Physics 506 Lecture 16

Introduction to scattering

Start with time-dependent Schroedinger equation in coordinate basis

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

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

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

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

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

equation of continuity (recall electromagnetism).

We will use this equation to find $\vec{J}$.

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

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

$$\cancel{\frac{d}{dt}\rho(\vec{r},t) = \frac{i\hbar}{2m}\left(\psi^*\nabla^2\psi + \psi^*\frac{V}{i\hbar}\psi - \nabla^2\psi^*\psi + V\psi^*\psi\right.}$$

$$\frac{d}{dt}\rho(\vec{r},t) = \frac{i\hbar}{2m}\left(\psi^*\nabla^2\psi - \nabla^2\psi^*\psi\right) + \frac{V}{i\hbar}\left(\psi^*\psi - \psi^*\psi\right)$$

$$= \vec{\nabla}\cdot\frac{i\hbar}{2m}\left(\psi^*\vec{\nabla}\psi - \vec{\nabla}\psi^*\psi\right)$$ because $\vec{\nabla}\psi^*\cdot\vec{\nabla}\psi$ terms cancel

$$\Rightarrow \boxed{\vec{J} = \frac{\hbar}{2im}\left(\psi^*\vec{\nabla}\psi - \vec{\nabla}\psi^*\psi\right)}$$

Check: for a free particle

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

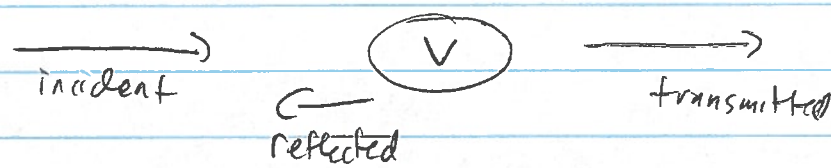
$$\vec{J} = \frac{\hbar\vec{k}}{2m} * 2\,\psi^*\psi = \frac{\hbar\vec{k}}{m}\,\psi^*(\vec{r},t)\,\psi(\vec{r},t)$$

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

Simple example of 1d scattering –
delta function potential at $x=0$

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

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



So for $x<0$ $\quad \psi(x,t) = \psi_{incident}(x,t) + \psi_{reflected}(x,t)$

for $x>0$ $\quad \psi(x,t) = \psi_{transmitted}(x,t)$ $\quad$ assume stationary so no t dependence

$$\psi(x) = \begin{cases} A\left(e^{ikx} + r e^{-ikx}\right) & x<0 \\ A t e^{ikx} & x>0 \end{cases}$$

goes right to left.

goes left to right

r = reflection amplitude $\quad$ t = transmission amplitude

$\psi(x)$ is continuous across $x=0$

⇒ $A(1+r) = At$ $\quad$ or $\quad$ $1+r = t$

But $\left.\frac{d\psi}{dx}\right|_{x=0^+} - \left.\frac{d\psi}{dx}\right|_{x=0^-} = \int_{x=0^-}^{x=0^+} dx \, \frac{d^2\psi}{dx^2} = \frac{-2m}{\hbar^2} \int_{x=0^-}^{x=0^+} dx \, \frac{-\hbar^2}{2m} \frac{d^2\psi}{dx^2}$

but $\frac{-\hbar^2}{2m} \frac{d^2\psi}{dx^2} = (E - V(x))\psi$ so

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

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

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

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

Note $|r|^2 + |t|^2 = 1$

$|r|^2 = R =$ reflection coefficient

$|t|^2 = T =$ transmission coefficient

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

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

Time dependent Schroedinger eq'n

$$i\hbar \frac{\partial}{\partial t} |\psi(t)\rangle = (\hat{H}_0 + \hat{V}) |\psi(t)\rangle \qquad \hat{H}_0 = \frac{\hat{p}^2}{2m} = \text{kinetic energy.}$$

Define the Green's function to satisfy

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

since the delta function acts like a unit matrix, one can think of the Green's function as the inverse of the leftmost operator in the above equation.

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

It is immediate that

$$\hat{G}_0(t,t') = \hat{G}_{0+}(t,t') + \hat{G}_{0-}(t,t')$$

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

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

solves the equation of motion, where

$$\theta(t) = \begin{cases} 0 & t<0 \\ 1 & t>0 \end{cases} \qquad \text{and} \qquad \frac{d}{dt}\theta(t) = \delta(t)$$

as can be seen by noting $\frac{d}{dt}\theta(t) = 0$ everywhere except at $t=0$ but $\int_{t=0^-}^{t=0^+} \frac{d}{dt}\theta(t)\,dt = \theta(t=0_+) - \theta(t=0^-)$
$= 1 - 0 = 1$

so $\frac{d}{dt}\theta(t) = 0$ everywhere but $\int_{0^-}^{0^+} dt\, \frac{d}{dt}\theta(t) = 1 \Rightarrow$ delta fcn.

Using $\hat{G}_0$ we find

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

where $|\psi_0(t)\rangle$ is the free wavefunction, which satisfies

$$i\hbar \frac{d}{dt} |\psi_0(t)\rangle = \hat{H}_0 |\psi_0(t)\rangle$$

Proof:

$$\underbrace{\left(i\hbar \frac{d}{dt} - \hat{H}_0\right)}_{\text{moved over from RHS}} |\psi(t)\rangle = \underbrace{\left(i\hbar \frac{d}{dt} - \hat{H}_0\right) |\psi_0(t)\rangle}_{\text{is zero}} + \underbrace{\hat{V}(t)|\psi(t)\rangle}_{\text{from full Schroedinger eq'n}}$$

Now multiply by the inverse operator $\left(i\hbar \frac{d}{dt} - \hat{H}_0\right)^{-1}$ on the left

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

t,t' matrix element of inverse

since matrix multiplication of operator is an integration over one index.

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

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

Now substitute in $\hat{G}_0 = \hat{G}_{0+}$ only because we are interested in retarded solutions which build up at time t 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

$$|\psi(t)\rangle = |\psi_0(t)\rangle - \frac{i}{\hbar} e^{-i\frac{\hat{H}_0 t}{\hbar}} \int_{-\infty}^{t} dt' \, e^{+i\frac{\hat{H}_0 t'}{\hbar}} \hat{V}(t')|\psi(t')\rangle$$

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

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

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

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

Then we get

$$|\psi\rangle = |\psi_0\rangle - \frac{i}{\hbar} e^{-i(\hat{H}_0 - E)t/\hbar} \int_{-\infty}^{t} dt' \, e^{i(\hat{H}_0 - E)t'/\hbar} \hat{V}|\psi\rangle$$

It is mathematically convenient to think of $\hat{V}$ being turned on over some time interval in the infinite past, so we let $\hat{V} \to \hat{V} e^{\delta t/\hbar}$ $\quad \delta \to 0^+$. 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

$$|\psi\rangle = |\psi_0\rangle - \frac{i}{\hbar} e^{-i(\hat{H}_0 - E)t/\hbar} \int_{-\infty}^{t} dt' \, e^{i(\hat{H}_0 - E)t'/\hbar} e^{\delta t'/\hbar} \hat{V} |\psi\rangle$$

$$= |\psi_0\rangle - \frac{i}{\hbar} e^{-i(\hat{H}_0 - E)t/\hbar} \left. \frac{\hbar \, e^{i(\hat{H}_0 - E)t'/\hbar + \delta t'/\hbar}}{i(\hat{H}_0 - E) + \delta} \right|_{-\infty}^{t} \hat{V} |\psi\rangle$$

The $e^{\delta t'/\hbar}$ makes the contribution vanish as $t' \to -\infty$

we take the limit $\delta \to 0^+$ for the $e^{\delta t/\hbar}$ term

so it approaches 1 and we get

$$|\psi\rangle = |\psi_0\rangle - \frac{e^{-i(\hat{H}_0 - E)t/\hbar} \, e^{i(\hat{H}_0 - E)t}}{\hat{H}_0 - E - i\delta} \hat{V} |\psi\rangle$$

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

called the Lippman-Schwinger equation.