

Lecture 20

Scattering. The Born approximation.

The time-independent Schrödinger equation

$$-\frac{\hbar^2}{2m} \nabla^2 \psi + V\psi = E\psi$$

can be written as

$$(\nabla^2 + k^2) \psi = Q,$$

$$k \equiv \frac{\sqrt{2mE}}{\hbar}, \quad Q \equiv \frac{2m}{\hbar^2} V\psi \leftarrow \text{note that } Q \text{ depends on } \psi.$$

(which has the form of Helmholtz equation).

If we find the function $G(\mathbf{r})$ that solves the Helmholtz equation with a delta function "source"

$$(\nabla^2 + k^2) G(\mathbf{r}) = \delta^3(\mathbf{r})$$

we could express ψ as an integral.

$$\psi(\mathbf{r}) = \int G(\mathbf{r} - \mathbf{r}_0) Q(\mathbf{r}_0) d^3\mathbf{r}_0$$

Question to the class: proof that this still satisfies the Schrödinger equation.

Hint: plug $\psi(\mathbf{r}) = \int G(\mathbf{r} - \mathbf{r}_0) Q(\mathbf{r}_0) d^3\mathbf{r}_0$ into
 $(\nabla^2 + k^2) \psi$.

$$\begin{aligned} (\nabla^2 + k^2) \psi &= \int \underbrace{[\nabla^2 + k^2] G(\mathbf{r} - \mathbf{r}_0)}_{\parallel \delta^3(\mathbf{r} - \mathbf{r}_0)} Q(\mathbf{r}_0) d^3\mathbf{r}_0 \\ &= \int \delta^3(\mathbf{r} - \mathbf{r}_0) Q(\mathbf{r}_0) d^3\mathbf{r}_0 = Q(\mathbf{r}). \quad \text{QED} \end{aligned}$$

Note that what we are trying to do is essentially to write Schrödinger equation in an integral form rather than solve it. The function $G(\mathbf{r})$ is called the Green's function for the Helmholtz equation.

Derivation (see pages 409-411 of the textbook) shows that it is

$$G(\vec{r}) = - \frac{e^{ikr}}{4\pi r}.$$

We can add to it any function that satisfies the homogeneous Helmholtz equation

$$(\nabla^2 + k^2) G_0(\vec{r}) = 0.$$

Now we arrive to the integral form of the Schrödinger equation

$$\psi(\vec{r}) = \int G(\vec{r} - \vec{r}_0) Q(\vec{r}_0) d^3 r_0 \quad Q \equiv \frac{2m}{\hbar^2} V\psi$$

$$\psi(\vec{r}) = \psi_0(\vec{r}) - \frac{m}{2\pi\hbar^2} \int \frac{e^{ik|\vec{r} - \vec{r}_0|}}{|\vec{r} - \vec{r}_0|} V(\vec{r}_0) \psi(\vec{r}_0) d^3 r_0$$

The First Born Approximation

We suppose that scattering potential $V(\mathbf{r}_0)$ is localized about $\mathbf{r}_0=0$, i.e. potential drops to zero outside of finite region. It is a typical case for a scattering problem. We would like to calculate the wave function far away from the scattering center. Therefore, we can assume

$$|\vec{r}| \gg |\vec{r}_0|$$

for all points in our integral.

$$|\vec{r} - \vec{r}_0|^2 = r^2 + r_0^2 - 2\vec{r} \cdot \vec{r}_0 \approx r^2 \left(1 - 2 \frac{\vec{r} \cdot \vec{r}_0}{r^2} \right)$$

↑
drop this term

Then, $|\vec{r} - \vec{r}_0| \approx r - \hat{r} \cdot \vec{r}_0$ (expand $\sqrt{\quad}$ of the above)

Let's use this approximation in $\frac{e^{i k |\vec{r} - \vec{r}_0|}}{|\vec{r} - \vec{r}_0|} \leftarrow e^{i k (r - \hat{r} \cdot \vec{r}_0)} = e^{i k r} e^{-i \vec{k} \cdot \vec{r}_0}$

$\vec{k} = k \hat{r}$

$\approx r$

Note that we need to be more careful with approximating the exponential term than the denominator.

$$\psi(\vec{r}) = \psi_0(\vec{r}) - \frac{m}{2\pi\hbar^2} \int \frac{e^{i k |\vec{r} - \vec{r}_0|}}{|\vec{r} - \vec{r}_0|} V(\vec{r}_0) \psi(\vec{r}_0) d^3 r_0$$

In case of scattering

$$\psi_0(\vec{r}) = A e^{i k z}, \text{ incident plane wave}$$

$$\frac{e^{i k r} e^{-i \vec{k} \cdot \vec{r}_0}}{r} \text{ from above}$$

Then, our wave function can be written in a form

$$\psi(\vec{r}) = \underbrace{A e^{i k z}}_{\text{incoming plane wave}} + \underbrace{A \frac{e^{i k r}}{r}}_{\text{outgoing spherical wave}} \left\{ - \frac{m}{2\pi\hbar^2} \int e^{-i \vec{k} \cdot \vec{r}_0} V(\vec{r}_0) \psi(\vec{r}_0) d^3 r_0 \right\}$$

↑
scattering amplitude f

So far, we only assumed $|\vec{r}| \gg |\vec{r}_0|$.

Now, we use the **Born approximation**. Let's assume that the potential does not significantly alter the wave function (weak potential approximation).

$$\psi(\vec{r}_0) \approx \psi_0(\vec{r}_0) = A e^{i k z_0} = A e^{i \vec{k}' \cdot \vec{r}_0}$$

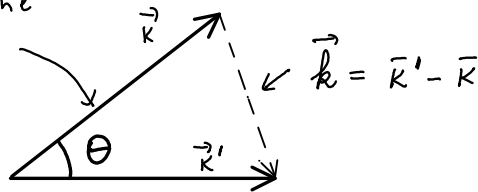
$\vec{k}' = k \hat{z}$

Then,
$$f(\theta, \phi) = -\frac{m}{2\pi\hbar^2} \int e^{-i \vec{k} \cdot \vec{r}_0} V(\vec{r}_0) \psi(\vec{r}_0) d^3 r_0$$

$A e^{i \vec{k}' \cdot \vec{r}_0}$

Let's clarify what are vectors \vec{k} and \vec{k}' :

\vec{k} points in the scattered direction



$\vec{k}' = k \hat{z}$ points in the incident direction

Scattering amplitude in Born approximation.

$$f(\theta, \phi) = -\frac{m}{2\pi\hbar^2} \int e^{-i(\vec{k}' - \vec{k}) \cdot \vec{r}_0} V(\vec{r}_0) d^3 r_0$$

As before, the differential and total cross sections are given by

$$\frac{d\sigma}{d\Omega} = |f|^2, \quad \sigma = \int |f|^2 d\Omega.$$

We can now consider two cases:

- (1) Low-energy scattering
- (2) Spherically symmetric potential.

Low energy scattering

In the case of low energy scattering, we can consider exponential factor to be constant over the scattering region and the Born approximation simplifies to

$$f(\theta, \phi) \approx - \frac{m}{2\pi\hbar^2} \int V(\vec{r}) d^3r$$

Exercise for the class: use low-energy scattering in Born approximation to calculate differential and total cross sections for **low-energy soft-sphere scattering**,

$$V(\vec{r}) = \begin{cases} V_0, & \text{if } r \leq a \\ 0, & \text{if } r > a \end{cases}$$

$$f = - \frac{m}{2\pi\hbar^2} \int V(r) d^3r = - \frac{m}{2\pi\hbar^2} \int_0^a V_0 r^2 dr 4\pi =$$

$$= - \frac{m}{2\pi\hbar^2} \frac{a^3}{3} 4\pi V_0 = - \frac{2ma^3 V_0}{3\hbar^2}$$

$$\frac{d\sigma}{d\Omega} = |f|^2 \approx \frac{4m^2 a^6 V_0^2}{9\hbar^4}$$

$$\sigma = 4\pi \left\{ \frac{4m^2 a^6 V_0^2}{9\hbar^4} \right\}$$

Spherically symmetric potential

$$V(\vec{r}) \equiv V(r)$$

Let's pick axis for \vec{r}_0 integral so

$$\underbrace{(\vec{k}' - \vec{k}) \cdot \vec{r}_0}_{\vec{k}} = kr_0 \cos \theta$$

$$\text{Then, } f(\theta) \approx -\frac{m}{2\pi\hbar^2} \int e^{i\vec{k} \cdot \vec{r}_0 \cos \theta} V(r_0) r_0^2 \sin \theta dr_0 d\theta_0 d\phi_0$$

$$f(\theta) = -\frac{m}{\hbar^2} \iint e^{i\vec{k} \cdot \vec{r}_0 \cos \theta} V(r_0) r_0^2 \sin \theta dr_0 d\theta_0$$

$$[\int d\phi_0 = 2\pi]$$

$$\int_0^\pi e^{i\vec{k} \cdot \vec{r}_0 \cos \theta} \sin \theta d\theta = -\frac{e^{i\vec{k} \cdot \vec{r}_0 \cos \theta}}{i\vec{k} \cdot \vec{r}_0} \Big|_0^\pi = \frac{2\sin(kr)}{kr}$$

$$\left\{ \sin x = \frac{e^{ix} - e^{-ix}}{2i} \right\}$$

$$f(\theta) = -\frac{2m}{\hbar^2 k} \int_0^\infty r_0 V(r_0) \sin(kr_0) dr_0$$

Where is dependence on θ ?

$$k^2 = |\vec{k} - \vec{k}'|^2 = (k^2 + k'^2 - 2\vec{k} \cdot \vec{k}') = k^2 + k'^2 - 2kk' \cos \theta \approx$$

$$\approx 2k^2(1 - \cos \theta) = 2k^2 \underbrace{(1 - \cos \theta)}_{= 2 \sin^2 \frac{\theta}{2}} = 4k^2 \sin^2 \frac{\theta}{2}$$

$$k = 2k \sin \frac{\theta}{2}$$

$$= 2 \sin^2 \frac{\theta}{2}$$