Phys 506 lecture 21: Introduction to Scattering II

1 Lippman-Schwinger Equation Continued

Last time, we derived the Lippman-Schwinger equation:

$$|\psi\rangle = |\psi_0\rangle + \frac{1}{E - \hat{H}_0 + i\delta}\hat{V}|\psi\rangle.$$

Let's examine it in coordinate space by multiplying by $\langle x|$ on the left and introducing the complete set of states $\int |x'\rangle\langle x'| = \mathbb{I}$ between the fraction and the $\hat{V}$:

$$\psi(x) = \psi_0(x) + \int dx' \, \langle x|\frac{1}{E - \hat{H}_0 + i\delta}|x'\rangle V(x')\psi(x').$$

Introduce the complete set of states $\int |p\rangle\langle p| \, dp = \mathbb{I}$ on the left to get:

$$\langle x|\frac{1}{E - \hat{H}_0 + i\delta}|x'\rangle = \int dp \, \langle x|p\rangle\langle p|\frac{1}{E - \hat{H}_0 + i\delta}|p\rangle\langle p|x'\rangle.$$

But $\langle x|p\rangle = \frac{e^{ipx/\hbar}}{\sqrt{2\pi\hbar}}$ and $\hat{H}_0|p\rangle = \frac{p^2}{2m}|p\rangle$, where $\frac{p^2}{2m}$ is a number. Thus:

$$\begin{aligned}\langle x|\frac{1}{E - \hat{H}_0 + i\delta}|x'\rangle &= \int dp \, \frac{e^{ipx/\hbar}}{\sqrt{2\pi\hbar}} \frac{1}{E - \frac{p^2}{2m} + i\delta} \frac{e^{-ipx'/\hbar}}{\sqrt{2\pi\hbar}} \\ &= \int dp \, \frac{e^{ip(x-x')/\hbar}}{2\pi\hbar} \frac{1}{\left(\sqrt{E + i\delta} - \frac{p^2}{2m}\right)\left(\sqrt{E + i\delta} + \frac{p^2}{2m}\right)}\end{aligned}$$

You can integrate this using residues. If you don't know how to do this, don't worry. The answer is:

$$\begin{aligned}\langle x|\frac{1}{E - \hat{H}_0 + i\delta}|x'\rangle &= -i\sqrt{\frac{2m}{\hbar^2}}\frac{1}{2\sqrt{E}}\left[\Theta(x-x')e^{i\sqrt{\frac{2mE}{\hbar^2}}(x-x')} + \Theta(x'-x)e^{-i\sqrt{\frac{2mE}{\hbar^2}}(x-x')}\right] \\ &= -i\frac{\sqrt{2mE}}{\hbar}\frac{1}{2E}\left[\Theta(x-x')e^{i\sqrt{2mE}(x-x')/\hbar} + \Theta(x'-x)e^{-i\sqrt{2mE}(x-x')/\hbar}\right]\end{aligned}$$

Let: $k = \sqrt{\frac{2mE}{\hbar^2}}$ and choose $\psi_0(x) = e^{ikx}$, corresponding to an incident wave moving to the right. Then:

$$\begin{aligned}\psi(x) &= e^{ikx} - \frac{ik}{2E}\int_{-\infty}^{x} e^{-ik(x-x')}V(x')\psi(x')\,dx' - \frac{ik}{2E}\int_{x}^{\infty} e^{ik(x-x')}V(x')\psi(x')\,dx' \\ &= e^{ikx}\left(1 - \frac{ik}{2E}\int_{-\infty}^{x} e^{-ik(x-x')}V(x')\psi(x')\,dx'\right) - \frac{ik}{2E}e^{-ikx}\int_{x}^{\infty} e^{ikx'}V(x')\psi(x')\,dx'.\end{aligned}$$

If we consider the limit when $x \to +\infty$:

$$t = 1 - \frac{ik}{2E}\int_{-\infty}^{\infty} e^{-ikx'}V(x')\psi(x')\,dx'$$

and in the limit when $x \to -\infty$:

$$r = -\frac{ik}{2E}\int_{-\infty}^{\infty} e^{ikx'}V(x')\psi(x')\,dx'.$$

Since $\psi(x)$ represents scattering to the right, we write $|\psi\rangle = |\psi_{\rightarrow}\rangle$ and so:

$$\psi_0(x) = e^{ikx} = \langle x|\psi_{0\rightarrow}\rangle \quad \text{and} \quad e^{-ikx} = \langle x|\psi_{0\leftarrow}\rangle$$

Thus, we can write:

$$r_{\rightarrow} = -\frac{ik}{2E}\langle\psi_{0\leftarrow}|\hat{V}|\psi_{\rightarrow}\rangle \quad \text{and} \quad t_{\rightarrow} = 1 - \frac{ik}{2E}\langle\psi_{0\rightarrow}|\hat{V}|\psi_{\rightarrow}\rangle.$$

2 Formal Solution and the Born Series

Let:

$$|\psi\rangle = |\psi_0\rangle + \frac{1}{E - \hat{H}_0 + i\delta}\hat{V}|\psi\rangle$$

and define

$$\frac{1}{E - \hat{H}_0 + i\delta} = \hat{G}_{0+}(E)$$

so:

$$|\psi\rangle = \left[1 - \hat{G}_{0+}(E)\hat{V}\right]^{-1}|\psi_0\rangle.$$

You may want to compare this with how we had organized pertrubation theory for bound states previously. The reflection $r_{\rightarrow}$ and transmission $t_{\rightarrow}$ coefficients are given by:

$$\begin{cases} r_{\rightarrow} = -\frac{ik}{2E}\langle\psi_0|\hat{V}\left[1 - \hat{G}_{0+}(E)\hat{V}\right]^{-1}|\psi_0\rangle \\ t_{\rightarrow} = 1 - \frac{ik}{2E}\langle\psi_0|\hat{V}\left[1 - \hat{G}_{0+}(E)\hat{V}\right]^{-1}|\psi_0\rangle. \end{cases}$$

Expand in a geometric series:

$$|\psi_{\rightarrow}\rangle = \sum_{n=0}^{\infty} \left(\hat{G}_{0+}(E)\hat{V}\right)^n |\psi_{0\rightarrow}\rangle,$$

giving us:

$$\begin{cases} r_{\rightarrow} = -\frac{ik}{2E}\sum_{n=0}^{\infty}\langle\psi_{0\leftarrow}|\hat{V}\left(\hat{G}_{0+}(E)\hat{V}\right)^n|\psi_{0\rightarrow}\rangle \\ t_{\rightarrow} = 1 - \frac{ik}{2E}\sum_{n=0}^{\infty}\langle\psi_{0\rightarrow}|\hat{V}\left(\hat{G}_{0+}(E)\hat{V}\right)^n|\psi_{0\rightarrow}\rangle. \end{cases}$$

This is a formal series, similar to perturbation theory for bound states, that we can expand to obtain subsequently more accurate approximations to the scattering problem solutions. The case when $n = 1$ is called the **Born Approximation**:

$$\begin{cases} |\psi_{\rightarrow}^{\text{Born}}\rangle = |\psi_{0\rightarrow}\rangle + \hat{G}_{0+}(E)\hat{V}|\psi_{0\rightarrow}\rangle \\ \psi_{\rightarrow}^{\text{Born}}(x) = e^{ikx} + \int_{-\infty}^{\infty} dx'\,\hat{G}_{0+}(x-x')V(x')e^{ikx'} \\ r_{\rightarrow}^{\text{Born}} = -\frac{ik}{2E}\langle\psi_{0\leftarrow}|\hat{V}|\psi_{0\rightarrow}\rangle = -\frac{ik}{2E}\int_{-\infty}^{\infty} dx\,V(x)e^{2ikx} \\ t_{\rightarrow}^{\text{Born}} = 1 - \frac{ik}{2E}\langle\psi_{0\rightarrow}|\hat{V}|\psi_{0\rightarrow}\rangle = 1 - \frac{ik}{2E}\int_{-\infty}^{\infty} dx\,e^{ikx}V(x)e^{ikx} \approx e^{\frac{ik}{2E}\int_{-\infty}^{\infty}dx\,V(x)} \end{cases}$$

Since we assume $\hat{V}$ is small, $r_{\rightarrow}^{\text{Born}} \sim 0$ and $t_{\rightarrow}^{\text{Born}} \sim 1$. Hence, the Born approximation works well when most of the wave is transmitted.

3 3D Scattering

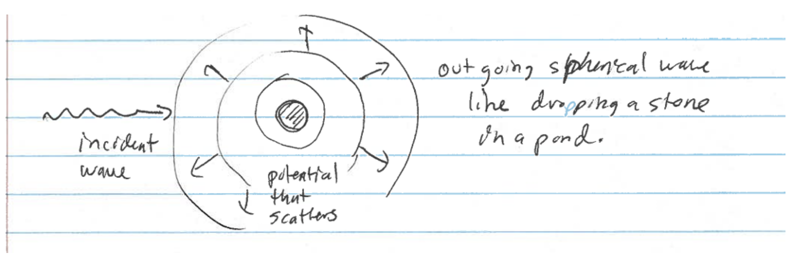

Figure 1: In spherical potential scattering, we have a plane wave come in, scatter of a center and come out in spherical waves, similar to what happens when a pebble is dropped into a pond.

Recall expansion of plane wave in spherical harmonics with $E = \frac{\hbar^2 k^2}{2m}$ and thus $k = \frac{\sqrt{2mE}}{\hbar}$:

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

where $j_\ell(kr) = \sqrt{\frac{\pi}{2kr}} J_{\ell+\frac{1}{2}}(kr)$ is a spherical Bessel function and $P_\ell(\cos\theta)$ a Legendre polynomial. Recall as well that as $r \to \infty$, we have:

$$j_\ell(kr) \to \frac{1}{kr} \sin\left(kr - \frac{\ell\pi}{2}\right).$$

Thus for $r \to \infty$:

$$f_\ell(r) \to C_\ell \sin\left(kr - \frac{\ell\pi}{2}\right) = C_\ell\left(e^{i(kr-\frac{\ell\pi}{2})} - e^{-i(kr-\frac{\ell\pi}{2})}\right),$$

where the term $e^{i(kr-\frac{\ell\pi}{2})}$ is an outgoing wave and $e^{-i(kr-\frac{\ell\pi}{2})}$ an incoming wave.

For an interacting case, where $V(r) \to 0$ faster than the centrifugal potential $\frac{\hbar^2\ell(\ell+1)}{2mr^2}$, we expect as $r \to \infty$

$$f_\ell(r) \to A_\ell(k)\left(e^{-ikr} + r_\ell(k)e^{ikr}\right)$$

where $A_\ell(k)$ is a constant, e^{-ikr} an incident wave, and $r_\ell(k)e^{ikr}$ a reflected wave. This is because nothing can transmit through $r = 0$ (recall analogy to a 1D infinite wall at $r = 0$). But in 1D we have $R + T = 1$ which implies if $T = 0$, then $R = 1$. Thus $r = e^{i\phi} =$ phase and we write:

$$r_\ell(k) = -e^{i(2\delta_\ell(k)-\ell\pi)}$$

with $\delta_\ell(k)$ being the ℓ-th partial wave phase shift. Substituting in to find:

$$\begin{aligned} f_\ell(r) &\to A_\ell(k)\left(e^{-ikr} - e^{i(2\delta_\ell(k)-\ell\pi+kr)}\right) \\ &= A_\ell(k)e^{i(\delta_\ell(k)-\frac{\ell\pi}{2})}2i\sin\left(kr + \delta_\ell(k) - \frac{\ell\pi}{2}\right) \\ &= B_\ell(k)\sin\left(kr + \delta_\ell(k) - \frac{\ell\pi}{2}\right). \end{aligned}$$

For the free case, $V = 0$ and $\delta_\ell(k) = 0$ for all ℓ and k.

Example 3.1. Consider a spherical well as pictured below.

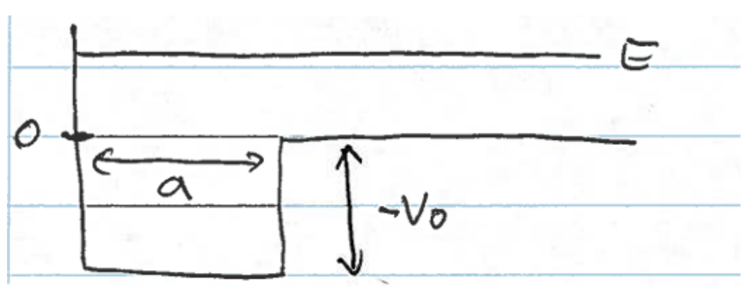

Figure 2: A spherical well with an infinite potential for the unphysical region with $r < 0$, a negative potential $-V_0$ for $0 < r < a$ and then 0 potential for $r > a$.

Define:

$$\begin{cases} k_1 = \frac{1}{\hbar}\sqrt{2m(E+V_0)} & \text{for } r < a, \\ k_2 = \frac{1}{\hbar}\sqrt{2mE} & \text{for } r > a, \end{cases}$$

with $E > 0$. Then we have:

$$R_\ell(r) = \begin{cases} A_\ell(E) j_\ell(k_1 r), & r < a, \\ B_\ell(E) j_\ell(k_2 r) + C_\ell(E)\eta_\ell(k_2 r), & r > a, \end{cases}$$

where there is no restriction on the wave functions for $r > a$ since $r = 0$ is not within this region. Now, continuity of ψ at $r = a$ tells us:

$$A_\ell(E) j_\ell(k_1 a) = B_\ell(E) j_\ell(k_2 a) + C_\ell(E)\eta_\ell(k_2 a).$$

And continuity of $\frac{d\psi}{dr} = \psi'$ at $r = a$ tells us:

$$k_1 A_\ell(E) j_\ell'(k_1 a) = k_2 B_\ell(E) j_\ell'(k_2 a) + k_2 C_\ell(E)\eta_\ell'(k_2 a).$$

We now want to solve for the coefficients $B_\ell(E)/A_\ell(E)$ and $C_\ell(E)/A_\ell(E)$. We find:

$$\frac{B_\ell(E)}{A_\ell(E)} = \frac{k_2 \eta_\ell(k_2 a) j_\ell'(k_1 a) - k_1 j_\ell(k_1 a)\eta_\ell'(k_2 a)}{k_2 \eta_\ell(k_2 a) j_\ell'(k_2 a) - k_2 j_\ell(k_2 a)\eta_\ell'(k_2 a)},$$

and:

$$\frac{C_\ell(E)}{A_\ell(E)} = \frac{k_2 j_\ell'(k_2 a) j_\ell(k_1 a) - k_1 j_\ell'(k_1 a) j_\ell(k_2 a)}{k_2 \eta_\ell(k_2 a) j_\ell'(k_2 a) - k_2 j_\ell(k_2 a)\eta_\ell'(k_2 a)}.$$

Note that:

$$\eta_\ell(p) \to -\frac{1}{p}\cos\left(p - \ell\frac{\pi}{2}\right).$$

Yes, it is a mess. One would want to ultimately extract the scattering phase shifts from this, but we are not going to show that here.