Phys 506 lecture 20: Introduction to scattering

1 Introduction to scattering

Start with time-dependent Schrodinger equation in coordinate basis

$$i\hbar\frac{\partial}{\partial t}\psi(\mathbf{r},t) = \left(-\frac{\hbar^2}{2m}\nabla^2 + V(\mathbf{r})\right)\psi(\mathbf{r},t).$$

The probability density to find the particle in the region around $\mathbf{r}$ is

$$\rho(\mathbf{r},t) = |\psi(\mathbf{r},t)|^2 = \psi^*(\mathbf{r},t)\psi(\mathbf{r},t).$$

The equation of continuity says that the change in the particle density must arise from the flow of currents, since particles are not created or destroyed. So

$$\frac{d}{dt}\rho(\mathbf{r},t) + \nabla\cdot\mathbf{J}(\mathbf{r},t) = 0$$

is the equation of continuity (recall electromagnetism).

We use this equation to find $\mathbf{J}$:

$$\frac{d}{dt}\rho(\mathbf{r},t) = \frac{\partial}{\partial t}\psi^*(\mathbf{r},t)\psi(r,t) + \psi^*(\mathbf{r},t)\frac{\partial}{\partial t}\psi(\mathbf{r},t).$$

But

$$\frac{\partial}{\partial t}\psi = \frac{i\hbar}{2m}\nabla^2\psi + \frac{V}{i\hbar}\psi \qquad \text{and} \quad \frac{\partial}{\partial t}\psi^* = -\frac{i\hbar}{2m}\nabla^2\psi^* + \frac{V}{i\hbar}\psi^*$$

So

$$\begin{aligned}\frac{d}{dt}\rho(\mathbf{r},t) &= \frac{i\hbar}{2m}\left(\psi^*\nabla^2\psi - \nabla^2\psi^*\psi\right) + \frac{V}{i\hbar}\left(\psi^*\psi - \psi^*\psi\right)\\ &= \nabla\cdot\frac{i\hbar}{2m}\left(\psi^*\nabla\psi - \nabla\psi^*\psi\right) \qquad \text{because } \nabla\psi^*\cdot\nabla\psi \text{ terms cancel}\\ \Rightarrow &\boxed{\mathbf{J} = \frac{\hbar}{2im}\left(\psi^*\nabla\psi - \nabla\psi^*\psi\right)}\end{aligned}$$

Check: for a free particle

$$\psi_{\text{free}}(\mathbf{r},t) = e^{i\mathbf{k}\cdot\mathbf{r} - i\frac{\hbar k^2}{2m}t}$$

$$\mathbf{J} = \frac{\hbar\mathbf{k}}{2m}\times 2\psi^*\psi = \frac{\hbar\mathbf{k}}{m}\psi^*(\mathbf{r},t)\psi(\mathbf{r},t)$$

But $\frac{\hbar\mathbf{k}}{m} = \mathbf{v} =$ velocity $\Rightarrow$ current takes probability to find particle at position $\mathbf{r}$ at time t and multiplies by the particle's velocity. This is what a current should be.

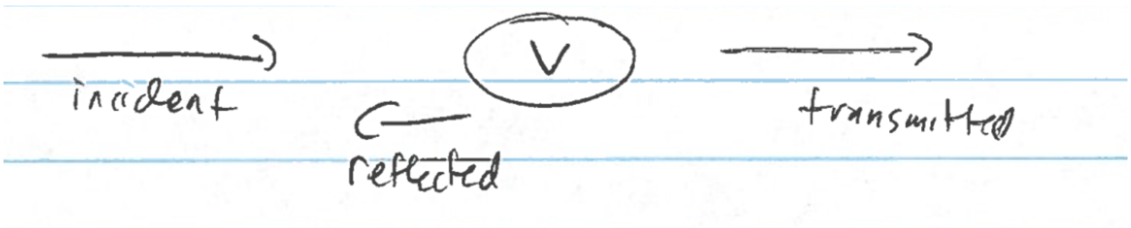

Figure 1: Schematic of a scattering experiment in one-d. The incident wave enters from the left, goes to the scattering center, denoted by V and then is either transmitted or reflected.

2 Example: Scattering in one dimension

Simple example of 1D scattering—delta function potential at $x = 0$:

$$V(x) = -\lambda\delta(x) \quad \lambda > 0$$

We have an incident wave from the left (looks like e^{ikx} far away)

So for

$$\begin{array}{ll} x < 0 & \psi(x,t) = \psi_{\text{incident}}(x,t) + \psi_{\text{reflected}}(x,t) \\ x > 0 & \psi(x,t) = \psi_{\text{transmitted}}(x,t) \quad \text{assume stationary so no } t \text{ dependence} \end{array}$$

$$\psi(x,t) = \begin{cases} A(e^{ikx} + re^{-ikx}) & x < 0 \\ Ate^{ikx} & x > 0 \end{cases}$$

$r =$ Reflection amplitude $\qquad t =$ Transmission amplitude

Now, we use the fact that $\psi(x)$ is continuous across $x = 0$. This implies that $A(1 + r) = At$ or $1 + r = t$.

Now, the potential vanishes everywhere except at $x = 0$. But, $\left.\frac{d\psi}{dx}\right|_{x=0^+} - \left.\frac{d\psi}{dx}\right|_{x=0^-} = \int_{x=0^-}^{x=0^+} dx \frac{d^2\psi}{dx^2} = -\frac{2m}{\hbar^2}\int_{x=0^-}^{x=0^+} dx \frac{-\hbar^2}{2m}\frac{d^2\psi}{dx^2}$ and $-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} = (E - V(x))\psi$, so

$$\left.\frac{d\psi}{dx}\right|_{x=0^+} - \left.\frac{d\psi}{dx}\right|_{x=0^-} = -\frac{2m}{\hbar^2}E\left(\underbrace{\psi\left(x{=}0^+\right) - \psi\left(x{=}0^-\right)}_{0 \text{ since } \psi \text{ is continuous}}\right) - \frac{2m\lambda}{\hbar^2}\psi(x{=}0)$$

From this result, we can read off what the amplitudes are, so

$$Aikt - Aik(1 - r) = -\frac{2m\lambda}{\hbar^2}At \qquad \text{with } r = t - 1.$$

Hence,

$$ik(t - 1 + t - 1) = -\frac{2m\lambda}{\hbar^2}t \qquad \text{and} \quad t = \frac{2ik}{2ik + \frac{2m\lambda}{\hbar^2}} = \frac{+i\frac{\hbar^2 k}{m\lambda}}{1 + \frac{i\hbar^2 k}{m\lambda}}.$$

Simplifying, we have

$$\boxed{r = t - 1 = -\frac{1}{1 + i\frac{\hbar^2 k}{m\lambda}} \quad \text{and} \quad t = \frac{+i\frac{\hbar^2 k}{m\lambda}}{1 + i\frac{\hbar^2 k}{m\lambda}}}$$

Note that these results satisfy $|r|^2+|t|^2=1$

$$|r|^2 = R = \text{ reflection coefficient}$$
$$|t|^2 = T = \text{ transmission coefficient}$$

$R+T=1$ is a consequence of conservation of probability, hence it always holds.

3 Formal theory for one-dimensional scattering

Now we treat a more formal theory of one -dimensional scattering.

We start from time dependent Schrodinger equation

$$i\hbar\frac{\partial}{\partial t}|\psi(t)\rangle = \left(\hat{H}_0+\hat{V}\right)|\psi(t)\rangle \quad \text{and} \quad \hat{H}_0 = \frac{\hat{P}^2}{2m} = \text{ kinetic energy.}$$

We define the Green's function to satisfy

$$\left(i\hbar\frac{\partial}{\partial t}-\hat{H}_0\right)\hat{G}_0\left(t,t'\right)=\delta\left(t-t'\right) \qquad \text{which is called the equation of motion}$$

Since the delta function acts like a unit matrix, one can think of Green's function as the inverse of the left most operator in the above equation ($M^{-1}M=\mathbf{I}$).

Since G_0 has a delta function in its equation of motion, it must be discontinuous at $t=t'$.

Immediately, we break up the Green's function into its two different pieces

$$\hat{G}_0\left(t,t'\right)=\hat{G}_{0+}\left(t,t'\right)+\hat{G}_{0-}\left(t,t'\right)$$
$$\hat{G}_{0+}\left(t,t'\right)=-\frac{i}{\hbar}\theta\left(t-t'\right)e^{-i\hat{H}_0(t-t')/\hbar} \quad \text{retarded}$$
$$\hat{G}_{0-}\left(t,t'\right)=\frac{i}{\hbar}\theta\left(t'-t\right)e^{-i\hat{H}_0(t-t')/\hbar} \quad \text{advanced}$$

This solves the equation of motion, where

$$\theta(t)=\left[\begin{array}{ll}0 & t<0\\ 1 & t>0\end{array}\right. \quad \text{and} \quad \frac{d}{dt}\theta(t)=\delta(t)$$

as can be seen by noting $\frac{d}{dt}\theta(t)=0$ everywhere except at $t=0$ where we have that $\int_{t=0-}^{t=0+}\frac{d}{dt}\theta(t)dt=\theta\left(t{=}0+\right)-\theta(t{=}0-)=1-0=1$. So $\frac{d}{dt}\theta(t)=0$ everywhere and $\int_{0-}^{0+}dt\frac{d}{dt}\theta(t)=1\Rightarrow$ delta function.

Using $\hat{G}_0$ we find

$$|\psi(t)\rangle=|\psi_0(t)\rangle+\int_{-\infty}^{+\infty}dt'\hat{G}_0\left(t,t'\right)\hat{V}\left(t'\right)|\psi(t)\rangle$$

Where $|\psi_0(t)\rangle$ is the free quantum state, which satisfies

$$i\hbar\frac{d}{dt}\bigg|\,\psi_0(t)\bigg\rangle=\hat{H}_0\left|\psi_0(t)\right\rangle.$$

Proof:
$$\underbrace{\left(i\hbar\frac{d}{dt}-\hat{H}_0\right)}_{\text{from R.H.S}}|\psi(t)\rangle=\underbrace{\left(i\hbar\frac{d}{dt}-\hat{H}_0\right)}_{\text{is zero}}|\psi_0(t)\rangle+\underbrace{\hat{V}(t)|\psi(t)\rangle}_{\text{from full Schro. eq'n}}.$$

Now multiply by the inverse-operator from the left

$$\left(i\hbar\frac{d}{dt}-\hat{H}_0\right)^{-1}\text{ on the left}$$
$$|\psi(t)\rangle=|\psi_0(t)\rangle+\int dt'\left(i\hbar\frac{d}{dt}-\hat{H}_0\right)^{-1}_{t,t'\text{ matrix element}}\underbrace{\hat{V}(t')\left|\psi\left(t'\right)\right\rangle}_{\text{vector}}$$

where the t,t' matrix element of the inverse operator is the Green's function. Note that matrix multiplication of a continuous operator requires an integration over one index.

But $\hat{G}_0(t,t')$ is the inverse operator from the equation of motion, so

$$|\psi(t)\rangle=|\psi_0(t)\rangle+\int dt'\hat{G}_0\left(t,t'\right)\hat{V}\left(t'\right)\left|\psi\left(t'\right)\right\rangle$$

Now substitute in $\hat{G}_0=\hat{G}_{0+}$ only because we are interested in retarded solutions which build up in time from the history of what happened for all earlier times. If you like, this is a postulate where we are introducing an "arrow of time".

So we get
$$|\psi(t)\rangle=|\psi_0(t)\rangle-\frac{i}{\hbar}e^{-i\hat{H}_0t/\hbar}\int_{-\infty}^{t}dt'e^{+i\hat{H}_0t'/\hbar}\hat{V}\left(t'\right)\left|\psi\left(t'\right)\right\rangle$$
as $t\to-\infty$ $\quad|\psi(t)\rangle\to|\psi_0(t)\rangle$ which is what we want if V is bounded.

Hence one can also view this choice as a way to satisfy the boundary condition.

Now, unlike bound state problems, when $E>V$, we expect there to be a continuum of possible states. Let E be the energy of the initial state such that

$$|\psi_0(t)\rangle=e^{-iEt/\hbar}\,|\psi_0\rangle\qquad\text{as }t\to-\infty$$
$$|\psi(t)\rangle=e^{-iEt/\hbar}|\psi\rangle\text{ as }t\to-\infty$$

Since we expect energy to be conserved if $\hat{V}$ is independent of time, we expect the energy to stay at E for all time. Hence we write

$$|\psi(t)\rangle=e^{-iEt/\hbar}|\psi\rangle\text{ for all }t.$$

Then we get
$$|\psi\rangle=|\psi_0\rangle-\frac{i}{\hbar}e^{-i\left(\hat{H}_0-E\right)t/\hbar}\int_{-\infty}^{t}dt'e^{i(H_0-E)t'/\hbar}\hat{V}|\psi\rangle.$$

It is mathematically convenient to think of $\hat{V}$ being turned on over some time interval in the infinite past, so we let $\hat{V}\to\hat{V}e^{\delta t/\hbar}\qquad\delta\to0^+$. This may sound like an odd thing to do, but it helps control some infinities one gets, if we do not do it.

Substituting in, we can now integrate

$$\begin{aligned} |\psi\rangle =& | \psi_0\rangle - \frac{i}{\hbar} e^{-i\left(\hat{H}_0 - E\right)t/\hbar} \int_{-\infty}^{t} dt' e^{i\left(\hat{H}_0 - E\right)t'/\hbar} e^{\delta t'/\hbar} \hat{V}|\psi\rangle \\ =& | \psi_0\rangle - \frac{i}{\hbar} e^{-i\left(\hat{H}_0 - E\right)t/\hbar} \frac{\hbar e^{i\left(\hat{H}_0 - E\right)t'/\hbar + \delta t'/\hbar}}{i\left(\hat{H}_0 - E\right) + \delta} \Bigg|_{-\infty}^{t} \hat{V}|\psi\rangle \end{aligned}$$

The $e^{\delta t'/\hbar}$ makes the contribution vanish as $t' \to -\infty$ and we take the limit $\delta \to 0^+$ for the $e^{\delta t/\hbar}$ term so it approaches 1 and we obtain

$$\begin{aligned} |\psi\rangle &= |\psi_0\rangle - \frac{e^{-i\left(\hat{H}_0 - E\right)t/\hbar} e^{i\left(\hat{H}_0 - E\right)t}}{\hat{H}_0 - E - i\delta} \hat{V}|\psi\rangle \\ |\psi\rangle &= |\psi_0\rangle + \frac{i}{E - \hat{H}_0 + i\delta} \hat{V}|\psi\rangle \end{aligned}$$

This is called the Lippman-Schwinger equation.