the volume.

[30]We consider a more unified expression for the behavior of spherical waves at infinite distant away via analytic continuation given the wavefunction in bound states. So, we can write

$$\begin{aligned}\Psi(\vec{r}) &\longrightarrow \frac{1}{(2\pi)^{3/2}}\left(e^{ikz} + \frac{f(\theta)}{r}e^{ik^+ r}\right)\\ k^+ &= k + i0 = k + i\epsilon\end{aligned}$$

We further suppose $R\epsilon >> 1$; i.e., we have the initial system of infinite large then, take the limit of $\epsilon \to 0$ at the end. Thus,

$$\begin{aligned}\Psi =& \frac{1}{(2\pi)^{3/2}}(e^{ikr\cos\theta} + \frac{f}{r}e^{ik^+ r})\\ V_0\Psi^*\boldsymbol{\nabla}\Psi\Big|_{r=R} =& (e^{-ikr\cos\theta} + \frac{f^*}{r}e^{-ik^- r})(ike^{ikr\cos\theta} + ik\frac{f}{r}e^{ik^+ r})\hat{\boldsymbol{r}}\Big|_{r=R} + \mathcal{O}(1/R^2)\\ =& \left(ik\cos\theta + ik\frac{f^*}{R}\cos\theta e^{iR(k\cos\theta - k^-)} + ik\frac{f}{R}e^{-iR(k\cos\theta - k^+)}\right)\hat{\boldsymbol{r}}\\ =& \left(ik\cos\theta + ik\frac{f^*}{R}\cos\theta e^{ikR(\cos\theta-1)-\epsilon R} + ik\frac{f}{R}e^{-ikR(\cos\theta-1)-\epsilon R}\right)\hat{\boldsymbol{r}}\\ V_0\Psi^*\boldsymbol{\nabla}\Psi\Big|_{r=R} - h.c. =& \left(2ik\cos\theta + ik\frac{f^*}{R}(1+\cos\theta)e^{ikR(\cos\theta-1)-\epsilon R} + ik\frac{f}{R}(1+\cos\theta)e^{-ikR(\cos\theta-1)-\epsilon R}\right)\hat{\boldsymbol{r}}\end{aligned}$$

In the following equations, the higher-prder terms are ignored $(1/R^2)$,and rewritten

$$\begin{aligned}0 =& \int_S d\vec{S}\cdot\vec{j}_\infty\\ =& \left(\frac{\hbar}{2mi}\right)\int_S dS\left(\Psi^*\frac{\partial\Psi}{\partial r} - h.c.\right)\\ =& \int_S d\vec{S}(\hat{z}\vec{j}_0 - \hat{z}\vec{j}_0) + \int d\Omega\left[R^2\cdot\frac{v}{V_0}\frac{|f(\theta)|^2}{R^2}\right] + \mathcal{O}\left(\frac{1}{R}\right)\\ &+ \left(\frac{\hbar}{2mi}\right)\int d\hat{\Omega}\,R^2\frac{1}{(2\pi)^3}\left(e^{-ikz}(ik)\frac{f(\theta)}{R}e^{ikR}\,\hat{r} + \frac{f^*(\theta)}{R}e^{-ikR}(ik)e^{ikz}\,\hat{z} - h.c.\right)\\ =& \frac{v}{V_0}\int d\Omega|f(\theta)|^2\\ &+ \left(\frac{i\hbar k}{2mi}\right)\int d\Omega\,R^2\frac{1}{(2\pi)^3}\left(e^{ikR(1-\cos\theta)}\frac{f(\theta)}{R} + \frac{f^*(\theta)}{R}e^{-ikR(1-\cos\theta)}\cos\theta\right.\\ &\qquad\left. + e^{-ikR(1-\cos\theta)}\frac{f^*(\theta)}{R} + \frac{f(\theta)}{R}e^{ikR(1-\cos\theta)}\cos\theta\right)\\ =& \frac{v}{V_0}\int d\Omega|f(\theta)|^2 + \frac{\hbar k}{2m}\frac{1}{(2\pi)^3}R\int d\Omega\,(1+\cos\theta)(f(\theta)e^{ikR(1-\cos\theta)} + f^*(\theta)e^{-ikR(1-\cos\theta)})\\ =& \frac{v}{V_0}\int d\Omega|f(\theta)|^2 + \frac{\hbar k}{2m}\frac{1}{(2\pi)^3}R2\cdot 2\pi\frac{1}{kR}i(f(0) - f^*(0)) + \text{const.}e^{\pm ikR}\end{aligned}$$

31 32

31

$$\begin{aligned}\int d\Omega\, e^{ikR(1-\cos\theta)} f(\theta) &= 2\pi f(0) \int_0^\pi d\theta \sin\theta e^{ikR(1-\cos\theta)} f(\theta) \to 2\pi f(0) \int_{-1}^1 dt\, e^{ikR(1-t)}, \quad kR \to \infty \\ &= 2\pi f(0) \frac{1}{-ikR} e^{ikR(1-t)} \Big|_{-1}^{1} = 2\pi f(0) \frac{i}{kR}(1 - e^{-2ikR}) \\ &= 2\pi \frac{1}{kR} i f(0) + \text{const.} e^{-2ikR} \\ \int d\Omega\, e^{-ikR(1-\cos\theta)} f^*(\theta) &= -2\pi \frac{1}{kR} i f^*(0) + \text{const.} e^{2ikR}\end{aligned}$$

32Our discussion in general can be

$$\begin{aligned}0 &= \int_S d\vec{S} \cdot \vec{j}_\infty \\ &= \left(\frac{\hbar}{2mi}\right) \int_S dS \left(\Psi^* \frac{\partial \Psi}{\partial r} - h.c.\right) \\ &= \int_S d\vec{S}(\hat{z}\vec{j}_0 - \hat{z}\vec{j}_0) + \int d\Omega \left[R^2 \cdot \frac{v}{V_0} \frac{|f(\theta)|^2}{R^2}\right] + \mathcal{O}\,(\frac{1}{R}) \\ &+ \left(\frac{\hbar}{2mi}\right) \int d\hat{\Omega}\, R^2 \frac{1}{(2\pi)^3} \left(e^{-ikz}(ik) \frac{f(\theta)}{R} e^{ikR}\, \hat{r} + \frac{f^*(\theta)}{R} e^{-ikR}(ik) e^{ikz}\, \hat{z} - h.c.\right) \\ &= \frac{v}{V_0} \int d\Omega |f(\theta)|^2 \\ &+ \left(\frac{i\hbar k}{2mi}\right) \int d\Omega\, R^2 \frac{1}{(2\pi)^3} \left(e^{ikR(1-\cos\theta)} \frac{f(\theta)}{R} + \frac{f^*(\theta)}{R} e^{-ikR(1-\cos\theta)} \cos\theta \right. \\ &\qquad \left. + e^{-ikR(1-\cos\theta)} \frac{f^*(\theta)}{R} + \frac{f(\theta)}{R} e^{ikR(1-\cos\theta)} \cos\theta \right) \\ &= \frac{v}{V_0} \int d\Omega |f(\theta)|^2 + \frac{\hbar k}{2m} \frac{1}{(2\pi)^3} R \int d\Omega\, (1 + \cos\theta)(f(\theta) e^{ikR(1-\cos\theta)} + f^*(\theta) e^{-ikR(1-\cos\theta)}) \\ &= \frac{v}{V_0} \int d\Omega |f(\theta)|^2 + \frac{\hbar k}{2m} \frac{1}{(2\pi)^3} R 2 \cdot 2\pi \frac{1}{kR} i(f(0) - f^*(0)) + \text{const.} e^{\pm ikR}\end{aligned}$$

We can take average of the above at infinitesimal region of R, which we can leave out the last term. Thus,

$$0 = \frac{v}{V_0} \int d\Omega |f(\theta)|^2 + \frac{v}{V_0} \frac{4\pi}{k} (-) \text{Im}\, f(0)$$

$$
\begin{aligned}
\vec{j}_\infty &= \left(\frac{\hbar}{2mi}\right)\left(\Psi^*\frac{\partial\Psi}{\partial r} - h.c.\right) \\
0 &= \int_S d\vec{S}\cdot\vec{j}_\infty \\
&= \left(\frac{\hbar}{2mi}\right)\int_S dS\left(\Psi^*\frac{\partial\Psi}{\partial r} - h.c.\right) \\
&= \int_S d\vec{S}(\hat{z}\vec{j}_0 - \hat{z}\vec{j}_0) + \int d\Omega\left[R^2\cdot\frac{v}{V_0}\frac{|f(\theta)|^2}{R^2}\right] + \mathcal{O}\ (\frac{1}{R}) \\
&+ \left(\frac{\hbar}{2mi}\right)\int d\hat{\Omega}\, R^2\frac{1}{(2\pi)^3}\left(e^{-ikz}(ik)\frac{f(\theta)}{R}e^{ikR}\,\hat{r} + \frac{f^*(\theta)}{R}e^{-ikR}(ik)e^{ikz}\,\hat{z} - h.c.\right)
\end{aligned}
$$

We average the above by the infinitesimal area on R to obtain

$$
\text{Im } f(0) = \frac{k}{4\pi}\int d\Omega|f(\theta)|^2 = \frac{k}{4\pi}\sigma_T
$$

Such relation between the forward scattering amplitude and the total cross section of the scatterer is called the optical theorem.

2.2 Lippmann-Schwinger Equation and the scattering Amplitude

We now consider determining the scattering amplitude via the integral equation derived from the Lippmann-Schwinger equation, which we discussed in our previous section. To begin with, we difine the Green's function $G_0(\vec{r}) = G_0^{\pm}(\vec{r}, E)$ of the three-dimentional free-particle system as the solution of the equation

$$
\begin{aligned}
(E - H_0(\vec{r}))G_0(\vec{r}) &= \delta(\vec{r}) \\
H_0(x) &= -\frac{\hbar^2\nabla^2}{2m}
\end{aligned}
$$

Specific forms of the equation above can be obtained by using the Fourier analysis in the same way we did to obtain the specific equation form in our previous section. [33]

$$
G_0(E) = \begin{cases}
G_0^{\pm}(\vec{r}) = & -\left(\frac{2m}{\hbar^2}\right)\frac{1}{4\pi}\frac{e^{\pm iKr}}{r}, \quad K \to K \pm i0 = \frac{\sqrt{2mE}}{\hbar} \pm i0, \quad E \to E \pm i0, E > 0 \\
G_0^{+}(\vec{r}, K \leftarrow i\kappa) = & -\left(\frac{2m}{\hbar^2}\right)\frac{1}{4\pi}\frac{e^{-\kappa r}}{r}, \qquad \kappa = \frac{\sqrt{2m|E|}}{\hbar}, \qquad E < 0
\end{cases}
$$

[33] On the one hand where $E \geq 0$, we may write

$$
E \pm i0 = \frac{\hbar^2 K_\pm^2}{2m}, \quad G_0^{\pm}(x) = \frac{1}{(2\pi)^{3/2}}\int d^3k\hat{G}_0^{\pm}(\vec{k})e^{i\vec{k}\cdot\vec{r}}
$$

In out present case, we consider the scattering states where $E > 0$, and having the plane wave of $\Phi(\vec{r}) = \frac{1}{(2\pi)^{3/2}} e^{ikz}$ traveling in z-axis direction as homogeneous solution to express the Lippmann-Schwinger integral equation

$$\Psi^{\pm} = \Phi + \frac{1}{E \pm i0 - H_0} V \Psi^{\pm}$$

In more specifin form we can write

$$\Psi^{\pm}(\vec{r}) = \frac{1}{(2\pi)^{3/2}} e^{ikz} - \left(\frac{2m}{\hbar^2}\right) \frac{1}{4\pi} \int d\vec{r}' \frac{e^{\pm ik|r-r'|}}{|\vec{r} - \vec{r}'|} V(\vec{r}') \Psi^{\pm}(\vec{r}')$$

Here we suppose there is the scatterer of a finite size ($V(\vec{r}) \approx 0, r >> a$). We consider the wavefunction at a point, a sufficient distance away from the scatterer.

The equation we initially defined and $\delta(\vec{r}) = \frac{1}{(2\pi)^3} \int d^3k e^{i\vec{k}\cdot\vec{r}}$ yields $\hat{G}_0^{\pm}(\vec{k}) = \left(\frac{2m}{\hbar^2}\right) \frac{1}{(2\pi)^{3/2}} \frac{1}{K^2 - k^2}$ so, we cn write

$$G_0^{\pm}(\vec{r}) = \frac{1}{(2\pi)^3} \left(\frac{2m}{\hbar^2}\right) \int d^3k \frac{1}{K^2 - k^2} e^{i\vec{k}\cdot\vec{r}}$$

This integral is evaluated in the polar coordinated (z-axis in $\vec{r}$ direction) such that

$$\int d^3k \frac{1}{K_{\pm}^2 - k^2} e^{i\vec{k}\cdot\vec{r}} = \int_0^{\infty} dk k^2 \frac{1}{K_{\pm}^2 - k^2} (2\pi) \int_0^{\pi} d\theta \sin\theta e^{ikr\cos\theta}$$

$$= \frac{\pi}{i} \frac{1}{r} \int_{\infty dk \frac{k}{K_{\pm}^2 - k^2}(e^{ikr} - e^{-ikr}) = \frac{\pi}{i}\frac{1}{r} 2 \int_{\infty} dk \frac{-k}{K_{\pm}^2 - k^2} e^{ikr}}$$

$$= \frac{\pi}{i} \frac{1}{r} \int_{-\infty}^{\infty} dk \left(\frac{1}{k + K \pm i0} + \frac{1}{k - K \mp i0}\right)(-e^{ikr}) = \frac{\pi^2}{r}(-2)e^{\pm iKr}$$

Thus,

$$G_0^{\pm}(\vec{r}) = -\left(\frac{2m}{\hbar^2}\right) \frac{1}{4\pi} \frac{e^{\pm iKr}}{r}$$

On the other where $E < 0$, same way we handled the one-dimensional systems, we write

$$K = i\kappa = i\frac{\sqrt{2m|E|}}{\hbar}, \quad \kappa > 0$$

In this case, we may directly evaluate the integral, in which we can apply $K \to K + i0$ ($E \to E + i0$) . Thus,

$$G_0(\vec{r}) = -\left(\frac{2m}{\hbar^2}\right) \frac{1}{4\pi} \frac{e^{-\kappa r}}{r}$$

Having $r >> a \;\; r' \approx a$, we can write [34]

$$\begin{aligned} |\vec{r}-\vec{r}'| &= r - \hat{r}\cdot\vec{r}' + \mathcal{O}(\left(\frac{a}{r}\right)) \\ \frac{a}{|\vec{r}-\vec{r}'|} &= \frac{a}{r} + \mathcal{O}(\left(\frac{a}{r}\right)^2) \end{aligned}$$

which giving

$$\Psi^{\pm}(\vec{r}) = \frac{1}{(2\pi)^{3/2}}\left[e^{ikz} + \frac{e^{\pm ikr}}{r}\left\{-\left(\frac{2m}{\hbar^2}\right)\frac{(2\pi)^{3/2}}{4\pi}\int d\vec{r}' e^{\mp i\vec{k}_r\cdot\vec{r}'}V(\vec{r}')\Psi^{\pm}(\vec{r}')\right\}\right] + \mathcal{O}(\left(\frac{a}{r}\right))$$

Here we note that $\vec{k}_r = k\hat{r}$ is the k-vector in the direction of the scattering. This in fact shows that $\Psi^+(\vec{r})$ is the solution, which satisfies the boundary condition. The scattering amplitude can be given from

$$f(\theta_{\vec{k}_r}) = -\left(\frac{2m}{\hbar^2}\right)\frac{(2\pi)^{3/2}}{4\pi}\int d\vec{r}' e^{-i\vec{k}_r\cdot\vec{r}'}V(\vec{r}')\Psi^{+}(\vec{r}')$$

Note that the incident wave is expressed as
$\Phi_{\vec{k}_z}(\vec{r}) = \frac{1}{(2\pi)^{3/2}}e^{i\vec{k}_z\cdot\vec{r}}, \;\; (\vec{k}_z = k\hat{z})$, we can write [35]

$$\begin{aligned} f(\theta_{\vec{k}_r}) &= -\left(\frac{2m}{\hbar^2}\right)\frac{(2\pi)^3}{4\pi}\langle\Phi_{\vec{k}_r}|V|\Psi^+\rangle \\ &= -\left(\frac{2m}{\hbar^2}\right)\frac{(2\pi)^3}{4\pi}\langle\Phi_{\vec{k}_r}|T|\Phi_{\vec{k}_z}\rangle \\ T &= V + V\frac{1}{E_k - H + i0}V \end{aligned}$$

2.3 Born Approximation

The approximation method that has solution Phi in the right side of $\Psi^{\pm}$ as the lowest order of the successive approximation steps within the integral equation to give a simplest form of approximation

$$\Psi^{\pm} \approx \frac{1}{(2\pi)^{3/2}}e^{ikz} = \frac{1}{(2\pi)^{3/2}}e^{ik\hat{z}\cdot\vec{r}}$$

[34]

$$\begin{aligned} |\vec{r}-\vec{r}'| = (r^2 + r'^2 - 2\vec{r}\cdot\vec{r}')^{1/2} &= r(1 - 2\frac{\hat{r}\cdot\vec{r}'}{r} + \frac{r'^2}{r^2})^{1/2} = r(1 - 2\frac{\hat{r}\cdot\vec{r}'}{r} + \mathcal{O}(\left(\frac{a}{r}\right)^2))^{1/2} \\ &= r - \hat{r}\cdot\vec{r}' + \mathcal{O}(\left(\frac{a}{r}\right)) \end{aligned}$$

[35]We used $\Psi^+ = (1 + G^+V)\Phi$

Is called the (first) Born approximation. The scattering amplitude in this approximation can be written

$$\begin{aligned} f_B(\theta_{\vec{k}}) &= -\left(\frac{2m}{\hbar^2}\right)\frac{1}{4\pi}\int d\vec{r} e^{i(\vec{k}'-\vec{k})\cdot\vec{r}} V(r) \\ \vec{k}' &= k\hat{z} \end{aligned}$$

Now let us have

$$\vec{K} = \vec{k}' - \vec{k}$$

Calculation is made with the polar coordinates $(\bar{r}, \bar{\theta}, \bar{\phi})$ in $\vec{K}$ direction to give [36]

$$\begin{aligned} f_B(\theta_{\vec{k}}) &= -\left(\frac{2m}{\hbar^2}\right)\frac{1}{4\pi}\int d\bar{\phi}\int d\bar{\theta}\sin\bar{\theta}\int d\bar{r}\bar{r}^2 e^{iK\bar{r}\cos\bar{\theta}} V(\bar{r}) \\ &= -\left(\frac{2m}{\hbar^2}\right)\frac{1}{2}\int d\bar{r}\bar{r}^2 \frac{1}{iK\bar{r}} e^{iK\bar{r}\cos\bar{\theta}}\Big|_{\cos\bar{\theta}=-1}^{\cos\bar{\theta}=1} V(\bar{r}) \\ &= -\left(\frac{2m}{\hbar^2}\right)\frac{1}{K}\int drr\sin(Kr)V(r) \end{aligned}$$

The differntial cross section can be written

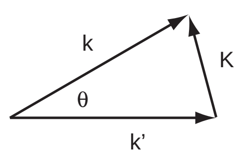
$$\sigma = \left(\frac{2m}{\hbar^2}\right)^2 \left|\frac{1}{K}\int_0^\infty drV(r)r\sin(Kr)\right|^2$$

A Case for Born Approximation (Rutherford Scattering)

Consider scattering by Yukawa potential

$$V(r) = \frac{Ae^{-\mu r}}{r}$$

36



$$K = |\vec{K}| = \sqrt{2k^2(1-\cos\theta)} = 2k\sin\frac{\theta}{2}$$

$$\begin{aligned} dK &= k\cos\theta/2d\theta \\ KdK &= k^2\sin\theta d\theta \\ \sin\theta d\theta &= \frac{1}{k^2}KdK \end{aligned}$$

In which we can write [37]

$$f_B(\theta) = -\frac{2m}{\hbar^2}\frac{A}{K^2+\mu^2}$$

We can rewrite the above equation with $\mu \to 0$, $A = -Ze^2$ to have

$$f_B \overset{\mu\to 0}{\longrightarrow} \frac{m}{2(\hbar k)^2}\frac{Ze^2}{\sin^2\theta/2}$$

This indeed is equivalent to the classical formula of the Rutherford scattering.

2.4 Partial Wave Decomposition

In the following sections we discuss the scattering problems with an approach by the partial wave decomposition. [38]

2.4.1 The Schroedinger Equation in Spherical Symmetric Field

The Schroedinger equation is expressed in the forms

$$\begin{aligned} H\Psi(\vec{r}) &= E\Psi(\vec{r}) \\ H &= \frac{\vec{p}^2}{2m} + V(r) \\ \vec{p} &= \frac{\hbar}{i}\vec{\nabla} \end{aligned}$$

Given that we consider to obtain the its eigenfunction in the following forms

$$\begin{aligned} \Psi(\vec{r}) &= R(r)\ \Theta(\theta)\ \Phi(\phi) \\ x &= r\sin\theta\cos\phi, \quad y = r\sin\theta\sin\phi, \quad z = r\cos\theta \end{aligned}$$

Let the angular momentum be

$$\begin{aligned} \vec{L} &\equiv \vec{r}\times\vec{p} \\ L_i &= \epsilon_{ijk}x_j p_k, \quad x_1 = x, \quad x_2 = y, \quad x_3 = z \end{aligned}$$

---

[37]

$$\begin{aligned} \int_0^\infty dr \sin Kr rV(r) &= A\int_0^\infty dr e^{-\mu r}\sin Kr = \frac{A}{2i}\int_0^\infty dr\left(e^{(-\mu+iK)r} - e^{(-\mu-iK)r}\right) \\ &= A\frac{-1}{2i}\left(\frac{1}{-\mu+iK} - \frac{1}{-\mu-iK}\right) = \frac{AK}{K^2+\mu^2} \end{aligned}$$

[38] Review the mathematical handbooks for the basic knowledge of the spherical function.

giving [39]

$$[L_i, L_j] = i\hbar\epsilon_{ijk}L_k$$

This exchange relationship generally makes clear of the fact (from the algebraic relation only) that the simultaneous eigenstates for $\vec{L}^2$ and L_z can be obtained as

$$\begin{aligned}
\vec{L}^2 Y_{\ell m} &= \hbar^2\ell(\ell+1)Y_{\ell m} \\
L_z Y_{\ell m} &= \hbar m Y_{\ell m} \\
m &= -\ell, \ell+1, \cdots, \ell-1, \ell
\end{aligned}$$

Furthermore, we may write [40]

$$\begin{aligned}
\vec{\nabla} &= \vec{e}_r \frac{\partial}{\partial r} + \vec{e}_\theta \frac{1}{r}\frac{\partial}{\partial\theta} + \vec{e}_\phi \frac{1}{r\sin\theta}\frac{\partial}{\partial\phi} \\
\vec{e}_r &= \widehat{\frac{\partial\vec{r}}{\partial r}} = (\sin\theta\cos\phi, \sin\theta\sin\phi, \cos\theta), \\
\vec{e}_\theta &= \widehat{\frac{\partial\vec{r}}{\partial\theta}} = (\cos\theta\cos\phi, \cos\theta\sin\phi, -\sin\theta), \\
\vec{e}_\phi &= \widehat{\frac{\partial\vec{r}}{\partial\phi}} = (-\sin\phi, \cos\phi, 0), \\
\vec{r} &= \vec{e}_r r
\end{aligned}$$

which gives a clear sense that $\vec{L}$ does not depend on r but depends on θ, and ϕ in

[39] $[x_i, p_j] = x_i p_j - p_j x_i = i\hbar\delta_{ij}$

$$\begin{aligned}
[L_i, L_j] &= \epsilon_{iab}\epsilon_{jcd}[x_a p_b, x_c p_d] = \epsilon_{iab}\epsilon_{jcd}(x_a[p_b, x_c p_d] + [x_a, x_c p_d]p_b) = \epsilon_{iab}\epsilon_{jcd}(x_a[p_b, x_c]p_d + x_c[x_a, p_d]p_b) \\
&= \epsilon_{iab}\epsilon_{jcd}(-i\hbar\delta_{bc}x_a p_d + i\hbar\delta_{ad}x_c p_b) = -i\hbar\epsilon_{iab}\epsilon_{jbd}x_a p_d + i\hbar\epsilon_{iab}\epsilon_{jca}x_c p_b \\
&= i\hbar(\delta_{ij}\delta_{ad} - \delta_{id}\delta_{aj})x_a p_d - i\hbar(\delta_{ij}\delta_{bc} - \delta_{ic}\delta_{bj})x_c p_b \\
&= i\hbar(\delta_{ij}x_a p_a - x_j p_i - \delta_{ij}x_b p_b + x_i p_j) = i\hbar(x_i p_j - x_j p_i) = i\hbar\epsilon_{ijk}L_k \\
&\quad (= i\hbar\epsilon_{ijk}\epsilon_{kab}x_a p_b = i\hbar(x_i p_j - x_j p_i))
\end{aligned}$$

[40] It is cleat that

$$\vec{r} = x\vec{e}_x + y\vec{e}_y + z\vec{e}_z$$

the function. We can write respsctively, [41]

$$
\begin{aligned}
L_x &= -i\hbar\Big(-\sin\phi\frac{\partial}{\partial\theta} - \cot\theta\cos\phi\frac{\partial}{\partial\phi}\Big)\\
L_y &= -i\hbar\Big(\cos\phi\frac{\partial}{\partial\theta} - \cot\theta\sin\phi\frac{\partial}{\partial\phi}\Big)\\
L_z &= -i\hbar\frac{\partial}{\partial\phi}\\
\vec{L}^2 &= -\hbar^2\Big\{\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\Big(\sin\theta\frac{\partial}{\partial\theta}\Big) + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\Big\}
\end{aligned}
$$

We use these specific in the above to determine the eigenvalue $\hbar^2\ell(\ell+1)$ for $\vec{L}^2$. In the first step, let us have $Y_{lm}(\theta,\phi) = \Theta(\theta)\Phi(\phi)$ and write out the equations according to the eigenfunction to have

$$
\begin{aligned}
\Big\{\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\Big(\sin\theta\frac{\partial}{\partial\theta}\Big) + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\Big\}\Theta(\theta)\Phi(\phi) &= -\ell(\ell+1)\Theta(\theta)\Phi(\phi)\\
\frac{1}{\Theta}\sin^2\theta\Big\{\frac{1}{\sin\theta}\frac{d}{d\theta}\Big(\sin\theta\frac{d\Theta}{d\theta}\Big) + \ell(\ell+1)\Theta\Big\} &= -\frac{1}{\Phi(\phi)}\frac{d^2\Phi}{d\phi^2}
\end{aligned}
$$

[41]

$$
\vec{L} = \vec{r}\times\vec{p} = -i\hbar\vec{e}_\phi\frac{\partial}{\partial\theta} + i\hbar\vec{e}_\theta\frac{1}{\sin\theta}\frac{\partial}{\partial\phi} = -i\hbar(-\sin\phi,\cos\phi,0)\frac{\partial}{\partial\theta} + i\hbar(\cot\theta\cos\phi,\cot\theta\sin\phi,-1)\frac{\partial}{\partial\phi}
$$

$$
\begin{aligned}
L_x^2 =& -\hbar^2\big(\sin\phi\,\partial_\theta + \cot\theta\cos\phi\,\partial_\phi\big)\big(\sin\phi\,\partial_\theta + \cot\theta\cos\phi\,\partial_\phi\big), \quad (\cot\theta)' = -\frac{1}{\sin^2\theta}\\
=& -\hbar^2\big(\sin^2\phi\,\partial_\theta^2 - \frac{1}{\sin^2\theta}\sin\phi\cos\phi\,\partial_\phi + \cot\theta\sin\phi\cos\phi\,\partial_\theta\,\partial_\phi\\
&+ \cot\theta\cos^2\phi\,\partial_\theta + \cot\theta\cos\phi\sin\phi\,\partial_\phi\,\partial_\theta\\
&- \cot^2\theta\sin\phi\cos\phi\,\partial_\phi + \cot^2\theta\cos^2\phi\,\partial_\phi^2\big)\\
L_y^2 =& -\hbar^2\big(\cos\phi\,\partial_\theta - \cot\theta\sin\phi\,\partial_\phi\big)\big(\cos\phi\,\partial_\theta - \cot\theta\sin\phi\,\partial_\phi\big)\\
=& -\hbar^2\big(\cos^2\phi\,\partial_\theta^2 + \frac{1}{\sin^2\theta}\sin\phi\cos\phi\,\partial_\phi - \cot\theta\sin\phi\cos\phi\,\partial_\theta\,\partial_\phi\\
&+ \cot\theta\sin^2\phi\,\partial_\theta - \cot\theta\sin\phi\cos\phi\,\partial_\theta\,\partial_\phi\\
&+ \cot^2\theta\sin\phi\cos\phi\,\partial_\phi + \cot^2\theta\sin^2\phi\,\partial_\phi^2\big)\\
L_x^2 + L_y^2 =& -\hbar^2\big(\partial_\theta^2 + \cot\theta\,\partial_\theta + \cot^2\theta\,\partial_\phi^2\big)\\
L_z^2 =& -\hbar^2\,\partial_\phi^2\\
\boldsymbol{L}^2 =& -\hbar^2\Big(\partial_\theta^2 + \cot\theta\,\partial_\theta + \frac{1}{\sin^2\theta}\,\partial)\phi^2\Big)\\
=& -\hbar^2\Big(\frac{1}{\sin\theta}\,\partial_\theta(\sin\theta\,\partial_\theta) + \frac{1}{\sin^2\theta}\,\partial)\phi^2\Big)
\end{aligned}
$$

We separate the equations above to give

$$\frac{d^2\Phi}{d\phi^2} = -m^2\Phi$$

$$\frac{1}{\sin\theta}\frac{d}{d\theta}\left(\sin\theta\frac{d\Theta}{d\theta}\right) + \{\ell(\ell+1) - \frac{m^2}{\sin^2\theta}\}\Theta = 0$$

The first equations above to give

$$\Phi(\phi) = e^{im\phi}, \quad m = 0, \pm1, \pm2, \pm3, \cdots ,$$

The condition for the m is being satisfied given the monodromy of the function. If we require the finite property in the whole region for θ in the function of Θ, we may use the associated Legendre differntial equation to write

$$\Theta(\theta) \propto P_l^{|m|}(\theta), \quad \ell = 0, 1, 2, \cdots , \ m = -\ell, \ell+1, \cdots , \ell$$

[42] With all the iformation we obtained from above, we now determine the normalization constant as in the following form

$$Y_{\ell m}(\theta, \phi) = (-1)^{\frac{m+|m|}{2}}\sqrt{\frac{2\ell+1}{4\pi}\frac{(\ell-|m|)!}{(\ell+|m|)!}}P_l^{|m|}(\cos\theta)e^{im\phi}$$

Thus, we can write the orthonormality,

$$\langle Y_{\ell' m'}|Y_{\ell m}\rangle \equiv \int d\Omega Y^*_{\ell' m'}(\theta, \phi)Y_{\ell m}(\theta, \phi) = \delta_{\ell,\ell'}\delta_{mm'}$$

the effects of ladder operator as,

$$L_\pm Y_{\ell m} \ = \ \hbar\sqrt{(\ell \mp m)(\ell \pm m+1)}Y_{\ell m\pm1}$$

and the complex conjugation as,

$$Y^*_{\ell m}(\theta, \phi) = (-)^m Y_{\ell -m}(\theta, \phi)$$

[42]With $x = \cos\theta$, we know $\frac{d}{d\theta} = \frac{dx}{d\theta}\frac{d}{dx} = -\sin\theta\frac{d}{dx}$ thus, we have $\frac{1}{\sin\theta}\frac{d}{d\theta}\left(\sin\theta\frac{d\Theta}{d\theta}\right) = \frac{d}{dx}\left(\sin^2\theta\frac{d\Theta}{dx}\right) = \frac{d}{dx}\left((1-x^2)\frac{d\Theta}{dx}\right)$ From that we obtain

$$\{(1-x^2)\frac{d\Theta}{dx}\} + \left(\ell(\ell+1) - \frac{m^2}{1-x^2}\right)\Theta = 0$$

(associated Legendre differntial equation)

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[43]Here we demonstrate step-by-step of deriving the spherical harmonics $Y_{\ell m}(\theta,\phi) = \Theta_{\ell m}(\theta)\Phi_m(\phi)$ via algebraic functions alone. First, we have $L_z Y_{\ell m} = m\hbar Y_{\ell m}$, which gives. $\Phi_m = \frac{1}{\sqrt{2\pi}}e^{im\phi}$ We may also write

$$\begin{aligned} L_+ =& L_x + iL_y = \hbar e^{i\phi}(\partial_\theta + i\cot\theta\partial_\phi) \\ L_- =& L_x - iL_y = \hbar e^{-i\phi}(-\partial_\theta + i\cot\theta\partial_\phi) \end{aligned}$$

So, from $L_+ Y_{\ell\ell} = 0$, we can write

$$\Theta'_{\ell\ell} - \ell\cot\theta\Theta_{\ell\ell} = 0, \to \Theta_{\ell\ell}(\theta) = C_\ell \sin^\ell\theta$$

Normalization may give

$$\begin{aligned} 1 =& |C_\ell|^2 \int_0^\pi d\theta\, \sin\theta\sin^{2\ell}\theta = 2|C_\ell|^2 \int_0^{\pi/2} d\theta\, \sin^{2\ell+1}\theta = C_\ell^2 B(\ell+1,1) = |C_\ell|^2 \frac{\Gamma(\ell+1)\Gamma(1/2)}{\Gamma(\ell+3/2)} \\ =& |C_\ell|^2 \frac{\ell!\Gamma(1/2)}{(\ell+1/2)(\ell-1/2)(\ell-3/2)\cdots(1/2)\Gamma(1/2)} \\ =& |C_\ell|^2 \frac{\ell! 2^\ell}{(\ell+1/2)(2\ell-1)!!} = |C_\ell|^2 \frac{\ell! 2^\ell \cdot (2\ell+1)2^\ell \ell!}{(\ell+1/2)(2\ell+1)!} = |C_\ell|^2 \frac{2(\ell! 2^\ell)^2}{(2\ell+1)!} \\ C_\ell =& e^{i\delta}\sqrt{\frac{(2\ell+1)!}{2}}\frac{1}{\ell! 2^\ell} \end{aligned}$$

Thus, we write

$$\begin{aligned} Y_{\ell m-1} =& \frac{1}{\sqrt{(\ell+m)(\ell-m+1)}} e^{-i\phi}(-\partial_\theta + i\cot\theta\partial_\phi)Y_{\ell m} \\ =& \frac{1}{\sqrt{(\ell+m)(\ell-m+1)}}(-)(\partial_\theta + m\cot\theta)\Theta_{\ell m}\Phi_{m-1}(\phi) = \Theta_{\ell m-1}\Phi_{m-1}(\phi) \\ \Theta_{\ell m-1} =& -\frac{1}{\sqrt{(\ell+m)(\ell-m+1)}}(\partial_\theta + m\cot\theta)\Theta_{\ell m} \end{aligned}$$

Here we note that

$$\begin{aligned} \sin^{1-m}\theta \frac{d}{d\cos\theta}(\sin^m\theta\Theta) =& \sin^{1-m}\theta\left(\frac{d\cos\theta}{d\theta}\right)^{-1}\frac{d}{d\theta}(\sin^m\theta\Theta) = -\sin^{-m}\theta(\Theta m\sin^{m-1}\theta\cos\theta + \sin^m\theta\partial_\theta\Theta) \\ =& -(\Theta m\cot\theta + \partial_\theta\Theta) \end{aligned}$$

which giving,

$$
\begin{aligned}
\Theta_{\ell m-1} =& \frac{1}{\sqrt{(\ell+m)(\ell-m+1)}} \sin^{1-m}\theta \frac{d}{d\cos\theta}(\sin^m\theta\Theta_{\ell m}) \\
\Theta_{\ell m-2} =& \frac{1}{\sqrt{(\ell+m-1)(\ell-m+2)}} \sin^{2-m}\theta \frac{d}{d\cos\theta}(\sin^{m-1}\theta\Theta_{\ell m-1}) \\
=& \frac{1}{\sqrt{(\ell+m)(\ell+m-1)\cdot(\ell-m+1)(\ell-m+2)}} \sin^{1-m}\theta \left(\frac{d}{d\cos\theta}\right)^2 (\sin^m\theta\Theta_{\ell m}) \\
\Theta_{\ell m-k} =& \frac{\sqrt{(\ell+m-k)!(\ell-m)!}}{\sqrt{(\ell+m)!(\ell-m+k)!}} \sin^{k-m}\theta \left(\frac{d}{d\cos\theta}\right)^k (\sin^m\theta\Theta_{\ell m}) \\
& Let us now have m \to \ell, k \to \ell - m so, we rewrite in the form \\
\Theta_{\ell m} =& \frac{\sqrt{(\ell+m)!(0)!}}{\sqrt{(2\ell)!(\ell-m)!}} \sin^{-m}\theta \left(\frac{d}{d\cos\theta}\right)^{\ell-m} (\sin^\ell\theta\Theta_{\ell\ell}) \\
=& e^{i\delta}\sqrt{\frac{2\ell+1}{2}\frac{(\ell+m)!}{(\ell-m)!}} \frac{1}{\ell!2^\ell}\frac{1}{\sin^m\theta}\left(\frac{d}{d\cos\theta}\right)^{\ell-m}(\sin^{2\ell}\theta) \\
& We especially consider m = 0 to obtai \\
\Theta_{\ell 0} =& e^{i\delta}\sqrt{\frac{2\ell+1}{2}}\frac{1}{\ell!2^\ell}\left(\frac{d}{d(\cos\theta)}\right)^\ell(\sin^{2\ell}\theta) = e^{i\delta}(-)^\ell\sqrt{\frac{2\ell+1}{2}}\frac{1}{\ell!2^\ell}\frac{d}{d(\cos\theta)}(\cos^2\theta-1)^\ell \\
=& e^{i\delta}(-)^\ell\sqrt{\frac{2\ell+1}{2}}P_\ell(\cos\theta) \\
& so, we put e^{i\delta} = (-)^\ell \\
\Theta_{\ell 0} =& \sqrt{\frac{2\ell+1}{2}}P_\ell(\cos\theta) \\
\Theta_{\ell m} =& (-)^\ell\sqrt{\frac{2\ell+1}{2}\frac{(\ell+m)!}{(\ell-m)!}}\frac{1}{\ell!2^\ell}\frac{1}{\sin^m\theta}\left(\frac{d}{d\cos\theta}\right)^{\ell-m}(\sin^{2\ell}\theta) \\
m \le 0, & \\
\Theta_{\ell m} =& \sqrt{\frac{2\ell+1}{2}\frac{(\ell+m)!}{(\ell-m)!}}\frac{1}{\sin^m\theta}\left(\frac{d}{d\cos\theta}\right)^{-m}P_\ell(\cos\theta) \\
=& \sqrt{\frac{2\ell+1}{2}\frac{(\ell-|m|)!}{(\ell+|m|)!}}\sin^{|m|}\theta\left(\frac{d}{d\cos\theta}\right)^{|m|}P_\ell(\cos\theta)
\end{aligned}
$$

On the other hand, we have

$$
\begin{aligned}
Y_{\ell m+1} =& \frac{1}{\sqrt{(\ell-m)(\ell+m+1)}}e^{i\phi}(\partial_\theta + i\cot\theta\partial_\phi)Y_{\ell m} \\
=& \frac{1}{\sqrt{(\ell-m)(\ell+m+1)}}(\partial_\theta - m\cot\theta)\Theta_{\ell m}\Phi_{\ell m+1} \\
\Theta_{\ell m+1} =& \frac{1}{\sqrt{(\ell-m)(\ell+m+1)}}(\partial_\theta - m\cot\theta)\Theta_{\ell m}
\end{aligned}
$$

While we can write using the algebraic functions alone, [44]

$$\vec{L}^2 = r^2\vec{p}^2 - r^2 p_r^2, \qquad p_r^2 = -\hbar^2(\partial_r^2 + \frac{2}{r}\partial_r)$$

Thus,

$$\frac{\vec{p}^2}{2m} = \frac{1}{2m}p_r^2 + \frac{1}{2m}\frac{\vec{L}^2}{r^2}$$

$$\sin^{m+1}\theta \frac{d}{d\cos\theta}(\sin^{-m}\theta\Theta) = \sin^{m+1}\theta \left(\frac{d\cos\theta}{d\theta}\right)^{-1}\frac{d}{d\theta}(\sin^{-m}\theta\Theta) = -\sin^m\theta(-\Theta m\sin^{-m-1}\theta\cos\theta + \sin^{-m}\theta\partial_\theta\Theta)$$
$$=(\Theta m\cot\theta - \partial_\theta\Theta)$$

which giving,

$$\Theta_{\ell m+1} =(-)\frac{1}{\sqrt{(\ell-m)(\ell+m+1)}}\sin^{m+1}\theta\frac{d}{d\cos\theta}(\sin^{-m}\theta\Theta_{\ell m})$$
$$\Theta_{\ell m+2} =(-)\frac{1}{\sqrt{(\ell-m-1)(\ell+m+2)}}\sin^{m+2}\theta\frac{d}{d\cos\theta}(\sin^{-m-1}\theta\Theta_{\ell m+1})$$
$$=(-)^2\frac{1}{\sqrt{(\ell-m)(\ell-m-1)\cdot(\ell+m+1)(\ell+m+2)}}\sin^{m+2}\theta\left(\frac{d}{d\cos\theta}\right)^2(\sin^{-m}\theta\Theta_{\ell m})$$
$$\Theta_{\ell m+k} =(-)^k\frac{\sqrt{(\ell-m-k)!(\ell+m)!}}{\sqrt{(\ell-m)!(\ell+m+k)!}}\sin^{m+k}\theta\left(\frac{d}{d\cos\theta}\right)^k(\sin^{-m}\theta\Theta_{\ell m})$$
$$We put m \to 0, k \to m (m > 0)$$
$$\Theta_{\ell m} =(-)^m\frac{\sqrt{(\ell-m)!\ell!}}{\sqrt{\ell!(\ell+m)!}}\sin^m\theta\left(\frac{d}{d\cos\theta}\right)^m\Theta_{\ell 0}$$
$$=(-)^m\sqrt{\frac{2\ell+1}{2}\frac{(\ell-m)!}{(\ell+m)!}}\sin^m\theta\left(\frac{d}{d\cos\theta}\right)^m P_\ell(\cos\theta)$$

$$Now, from P_\ell^{|m|}(\cos\theta) = \sin^{|m|}\theta\left(\frac{d}{d\cos\theta}\right)^{|m|}P_\ell(\cos\theta) we obtain,$$

$$\Theta_{\ell m} =(-1)^{\frac{m+|m|}{2}}\sqrt{\frac{2\ell+1}{2}\frac{(\ell-|m|)!}{(\ell+|m|)!}}P_\ell^{|m|}(\cos\theta)$$
$$With m \le 0, we can write \Theta_{\ell -m} = (-)^m\Theta_{\ell m}$$

[44]GIven that we have $\vec{r}\cdot\vec{p} = -i\hbar x_i\partial_i = -i\hbar r\frac{x_i}{r}\partial_i = -i\hbar r\frac{\partial x_i}{\partial r}\partial_i = -i\hbar r\partial_r$,

$$\begin{aligned}
\vec{L}^2 &= \epsilon_{ijk}\epsilon_{ilm}x_jp_kx_lp_m = (\delta_{jl}\delta_{km} - \delta_{jm}\delta_{kl})x_jp_kx_lp_m \\
&= x_jp_kx_jp_k - x_jp_lx_lp_j = x_j(x_jp_k - i\hbar\delta_{jk})p_k - x_j(x_lp_l - i\hbar\delta_{ll})p_j \\
&= r^2\vec{p}^2 - i\hbar\vec{r}\cdot\vec{p} - x_j(p_jx_l + i\hbar\delta_{lj})p_l + 3i\hbar\vec{r}\cdot\vec{p} = r^2\vec{p}^2 - (\vec{r}\cdot\vec{p})^2 + i\hbar\vec{r}\cdot\vec{p} \\
&= r^2\vec{p}^2 - r^2p_r^2 \\
p_r^2 &= \frac{1}{r^2}\left\{(\vec{r}\cdot\vec{p})^2 - i\hbar\vec{r}\cdot\vec{p}\right\} = \frac{\hbar^2}{r^2}\left\{-r\partial_r r\partial_r - r\partial_r\right\} = -\hbar^2(\partial_r^2 + \frac{2}{r}\partial_r)
\end{aligned}$$

Here we suppose $\Psi(\vec{r}) = R(r)Y_{lm}(\theta,\phi)$, the Schroedinger equation may give

$$\begin{aligned}\left\{-\left(\frac{d^2}{dr^2}+\frac{2}{r}\frac{d}{dr}\right)\right. &+& \left.\frac{\ell(\ell+1)}{r^2}+U(r)\right\}R_\ell(r) = k^2 R_\ell(r)\\ \frac{\hbar^2k^2}{2m} &=& E, \quad \frac{\hbar^2}{2m}U(r) = V(r)\end{aligned}$$

Especially in the case where the potential employs the constant $V = V_0$, we define $x = kr,\ E - V_0 = \frac{\hbar^2k^2}{2m}$, and write

$$\left\{\left(\frac{d^2}{dx^2}+\frac{2}{x}\frac{d}{dx}\right)+1-\frac{\ell(\ell+1)}{x^2}\right\}F_\ell(x) = 0$$

This equation is caled the spherical Bessel equation, and its second-order of the differntial equation has two independent solutions. [45] General solutions of the Schroedinger equaiton can be obtained by using those two independent solutions, and written

$$\Psi(\vec{r}) = \sum_{\ell m} c_{\ell m}R_\ell(r)Y_{\ell m}(\theta,\phi), \quad E = \frac{\hbar^2k^2}{2m}$$

Here we summarize the requirements for the radial of the wavefunction R_ℓ.

- Behavior at origin periphery

  Where $V(r)$ has no uniqueness at origin periphery [46]

$$R_\ell(kr) \stackrel{\vec{r}\to 0}{\longrightarrow} (kr)^\ell$$

- Conservation

[45]Either the pairs of the spherical Bessel function $j_\ell(x)$ and the spherical Neumann function $n_\ell(x)$, or the Hankel function of the first kind $h_\ell^{(1)}(x)$ and the Hankel function of the second kind $h^{(2)}\ell(x)$, can be used as the independent solutions.

$$F_\ell(x) = A_\ell j_\ell(x) + B_\ell n_\ell(x) = C_\ell h_\ell^{(1)}(x) + D_\ell h_\ell^{(2)}(x)$$

and more specifically given

$$\begin{aligned} j_\ell(x) &=& (-x)^\ell\left(\frac{1}{x}\frac{d}{dx}\right)^\ell\left(\frac{\sin x}{x}\right) \stackrel{x\to 0}{\longrightarrow} \frac{x^\ell}{(2\ell+1)!!}\\ n_\ell(x) &=& -(-x)^\ell\left(\frac{1}{x}\frac{d}{dx}\right)^\ell\left(\frac{\cos x}{x}\right) \stackrel{x\to 0}{\longrightarrow} -\frac{(2\ell-1)!!}{x^{\ell+1}}\end{aligned}$$

[46]Let us suppose $R_\ell \sim r^n$ at the origin periphery, the Schoedinger equation may give $\{-n(n-1)-2n+\ell(\ell+1)\}r^{n-2} \sim 0$. From which, we write

$$-n^2 - n + \ell^2 + \ell = (\ell - n)(\ell + n + 1) = 0$$

This gives r^ℓ,and $\frac{1}{r^{\ell+1}}$ yat, the probability amplitude is required not to diverge at the origin.

Especially the case where the potential is the real [47]

$$\det\begin{pmatrix} rR_\ell & rR_\ell^* \\ (rR_\ell)' & (rR_\ell^*)' \end{pmatrix} = 0$$

This becomes the conserved quantity; independent of the coordinate systems. (Consider where $r \to 0$)

2.4.2 Phase Shift

We now consider the potential that is resticted to the finite region. In this case, the region with no potential possesses the free particles, and the wavefunction can be written [48]

$$\Psi(\vec{r}) = \sum_\ell A_\ell \{ S_\ell h_\ell^{(1)}(kr) + h_\ell^{(2)}(kr) \} P_\ell(\cos\theta)$$

[47]Suppose we define, $R(x) = x^n \mathcal{R}(x)$ we can write, $R' = nx^{n-1}\mathcal{R} + x^n\mathcal{R}'$, $R'' = n(n-1)x^{n-2}\mathcal{R} + 2nx^{n-1}\mathcal{R}' + x^n\mathcal{R}''$ which giving

$$R''+2x^{-1}R' = n(n-1)x^{n-2}\mathcal{R}+2nx^{n-1}\mathcal{R}'+x^n\mathcal{R}''+2nx^{n-2}\mathcal{R}+2x^{n-1}\mathcal{R}' = x^n\mathcal{R}''+2(1+n)x^{n-1}\mathcal{R}'+\cdots$$

If we take $R(x) = x^{-1}\mathcal{R}(x)$, there are no first order differntials for the differntial equation of $\mathcal{R}$ so, Wronskians will be invariable when solutions for the differential equation be $\mathcal{R}_1$, and $\mathcal{R}_2$. Especially in this case, we consider the Wronskians of R and R^* for the real potential, giving

$$\det\begin{pmatrix} rR & rR^* \\ (rR)' & (rR^*)' \end{pmatrix}$$

This does not depend on the coordinate system

[48]The point of measurement for the angle of ϕ can be selected at any points, and therefore, the wavefunction does not depend on ϕ but, depends only on $Y_{\ell m=0}$.

. Let us first define the amplitude A_ℓ of each partial wave as we consider the asymptotic conditions for the point where infinite distance away. We can write [49]

$$\begin{aligned}\Psi(\vec{r}) &= \frac{1}{(2\pi)^{3/2}}\sum_{\ell=0}^{\infty}\frac{(2\ell+1)}{2}i^\ell\big\{S_\ell h_\ell^{(1)}(kr)+h_\ell^{(2)}(kr)\big\}P_\ell(\cos\theta)\\ &\longrightarrow \sum_\ell \frac{1}{(2\pi)^{3/2}}\frac{-i(2\ell+1)}{2}\frac{1}{kr}\big\{S_\ell e^{ikr}-(-1)^\ell e^{-ikr}\big\}P_\ell(\cos\theta)\end{aligned}$$

[49]The asymptotic form for a large argument can be written

$$j_\ell(x)\overset{x\to\infty}{\longrightarrow}\frac{1}{x}\sin\big(x-\frac{\ell\pi}{2}\big),\qquad n_\ell(x)\overset{x\to\infty}{\longrightarrow}-\frac{1}{x}\cos\big(x-\frac{\ell\pi}{2}\big)$$

$$h_\ell^{(1)}(x)\overset{x\to\infty}{\longrightarrow}(-i)^{\ell+1}\frac{e^{ix}}{x}\qquad h_\ell^{(2)}(x)\overset{x\to\infty}{\longrightarrow}(i)^{\ell+1}\frac{e^{-ix}}{x}$$

giving,

$$\Psi(\vec{r})\longrightarrow\sum_\ell A_\ell\frac{(-i)^{\ell+1}}{kr}\big\{S_\ell e^{ikr}-(-1)^\ell e^{-ikr}\big\}P_\ell(\cos\theta)$$

We expand the scattering amplitude in terms of the complete set $f(\theta)=\sum_{\ell=0}^{\infty}a_\ell P_\ell(\cos\theta)$, and further expand the incident wave in terms of the partial wave as following

$$e^{ikr\cos\theta}=\sum_{\ell=0}^{\infty}(2\ell+1)i^\ell j_\ell(kr)P_\ell(\cos\theta)$$

$$j_\ell(x)\overset{x\to\infty}{\longrightarrow}\frac{1}{x}\sin\big(x-\frac{\ell\pi}{2}\big)=\frac{1}{2ix}\big(e^{ix-i\frac{\ell\pi}{2}}-e^{-ix+i\frac{\ell\pi}{2}}\big)=\frac{1}{2ix}\big((-i)^\ell e^{ix}-i^\ell e^{-ix}\big)$$

From the above, we can express the expansion of the boundary condition at infinity point in terms of the Partial wave in the followin form

$$\begin{aligned}&\frac{1}{(2\pi)^{3/2}}\left(e^{ikr\cos\theta}+\frac{f(\theta)}{r}e^{ikr}\right)\\ &= \frac{1}{(2\pi)^{3/2}}\frac{1}{2ikr}\sum_{\ell=0}^{\infty}\left\{(2\ell+1)i^\ell\big((-i)^\ell e^{ikr}-i^\ell e^{-ikr}\big)+2ika_\ell e^{ikr}\right\}P_\ell(\cos\theta)\\ &= \frac{1}{(2\pi)^{3/2}}\frac{1}{2ikr}\sum_{\ell=0}^{\infty}(2\ell+1)\left\{\big(1+\frac{2ika_\ell}{(2\ell+1)}\big)e^{ikr}-(-)^\ell e^{-ikr}\right\}P_\ell(\cos\theta)\end{aligned}$$

Compare the two equqaions from above and write

$$a_\ell=\frac{(2\ell+1)}{2ik}(S_\ell-1)$$

$$A_\ell\frac{(-i)^{\ell+1}}{kr}=\frac{1}{(2\pi)^{3/2}}\frac{(2\ell+1)}{2ikr}$$

Thus,

$$A_\ell=\frac{1}{(2\pi)^{3/2}}\frac{(2\ell+1)}{2}i^\ell$$

We use S_ℓ to write the scattering amplitude as

$$f(\theta) = \frac{1}{2ik}\sum_{\ell=0}^{\infty}(2\ell+1)(S_\ell - 1)P_\ell(\cos\theta)$$

Note that this undefined coefficient S_ℓ is called the scattering matrix, which can be difined by the boundary condition of a region with a presence of the potential. We precede the rest of our discussion based on that we assume having defined the coefficient.

Now we apply the conservation law from our earlier discussion to each partial wave ℓ of the radial part, which corresponds to the conservation law for the number of the particle, and gives [50]

$$|S_\ell| = 1$$

Thus,

$$S_\ell = e^{i2\delta_\ell}, \quad \delta\text{: real}$$

Rewrite the asymptotic form as [51]

$$\Psi(\vec{r}) \longrightarrow \frac{1}{(2\pi)^{3/2}}\sum_\ell \frac{(2\ell+1)}{kr} i^\ell e^{i\delta_\ell}\sin(kr - \frac{\pi}{2}\ell + \delta_\ell)P_\ell(\cos\theta)$$

Compare the above with the asymptotic form for no potential,

$$\frac{1}{(2\pi)^{3/2}}e^{ikr\cos\theta} = \frac{1}{(2\pi)^{3/2}}\sum_{\ell=0}^{\infty}\frac{(2\ell+1)}{kr} i^\ell \sin(kr - \frac{\pi}{2}\ell)P_\ell(\cos\theta)$$

This makes us aware that there is a shift in the phase, and the shift occurred as much as δ_ℓ. δ_ℓ is called the phase shift.

50

$$\begin{aligned} 0 &= \det\begin{pmatrix} S_\ell e^{ikr} - (-1)^\ell e^{-ikr} & S_\ell^* e^{-ikr} - (-1)^\ell e^{ikr} \\ ikS_\ell e^{ikr} + ik(-1)^\ell e^{-ikr} & -ikS_\ell^* e^{-ikr} - ik(-1)^\ell e^{ikr} \end{pmatrix} \\ &= \det\begin{pmatrix} S_\ell e^{ikr} - (-1)^\ell e^{-ikr} & S_\ell^* e^{-ikr} - (-1)^\ell e^{ikr} \\ 2ik(-1)^\ell e^{-ikr} & -2ikS_\ell^* e^{-ikr} \end{pmatrix} \\ &= \det\begin{pmatrix} S_\ell e^{ikr} - (-1)^\ell e^{-ikr} & \{|S_\ell|^2 - 1\}(-1)^\ell e^{ikr} \\ 2ik(-1)^\ell e^{-ikr} & 0 \end{pmatrix} = -2ik\{|S_\ell|^2 - 1\} \end{aligned}$$

51

$$\begin{aligned} e^{i(2\delta_\ell + kr)} - e^{i(\pi\ell - kr)} &= e^{i(\delta_\ell + \frac{\pi}{2}\ell)}(e^{i(\delta_\ell + kr - \frac{\pi}{2}\ell)} - e^{i(-\delta_\ell + \frac{\pi}{2}\ell - kr)}) \\ &= e^{i(\delta_\ell + \frac{\pi}{2}\ell)}2i\sin(kr - \frac{\pi}{2}\ell + \delta_\ell) \end{aligned}$$

The total scattering cross section satisfies [52]

$$\sigma_T = \frac{4\pi}{k} f(0) = \sum_\ell \frac{4\pi}{k^2}(2\ell+1)\sin^2\delta_\ell$$

This first equation is called the optical theorem. We understand that when $\delta_\ell = (n+\frac{1}{2})\pi, n$: (integer), the scattering cross section of ℓ becomes the largest, while the area becomes 0 when $\delta_\ell = n\pi$.

2.4.3 Lograrithmic Differntiation and the Phase Shift

In determining the phase shift more exactly, let us first consider the junction conditions for the wavefunction within the radius $r = a$ and the wavefunction in radius part; outside the radius, by each partial wave.

$$\begin{aligned} R_\ell^{in}(a) &= R_\ell^{out}(a) \\ R_\ell^{in\prime}(a) &= R_\ell^{out\prime}(a) \end{aligned}$$

We can write the wavefunction of the outer part as

$$R_\ell^{out}(r) = C(S_\ell h_\ell^{(1)}(kr) + h_\ell^{(2)}(kr))$$

Since the noemalization factor C is unknown, the condition we can obtain now is

$$\left.\frac{d\log R_\ell^{in}(r)}{dr}\right|_{r=a} = \left.\frac{d\log R_\ell^{out}(r)}{dr}\right|_{r=a} = k\frac{S_\ell h_\ell^{(1)\prime}(ka) + h_\ell^{(2)\prime}(ka)}{S_\ell h_\ell^{(1)}(ka) + h_\ell^{(2)}(ka)}$$

Here we have

$$h^{(1,2)\prime}(ka) = \left.\frac{dh^{(1,2)}(x)}{dx}\right|_{x=ka}$$

from which we write the effects of the potential for the inner part

$$f_\ell^{in} = \frac{1}{k}\left.\frac{d\log R_\ell^{in}(r)}{dr}\right|_{r=a}$$

52

$$\begin{aligned} \sigma_T &= \int d\Omega |f(\theta)|^2 = \frac{1}{4k^2}\sum_\ell (2\ell+1)^2 |S_\ell - 1|^2 2\pi \frac{2}{(2\ell+1)} \\ &= \frac{\pi}{k^2}\sum (2\ell+1)|S_\ell - 1|^2 \end{aligned}$$

$$\begin{aligned} f(0) &= \frac{f(0) - f^*(0)}{2i} = \frac{1}{2i}\frac{1}{2ik}\sum(2\ell+1)(S_\ell + S_\ell^* - 2)P_\ell(\cos\theta) \\ &= -\frac{1}{4k}\sum_\ell (2\ell+1)(-1)(1-S_\ell)(1-S_\ell^*) = \frac{1}{4k}\sum_\ell (2\ell+1)|1-S_\ell|^2 = \frac{1}{4k}4\sum_\ell (2\ell+1)\sin^2\delta_\ell \end{aligned}$$

We parametralize the above to write

$$S_\ell = -\frac{h_\ell^{(2)}(ka) f_\ell^{in} - h_\ell^{(2)'}(ka)}{h_\ell^{(1)}(ka) f_\ell^{in} - h_\ell^{(1)'}(ka)}$$

While we have [53]

$$\tan \delta_\ell = \frac{j_\ell(ka) f_\ell^{in} - j'_\ell(ka)}{n_\ell(ka) f_\ell^{in} - n'_\ell(ka)}$$

This indicates that the wavefunction in the outer oart region is defined only by the logarithmic differntiation of the boundary of the scattering region, and not by the details of the potential.

The Low Energy Scattering

In the case for the low energy scattering

$$ka << 1$$

This gives [54] [55]

$$\delta_\ell \propto (ka)^2 \quad \ell = 0 (ka)^{2\ell+1} \quad \ell \geq 1$$

Thus, [56]

$$f(\theta) = \frac{\delta_0}{k}$$

53

$$\tan \delta_\ell = \frac{1}{i} \frac{S_\ell - S_\ell^*}{S_\ell + S_\ell^* + 2}$$

54

$$\begin{aligned} \tan \delta_\ell &\rightarrow -\frac{1}{(2\ell+1)!!(2\ell-1)!!} (ka)^{2\ell+1} \frac{f_\ell^{in} - \ell/(ka)}{f_\ell^{in} + (\ell+1)/(ka)} \\ &= -\frac{1}{(2\ell+1)!!(2\ell-1)!!} \frac{ka f_\ell^{in} - \ell}{ka f_\ell^{in} + \ell + 1} (ka)^{2\ell+1} \\ &\propto (ka)^2 \quad \ell = 0 (ka)^{2\ell+1} \quad \ell \geq 1 \end{aligned}$$

55 This does not apply hor the hard sphere.

56

$$\begin{aligned} f(\theta) &= \frac{1}{2ik} \sum_{\ell=0}^{\infty} (2\ell+1)(S_\ell - 1) P_\ell(\cos\theta) \\ &\rightarrow \frac{1}{2ik} 2i\delta_0 = \frac{\delta_0}{k} \end{aligned}$$

The Hard Sphere Case

Suppose we have a hard sphere of radius $r = a$ we can assume $R(a) = 0$ when $r = a$, and written

$$f_\ell^{in} = \infty$$

Based on the above, we can write

$$\tan\delta_\ell = \frac{j_\ell(ka)}{n_\ell(ka)}$$

Here in particular, we consider the low energy case where $ka << 1$, and using the asymptotic form, which gives [57]

$$\tan\delta_\ell = -\frac{(ka)^{2\ell+1}}{(2\ell+1)!!(2\ell-1)!!}$$

2.4.4 Jost Function and the Bound States

The equation for the partial wave of the radius part in terms of

$$\mathcal{R}(r) = rR(r)$$

can be written as we discussed earlier,

$$\mathcal{R}'' - \left(U(r) + \frac{\ell(\ell+1)}{r^2}\right)\mathcal{R} = -k^2\mathcal{R}$$

The first order differential terms are absent in the equation above, and that the Wronskians for the equation will become the conserved quantity. Now, let us consider the solutions, which satisfy the three different boundary conditions.

- Solutions in physical term

  Require the regularity at the origin to have normalization

  $$\mathcal{R} = \psi^\ell(k,r) \to r^{\ell+1} \qquad (r \to 0)$$

  This is the solution, which we have been discussing expect for the normalization.

57

$$j_\ell(x) \overset{x\to 0}{\to} \frac{x^\ell}{(2\ell+1)!!}$$

$$n_\ell(x) \overset{x\to 0}{\to} -\frac{(2\ell-1)!!}{x^{\ell+1}}$$

- Jost solution

$$\mathcal{R} = f_\pm^\ell(k,r) \to e^{\pm ikr} \qquad (k>0, \quad r\to\infty)$$

Here we calculate the Wronskians among these solutions, which giving the conserved quantity for all. Thus, solution is independent of the coordinate systems [58]

$$W(f_+^\ell(k,r), f_-^\ell(k,r)) = -2ik$$

Now, let us write down

$$W(f_\pm^\ell(k,r), \psi^\ell(k,r)) = f_\pm^\ell(k)$$

in which we call

$$f_\pm^\ell(k)$$

the Jost function.

Given the function is the second order, the solution for the physical terms can be multiplied by the Jost solution. Whose coefficient can be given by the Jost function in the form,

$$\psi^\ell(k,r) = \frac{-i}{2k}\{f_-^\ell(k)f_+^\ell(k,r) - f_+^\ell(k)f_-^\ell(k,r)\}$$

Furthermore, we consider the asymptotic form of the solution in the physical terms, and which bein compared with the definition of the scatterin matrix to give [59]

$$f_\pm^\ell(k) = (\pm)^\ell f^\ell(k) e^{\mp i\delta_\ell(k)}$$

Note that

$$S_\ell = (-1)^\ell \frac{f_-^\ell}{f_+^\ell}$$

58

$$W(f_+^\ell(k,r), f_-^\ell(k,r)) = \det\begin{pmatrix} f_+ & f_- \\ f_+' & f_-' \end{pmatrix} = \det\begin{pmatrix} e^{ikr} & e^{-ikr} \\ ike^{ikr} & -ike^{-ikr} \end{pmatrix} = \det\begin{pmatrix} e^{ikr} & e^{-ikr} \\ 2ike^{ikr} & 0 \end{pmatrix} = -2ik$$

59

$$\psi^\ell(k,r) = \frac{-if_+^\ell(k)}{2k}\left(\frac{f_-^\ell}{f_+^\ell}e^{ikr} - e^{-ikr}\right) \qquad (r\to\infty)$$

The definition of the scattering matrix gives

$$S_\ell = (-1)^\ell \frac{f_-^\ell}{f_+^\ell}$$

Thus,

$$f_\pm^\ell(k) = (\pm i)^\ell f^\ell(k) e^{\mp i\delta_\ell(k)}$$

We consider carrying out the analytic continuation of the wave number k to reach the comlex number with the real energy, we have て

$$k = i\kappa, \qquad \kappa > 0$$

Whose physical terms solution can be

$$\psi(i\kappa, r) \to f_-^\ell(i\kappa)e^{-\kappa r} - f_+^\ell(i\kappa)e^{\kappa r}$$

As long as we have

$$f_+^\ell(k = i\kappa) = 0$$

The solution can be normalized in the whole space thus; the solution represents the bound state. the above equation also indicates that the
scattering mtrix possesses the polar in the bound state energy.

$$\frac{1}{S(k = i\kappa)} = 0$$

Since the potential is real, the following symmetric properties are being also obeyed.

- $\psi^\ell(k, r) = \psi^\ell(-k, r) = \psi^{\ell*}(k, r)$
- $f_+^\ell(k, r) = f_-^\ell(-k, r)$ thus giving $f_+^\ell(k) = f_-^\ell(-k)$
- $f_+^{\ell\,*}(k, r) = f_-^\ell(k, r)$ giving $f_+^{\ell\,*}(k) = f_-^\ell(k)$

In our discussion of carrying the analytic continuations of the Jost function and the phase shift on the complexplanes, we can observe that
the number of the bound states is defined by the phase shift analysis. This we call, Levinson's theorem.

The S-wave Scattering in the Three-dimentional Square Well Potential

Now we consider the function that the wavefunction $\mathcal{R} = rR$ satisfies, and consider especially the case for the s-waves $\ell = 0$.

$$\mathcal{R}'' + (k^2 - U(r))\mathcal{R} = 0$$

For the square well potential we suppose

$$U(x) = \begin{cases} U_0 & r \le a \\ 0 & \text{otherwise} \end{cases}$$

and we define

$$K^2 = k^2 - U_0$$

Which gives [60]

$$f_0^{in} = \frac{1}{ka}(Ka\cot Ka - 1)$$

Thus, [61]

$$\tan\delta_0 = \frac{ka\cot ka - Ka\cot Ka}{ka + Ka\cot Ka\cot ka}$$

Under the low energy $ka << 1$, we can write [62]

$$\tan\delta_0 = ka\,\frac{1 - a\sqrt{-U_0}\cot a\sqrt{-U_0}}{a\sqrt{-U_0}\cot a\sqrt{-U_0}}$$

For the hard sphere, we have $U_0 \to \infty$, which gives

$$\tan\delta_0 = -ka$$

This matches with our first result. Generally speaking, we may expand the equation above about $a\sqrt{-U_0}$ if we have the potential that is very weak. So, we have

[60] Require the boundary condition

$$\mathcal{R}|_{r=0} = rR|_{r=0} = 0$$

Thus, we write

$$\begin{aligned} \mathcal{R} &= C\sin Kr \\ \frac{d\log R}{dr} &= \frac{d\log(r^{-1}\mathcal{R})}{r} = -\frac{1}{r} + K\frac{\cos Kr}{\sin Kr} \\ f_0^{in} &= \frac{1}{k}\frac{d\log R}{dr}\bigg|_{r=a} = \frac{1}{ka}(Ka\cot Ka - 1) \end{aligned}$$

[61]

$$j_0(x) = \frac{\sin x}{x},\quad j_0'(x) = \frac{x\cos x - \sin x}{x^2},\quad n_0(x) = -\frac{\cos x}{x},\quad n_0'(x) = \frac{x\sin x + \cos x}{x^2},$$

From the above, we let $x = ka$, and write

$$\begin{aligned} \tan\delta_0 &= \frac{j_0(x)f_0^{in} - j_0'(x)}{n_0(x)f_0^{in} - n_0'(x)} = \frac{\frac{\sin x}{x}\frac{1}{x}(Ka\cot Ka - 1) - \frac{x\cos x - \sin x}{x^2}}{-\frac{\cos x}{x}\frac{1}{x}(Ka\cot Ka - 1) - \frac{x\sin x + \cos x}{x^2}} \\ &= \frac{\sin xKa\cot Ka - x\cos x}{-\cos xKa\cot Ka - x\sin x} = \frac{ka\cot ka - Ka\cot Ka}{ka + Ka\cot Ka\cot ka} \end{aligned}$$

[62]

$$\begin{aligned} Ka &\overset{ka\to 0}{\to} a\sqrt{-U_0} \\ \tan\delta_0 &\overset{ka\to 0}{\to} ka\,\frac{1 - a\sqrt{-U_0}\cot a\sqrt{-U_0}}{a\sqrt{-U_0}\cot a\sqrt{-U_0}} \end{aligned}$$

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$$\tan\delta_0 \to -\frac{U_0 k a^3}{3} \approx \delta_0$$

In other words, the gravity may give $\delta_0 > 0$ while the repulsion may give $\delta_0 < 0$. In order to discuss the bound states by the method using the integral equation; that is inndeed the main focus of our present section, recall that we define k, which is defined by $E = \frac{\hbar^2 k^2}{2m}$ in $E < 0$ to be as k を $k \to i\kappa$, $(\kappa > 0)$:

$$\mathcal{R} \approx S_\ell h^{(1)}(kr) + h^{(2)}(kr) = S_\ell h_0^{(1)}(i\kappa r) + h_0^{(2)}(i\kappa r)$$

$$h_0^{(1)}(i\kappa r) = j_0(i\kappa r) + i n_0(i\kappa r) = \frac{e^{-\kappa r}}{i\kappa r}, \quad h_0^{(2)}(i\kappa r) = j_0(i\kappa r) - i n_0(i\kappa r) = \frac{e^{\kappa r}}{i\kappa r},$$

This clearly tells that we need

$$S_\ell \to \infty$$

for the wavefunctions that are not being normalized. We ensured that the energy in the bound state indeed gives the polar of the scattering matrix. In our specific case, we have [64]

$$\tan\delta_0 + i = 0$$

3 Time-dependent Scattering Theory

3.1 Lippmann-Schwinger Equation

In this section we aim to understand the scatering theory in the time-dependent forms, which contrasting with the scattering in the stationary states from our ealier discussions. The Schroedinger equation can be written

$$\begin{aligned} i\hbar\frac{\partial}{\partial t}|\Psi(t)\rangle_S =& H|\Psi(t)\rangle_S \\ H =& H_0 + V \end{aligned}$$

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$$\cot x = \frac{1}{x} - \frac{1}{3}x \cdots$$

Thus,

$$\tan\delta_0 \to ka\frac{1}{3}(a\sqrt{-U_0})^2 = -\frac{U_0 k a^3}{3}$$

64

$$S_0 = \frac{e^{i\delta_0}}{e^{-i\delta_0}} = \frac{\cot\delta_0 + i}{\cot\delta_0 - i}$$

To be careful with the formal solution at $V = 0$, and we write

$$|\Psi(t)\rangle_S = e^{-iH_0 t/\hbar}|\Psi(t)\rangle$$

This gives, ($|\Psi(t)\rangle$ is called the interaction representation) [65]

$$\begin{aligned} i\hbar\frac{\partial}{\partial t}|\Psi(t)\rangle &= V(t)|\Psi(t)\rangle \\ V(t) &= e^{iH_0 t/\hbar} V e^{-iH_0 t/\hbar} \end{aligned}$$

Given that we write

$$|\Psi(t)\rangle = U_+(t)|\Psi(-\infty)\rangle$$

Thus, [66]

$$U_+(t) = 1 + \frac{1}{i\hbar}\int_{-\infty}^{t} d\tau\, V(\tau)U_+(\tau)$$

Especially in our case, we let

$$|\Psi(+\infty)\rangle = S|\Psi(-\infty)\rangle$$

be given, and have $S = U_+(+\infty)$ thus,

$$S = 1 + \frac{1}{i\hbar}\int_{-\infty}^{\infty} d\tau\, V(\tau)U_+(\tau)$$

65

$$\begin{aligned} i\hbar\frac{\partial}{\partial t}|\Psi(t)\rangle_S &= H_0 e^{-iH_0 t/\hbar}|\Psi(t)\rangle + e^{-iH_0 t/\hbar} i\hbar\frac{\partial}{\partial t}|\Psi(t)\rangle = (H_0 + V)e^{-iH_0 t/\hbar}|\Psi(t)\rangle \\ i\hbar\frac{\partial}{\partial t}|\Psi(t)\rangle &= e^{iH_0 t/\hbar} V e^{-iH_0 t/\hbar}|\Psi(t)\rangle \\ i\hbar\frac{\partial}{\partial t}|\Psi(t)\rangle &= V(t)|\Psi(t)\rangle \\ V(t) &= e^{iH_0 t/\hbar} V e^{-iH_0 t/\hbar} \end{aligned}$$

66

$$\begin{aligned} i\hbar\frac{\partial}{\partial t}U_+(t) &= V(t)U_+(t) \\ U_+(-\infty) &= 1 \end{aligned}$$

In the integral form we have

$$U_+(t) = 1 + \frac{1}{i\hbar}\int_{-\infty}^{t} d\tau\, V(\tau)U_+(\tau)$$

We now consider a case where the interactoin vanishes adiabatically at $t \to \pm\infty$ to have $H \to H_0$. For that we suppose

$$V(t) \to V(t)e^{-0|t|/\hbar} = V^\epsilon(t)$$

Under such condition, we take the eigenstate $|\Phi_i\rangle = \frac{1}{\sqrt{(2\pi)^3}} e^{i\boldsymbol{k}_i\cdot\boldsymbol{r}}$ for H_0 for the initial state. [67] [68] Which we write

$$\begin{aligned}|\Psi(-\infty)\rangle =& |\Phi_i\rangle \\ H_0|\Phi_i\rangle =& E_i|\Phi_i\rangle \\ \langle\Phi_i|\Phi_j\rangle =& 1_{ij} = \delta(\boldsymbol{k}_i - \boldsymbol{k}_j)\end{aligned}$$

We write the transition probability W_{ji} at $t : -\infty \to +\infty$ as

$$W_{ji} = |\langle\Phi_j|S\Phi_i\rangle|^2 = |S_{ji}|^2$$

Here we define

$$T = S - 1$$

which gives

$$\begin{aligned}i \neq j, \quad W_{ji} = |T_{ji}|^2 \\ T_{ji} =& \frac{1}{i\hbar}\int_{-\infty}^{\infty} d\tau\, \langle\Phi_j|V^\epsilon(\tau)U_+^\epsilon(\tau)|\Phi_i\rangle \\ =& \frac{1}{i\hbar}\int_{-\infty}^{\infty} d\tau\, e^{iE_j\tau/\hbar}\langle\Phi_j|Ve^{-iH_0\tau/\hbar}e^{-0|\tau|/\hbar}U_+(\tau)|\Phi_i\rangle\end{aligned}$$

Thus, we can write

$$|\Psi_i^{(+)}(E)\rangle = \int_{-\infty}^{\infty} d\tau\, e^{i(E-H_0)\tau/\hbar}e^{-0|\tau|/\hbar}U_+(\tau)|\Phi_i\rangle$$

This equation yields,

$$T_{ji} = \frac{1}{i\hbar}\langle\Phi_j|V|\Psi_i^{(+)}(E_j)\rangle$$

[67] The wavefunction for the interaction representation at $V = 0$ will be the wavefunction for the stationary states.

[68]

$$\langle\Phi_i|\Phi_j\rangle = \frac{1}{(2\pi)^3}\int d\boldsymbol{r}\, e^{-i(\boldsymbol{k}_i - \boldsymbol{k}_j)\cdot\boldsymbol{r}} = 1_{ij} = \delta(\boldsymbol{k}_i - \boldsymbol{k}_j)$$

The integral equation for U_+ gives [69] [70]

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$$
\begin{aligned}
|\Psi_i^{(+)}(E)\rangle =& \int_{-\infty}^{\infty} d\tau\, e^{i(E-H_0)\tau/\hbar} e^{-0|\tau|/\hbar} |\Phi_i\rangle \\
&+ \frac{1}{i\hbar}\int_{-\infty}^{\infty} d\tau\, e^{i(E-H_0)\tau/\hbar} e^{-0|\tau|/\hbar} \left(\int_{-\infty}^{\tau} d\tau'\, V^\epsilon(\tau') U_+^\epsilon(\tau')\right)|\Phi_i\rangle \\
=& \int_{-\infty}^{\infty} d\tau\, e^{i(E-H_0)\tau/\hbar} e^{-0|\tau|/\hbar} |\Phi_i\rangle \\
&+ \frac{1}{i\hbar}\int_{-\infty}^{\infty} d\tau' \int_{\tau'}^{\infty} d\tau\, e^{i(E-H_0)\tau/\hbar} e^{-0|\tau|/\hbar} V^\epsilon(\tau') U_+^\epsilon(\tau')|\Phi_i\rangle \\
=& \int_{-\infty}^{\infty} d\tau\, e^{i(E-H_0)\tau/\hbar} e^{-0|\tau|/\hbar} |\Phi_i\rangle \\
&+ \frac{1}{i\hbar}\int_{-\infty}^{\infty} d\tau' \int_{\tau'}^{\infty} d\tau\, e^{i(E-H_0)\tau/\hbar} e^{-0|\tau|/\hbar} e^{-0|\tau'|/\hbar} e^{iH_0\tau'/\hbar} V e^{-iH_0\tau'/\hbar} U_+^\epsilon(\tau')|\Phi_i\rangle \\
=& \int_{-\infty}^{\infty} d\tau\, e^{i(E-H_0)\tau/\hbar} e^{-0|\tau|/\hbar} |\Phi_i\rangle \\
&+ \frac{1}{i\hbar}\int_{-\infty}^{\infty} d\tau' e^{-0|\tau'|/\hbar} \int_{\tau'}^{\infty} d\tau e^{-0|\tau|/\hbar}\, e^{i(E-H_0)\tau/\hbar} e^{iH_0\tau'/\hbar} V e^{-iH_0\tau'/\hbar} U_+^\epsilon(\tau')|\Phi_i\rangle \\
=& \int_{-\infty}^{\infty} d\tau\, e^{i(E-H_0)\tau/\hbar} e^{-0|\tau|/\hbar} |\Phi_i\rangle \\
&+ \frac{1}{i\hbar}\int_{-\infty}^{\infty} d\tau' e^{-0|\tau'|/\hbar} \int_{\tau'}^{\infty} d\tau e^{-0|\tau|/\hbar}\, e^{i(E-H_0)(\tau-\tau')/\hbar} V e^{i(E-H_0)\tau'/\hbar} U_+^\epsilon(\tau')|\Phi_i\rangle \\
=& \int_{-\infty}^{\infty} d\tau\, e^{i(E-H_0)\tau/\hbar} e^{-0|\tau|/\hbar} |\Phi_i\rangle \\
&+ \frac{1}{i\hbar}\int_{-\infty}^{\infty} d\tau' e^{-0|\tau'|/\hbar} \int_{0}^{\infty} d\tau e^{-0|\tau|/\hbar}\, e^{i(E-H_0)\tau/\hbar} V e^{i(E-H_0)\tau'/\hbar} U_+^\epsilon(\tau')|\Phi_i\rangle \\
=& \int_{-\infty}^{\infty} d\tau\, e^{i(E-H_0)\tau/\hbar} e^{-0|\tau|/\hbar} |\Phi_i\rangle \\
&+ \frac{1}{i\hbar}\int_{0}^{\infty} d\tau e^{-0|\tau|/\hbar}\, e^{i(E-H_0)\tau/\hbar} V \int_{-\infty}^{\infty} d\tau' e^{-0|\tau'|/\hbar}\, e^{i(E-H_0)\tau'/\hbar} U_+^\epsilon(\tau')|\Phi_i\rangle \\
=& \int_{-\infty}^{\infty} d\tau\, e^{i(E-H_0)\tau/\hbar} e^{-0|\tau|/\hbar} |\Phi_i\rangle \\
&+ \frac{1}{i\hbar}\int_{0}^{\infty} d\tau e^{-0\tau/\hbar}\, e^{i(E-H_0)\tau/\hbar} V |\Psi_i^{(+)}(E)\rangle
\end{aligned}
$$

70 Recall the definition of the delta function

$$
\begin{aligned}
\frac{1}{x \pm i0} =& P\frac{1}{x} \mp i\pi\delta(x) \\
\delta(x) =& -\frac{1}{2\pi i}\left(\frac{1}{x+i0} - \frac{1}{x-i0}\right) = \frac{1}{\pi}\mathrm{Im}\,\frac{1}{x-i0}
\end{aligned}
$$

$$\begin{aligned}|\Psi_i^{(+)}(E)\rangle =& \int_{-\infty}^{\infty} d\tau\, e^{i(E-E_i)\tau/\hbar} e^{-0|\tau|/\hbar} |\Phi_i\rangle \\ &+ \frac{1}{i\hbar}\int_0^{\infty} d\tau e^{-0\tau/\hbar}\, e^{i(E-H_0)\tau/\hbar} V|\Psi_i^{(+)}(E)\rangle \\ =& 2\pi\hbar\delta(E-E_i)|\Phi_i\rangle + \frac{1}{E+i0-H_0} V|\Psi_i^{(+)}(E)\rangle\end{aligned}$$

We can write the eqution above in the form

$$|\Psi_i^{(+)}(E)\rangle = 2\pi\hbar\delta(E-E_i)|\Psi_i^{(+)}\rangle \qquad (*)$$

This enables us to derive the Lippmann-Schwinger equation

$$|\Psi_i^{(+)}\rangle = |\Phi_i\rangle + \frac{1}{E+i0-H_0} V|\Psi_i^{(+)}\rangle$$

Note that $(*)$ is [71]

$$e^{-iH_0t/\hbar} U_+(t)|\Phi_i\rangle = e^{-iE_it/\hbar}|\Psi_i^{(+)}\rangle$$

The left-hand side of the equation above represents the wavefunction for the Schroedinger representation, while we regard $|\Psi_i^{(+)}\rangle$ as the wavefunction for the stationary states. [72]

$$\int_0^{\infty} d\tau\, e^{-0\,\tau/\hbar + i(E-H_0)\tau/\hbar} = \int_0^{\infty} d\tau\, e^{i(E+i0-H_0)\tau/\hbar} = -\frac{\hbar}{i}\frac{1}{E+i0-H_0} = -\frac{\hbar}{i}\left(P\frac{1}{E-H_0} - i\pi\delta(E-H_0)\right)$$

[71]

$$\begin{aligned}|\Psi_i^{(+)}(E)\rangle &= \int_{-\infty}^{\infty} d\tau\, e^{i(E-H_0)\tau/\hbar} U_+(\tau)|\Phi_i\rangle \\ &= \int_{-\infty}^{\infty} d\tau\, e^{i(E-E_i)\tau/\hbar}|\Psi_i^{(+)}\rangle \\ e^{-iH_0\tau/\hbar}U_+(\tau)|\Phi_i\rangle &= e^{-iE_i\tau/\hbar}|\Psi_i^{(+)}\rangle\end{aligned}$$

[72] The relationship between the state vector $|\Psi(t)\rangle$ in the interaction representation and the state vector $|\Psi(t)\rangle_S$ in the Schroedinger representation gives

$$e^{-iH_0t/\hbar}U_+(t)|\Phi_i\rangle = e^{-iH_0t/\hbar}|\Psi_i(t)\rangle = |\Psi_i(t)\rangle_S = e^{-iE_it/\hbar}|\Psi_i^{(+)}\rangle$$

In our last discussion, we let $|\Psi_i(t)\rangle$ prossess the same energy E_i of $|\Phi_i\rangle$. Precisely, we consider the system in the box with the length of each ede to be L. The interaction is adiabactically applied slower than the energy resolution occurring the same time. We assume the interaction to take the limit of $L \to \infty$ knowing that the interaction may give the energy hift of about $1/L^3$ from the fact that the potential is much local.

3.2 Optical Theory

We further write [73]

$$
\begin{aligned}
T_{ji} \equiv& -2\pi i\delta(E_i - E_j)\boldsymbol{T}_{ji} togive \\
\boldsymbol{T}_{ji} =& \langle\Phi_j|V|\Psi_i^{(+)}\rangle
\end{aligned}
$$

The scattering probability for $i \to j$ per unit of time can be written [74]

$$
w_{ji} = \frac{2\pi}{\hbar}\delta(E_i - E_j)|\boldsymbol{T}_{ji}|^2
$$

If the equation above is approximated by $|\Psi_i^{(+)}\rangle \approx |\Phi_i\rangle$, which will be called the Fermi's golden rule.

We write the Green's function first;

$$
\begin{aligned}
G_0^+ =& \frac{1}{E + i0 - H_0} \\
G^+ =& \frac{1}{E + i0 - H} = \frac{1}{E + i0 - H_0 - V} = [(G_0^+)^{-1} - V]^{-1} = [(1 - VG_0^+)G_0^{+\,-1}]^{-1} \\
=& G_0^+(1 - VG_0^+)^{-1} = G_0^+ + G_0^+(VG_0^+) + G_0^+(VG_0^+)^2 + \cdots \\
=& G_0^+ + (G_0^+V)G_0^+ + (G_0^+V)^2G_0^+ + \cdots = (1 - G_0^+V)^{-1}G_0^+
\end{aligned}
$$

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$$
\begin{aligned}
|\Psi_i^{(+)}(E)\rangle =& 2\pi\hbar\delta(E - E_i)|\Psi_i^{(+)}\rangle \\
T_{ji} =& \frac{1}{i\hbar}\langle\Phi_i|V|\Psi_i^{(+)}(E_j)\rangle \\
=& -2\pi i\delta(E_j - E_i)\boldsymbol{T}_{ji} gives \\
\boldsymbol{T}_{ji} =& \langle\Phi_j|V|\Psi_i^{(+)}\rangle
\end{aligned}
$$

74

$$
\begin{aligned}
W_{ji} =& 4\pi^2\big(\delta(E_i - E_j)\big)^2|\boldsymbol{T}_{ji}|^2 \\
=& 4\pi^2\delta(E_i - E_j)|\boldsymbol{T}_{ji}|^2(\frac{1}{2\pi\hbar})\int_{-\infty}^{\infty} d\tau\, e^{i(E_i - E_j)\tau/\hbar} \\
=& \frac{2\pi}{\hbar}\delta(E_i - E_j)|\boldsymbol{T}_{ji}|^2\int_{-\infty}^{\infty} d\tau\, 1 \\
w_{ji} =& \frac{W_{ji}}{\int_{-\infty}^{\infty} d\tau\, 1} = \frac{2\pi}{\hbar}\delta(E_i - E_j)|\boldsymbol{T}_{ji}|^2
\end{aligned}
$$

Here we rewrite the Lippmann-Schwinger equation:

$$
\begin{aligned}
|\Psi_i^{(+)}\rangle =&|\Phi_i\rangle + G_{0,i}^{(+)}V|\Psi_i^{(+)}\rangle = (1+G_{0,i}^{+}V+(G_{0,i}^{+}V)^2+\cdots)|\Phi_i\rangle = (1+G_i^{+}V)|\Phi_i\rangle,\\
&G_{0,i}^{+}=G_0^{+}(E_i),\ G_i^{+}=G^{+}(E_i)\\
V|\Psi_i^{(+)}\rangle =&V(1+G_i^{+}V)|\Phi_i\rangle \equiv T(E_i)|\Phi_i\rangle\\
T(E) =&V(1+G^{+}(E)V)\\
|\Psi_i^{(+)}\rangle =&\big(1+G_0^{+}(E_i)T(E_i)\big)|\Phi_i\rangle
\end{aligned}
$$

Since $|\Psi_i^{(+)}\rangle$ and $|\Phi_i\rangle$ are linked by a unitary transformation, we can write

$$\langle\Psi_j^{(+)}|\Psi_i^{(+)}\rangle =\langle\Phi_j|\Phi_i\rangle$$

While we can write

$$\boldsymbol{T}_{ji} =\langle\Phi_j|V|\Psi_i^{(+)}\rangle = \langle\Phi_j|T_i|\Phi_i\rangle$$

which yields to

$$\langle\Psi_j^{(+)}|\Psi_i^{(+)}\rangle =\langle\Phi_j|\Phi_i\rangle + \langle\Phi_j|G_{0i}^{+}T_i|\Phi_i\rangle + \langle\Phi_j|T_j^{*}G_{0,j}^{+*}|\Phi_i\rangle + \langle\Phi_j|T_j^{*}G_{0,j}^{+*}G_{0,i}^{+}T_i|\Phi_i\rangle$$

Thus, [75]

$$-\mathrm{Im}\,\boldsymbol{T}_{ii} =\pi\sum_k \delta(E_i-E_k)|\boldsymbol{T}_{ik}|^2$$

---

[75]

$$
\begin{aligned}
0 =&\frac{1}{E_i-E_j+i0}\langle\Phi_j|T_i|\Phi_i\rangle + \frac{1}{E_j-E_i-i0}\langle\Phi_j|T_j^{*}|\Phi_i\rangle\\
&+\sum_k\langle\Phi_j|T_j^{*}G_{0,j}^{+*}|\Phi_k\rangle\langle\Phi_k|G_{0,i}^{+}T_i|\Phi_i\rangle\\
=&\frac{1}{E_i-E_j+i0}\langle\Phi_j|T_i|\Phi_i\rangle + \frac{1}{E_j-E_i-i0}\langle\Phi_j|T_j^{*}|\Phi_i\rangle\\
&+\sum_k \frac{1}{E_j-E_k-i0}\frac{1}{E_i-E_k+i0}\langle\Phi_j|T_j^{*}|\Phi_k\rangle\langle\Phi_k|T_i|\Phi_i\rangle\\
=&\left(P\frac{1}{E_i-E_j}-i\pi\delta(E_i-E_j)\right)(\boldsymbol{T}_{ji}-\boldsymbol{T}_{ij}^{*})\\
&+\frac{1}{E_j-E_i-i0}\sum_k\left(\frac{1}{E_i-E_k+i0}-\frac{1}{E_j-E_k-i0}\right)\boldsymbol{T}_{kj}^{*}\boldsymbol{T}_{ki}\\
=&\left(P\frac{1}{E_i-E_j}-i\pi\delta(E_i-E_j)\right)(\boldsymbol{T}_{ji}-\boldsymbol{T}_{ij}^{*})\\
&+\frac{1}{E_j-E_i-i0}\sum_k\left(P\frac{1}{E_i-E_k}-P\frac{1}{E_j-E_k}-i\pi\big(\delta(E_i-E_k)+\delta(E_j-E_k)\big)\right)\boldsymbol{T}_{kj}^{*}\boldsymbol{T}_{ki}\\
=&\left(P\frac{1}{E_i-E_j}-i\pi\delta(E_i-E_j)\right)(\boldsymbol{T}_{ji}-\boldsymbol{T}_{ij}^{*})\\
&-\left(P\frac{1}{E_i-E_j}-i\pi\delta(E_i-E_j)\right)\sum_k\left(P\frac{1}{E_i-E_k}-P\frac{1}{E_j-E_k}-i\pi\big(\delta(E_i-E_k)+\delta(E_j-E_k)\big)\right)\boldsymbol{T}_{kj}^{*}\boldsymbol{T}_{ki}
\end{aligned}
$$

This equation in fact is equivalent to $S^\dagger S = 1$. [76]

The optical theorem written below takes the same value as the equation above. [77]

$$\mathrm{Im}\, f(0) = \frac{k_i}{4\pi} \int d\Omega_k |f(\theta_k)|^2$$

Thus,

$$(\boldsymbol{T}_{ji} - \boldsymbol{T}^*_{ij}) = \sum_k \Big(P\frac{1}{E_i - E_k} - P\frac{1}{E_j - E_k} - i\pi\big(\delta(E_i - E_k) + \delta(E_j - E_k)\big)\Big) \boldsymbol{T}^*_{kj} \boldsymbol{T}_{ki}$$

Let us have $i = j$, and we obtain

$$2i\mathrm{Im}\, \boldsymbol{T}_{ji} = \sum_k -2i\pi\delta(E_i - E_k)|\boldsymbol{T}_{ki}|^2$$

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$$\begin{aligned}
(1 + T^\dagger)(1 + T) =& 1 \\
-(T + T^\dagger) =& T^\dagger T \\
2\pi i\delta(E_i - E_j)(\boldsymbol{T}_{ij} - \boldsymbol{T}^\dagger_{ij}) =& -(2\pi i)^2 \sum_k \delta(E_i - E_k)\delta(E_k - E_j)\boldsymbol{T}^\dagger_{ik}\boldsymbol{T}_{kj} \\
2\pi i\delta(E_i - E_j)(\boldsymbol{T}_{ij} - \boldsymbol{T}^*_{ji}) =& 4\pi^2\delta(E_i - E_j) \sum_k \delta(E_i - E_k)\boldsymbol{T}^*_{ki}\boldsymbol{T}_{kj} \\
where i = j, we obtain \quad - \mathrm{Im}\, \boldsymbol{T}_{ii} =& \pi \sum_k \delta(E_i - E_k)|\boldsymbol{T}_{ik}|^2
\end{aligned}$$

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$$\begin{aligned}
\sum_k \delta(E_i - E_k) =& \int dk\, k_k^2 \delta(\frac{\hbar^2}{2m}(k_i^2 - k_k^2)) \int d\Omega_k \\
=& \frac{2m}{\hbar^2} \int dk\, k_k^2 \frac{1}{2k_k}\delta(k_i - k_k) \int d\Omega_k \\
f(\theta_{ij}) =& -\frac{2m}{\hbar^2}\frac{(2\pi)^3}{4\pi}\boldsymbol{T}_{ij} \\
\mathrm{Im}\, f(0) =& \pi\frac{2m}{\hbar^2} \int dk_k \frac{1}{2k_k}\delta(k_i - k_k)k_k^2 \frac{\hbar^2}{2m}\frac{4\pi}{(2\pi)^3} \int d\Omega_k |f(\theta_k)|^2 \\
=& \frac{k_i}{4\pi} \int d\Omega_k |f(\theta_k)|^2
\end{aligned}$$