

The Born Approximation

The SE, $-\frac{\hbar^2}{2m} \nabla^2 \psi + V\psi = E\psi$, can be formally written as $(\nabla^2 + k^2)\psi = Q$ - the Helmholtz equation where $k = \frac{\sqrt{2mE}}{\hbar}$ $Q = \frac{2m}{\hbar^2} V\psi$. The inhomogeneity here depends on ψ , however.

Suppose now that we could solve such an equation when the inhomogeneity is a delta-function:

$$(\nabla^2 + k^2)G(\vec{r}) = \delta(\vec{r}) = \delta(x)\delta(y)\delta(z)$$

$G(\vec{r})$ is called the Green's function. The solution of $(\nabla^2 + k^2)\psi = Q$ could be then expressed as

$$\psi(\vec{r}) = \int G(\vec{r} - \vec{r}_0) Q(\vec{r}_0) d\vec{r}_0$$

Indeed, the direct substitution yields

$$\begin{aligned} (\nabla^2 + k^2)\psi(\vec{r}) &= \int [(\nabla^2 + k^2)G(\vec{r} - \vec{r}_0)] Q(\vec{r}_0) d\vec{r}_0 = \\ &= \int \delta(\vec{r} - \vec{r}_0) Q(\vec{r}_0) d\vec{r}_0 = Q(\vec{r}) \end{aligned}$$

Let us then solve the equation for $G(\vec{r})$. One way of doing it is by taking the Fourier transform

$$G(\vec{r}) = \frac{1}{(2\pi)^{3/2}} \int e^{i\vec{s}\cdot\vec{r}} g(\vec{s}) d\vec{s}$$

$$\begin{aligned} (\nabla^2 + k^2)G(\vec{r}) &= \frac{1}{(2\pi)^{3/2}} \int [(\nabla^2 + k^2)e^{i\vec{s}\cdot\vec{r}}] g(\vec{s}) d\vec{s} = \\ &= \frac{1}{(2\pi)^{3/2}} \int (-s^2 + k^2) e^{i\vec{s}\cdot\vec{r}} g(\vec{s}) d\vec{s} = \delta(\vec{r}) = \frac{1}{(2\pi)^3} \int e^{i\vec{s}\cdot\vec{r}} d\vec{s} \end{aligned}$$

Clearly

$$g(\vec{s}) = \frac{1}{(2\pi)^{3/2}} \frac{1}{k^2 - s^2}$$

Now we do the inverse Fourier transform

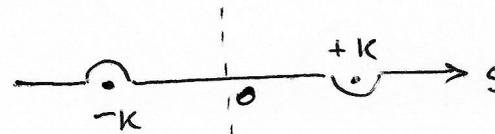
$$G(\vec{r}) = \frac{1}{(2\pi)^{3/2}} \int g(\vec{s}) e^{i\vec{s}\cdot\vec{r}} d\vec{s} = \frac{1}{(2\pi)^3} \int \frac{e^{i\vec{s}\cdot\vec{r}}}{k^2 - s^2} d\vec{s} = \frac{1}{(2\pi)^3} \cdot 2\pi \cdot \int_0^\pi \int_0^{2\pi} \frac{e^{isr \cos\theta}}{k^2 - s^2} s^2 \sin\theta d\theta ds$$

The integral over θ is : $\int_0^\pi e^{isr \cos\theta} \sin\theta d\theta = \frac{2 \sin sr}{sr}$

Then

$$G(\vec{r}) = \frac{1}{(2\pi)^2} \frac{2}{r} \int_0^\infty \frac{s \sin sr}{k^2 - s^2} ds = \frac{1}{4\pi^2 r} \int_{-\infty}^{+\infty} \frac{s \sin sr}{k^2 - s^2} ds = \frac{1}{4\pi^2 r} I = \frac{1}{4\pi r} e^{ikr}$$

The above integral I can be evaluated as follows

$$I = \int_{-\infty}^{+\infty} \frac{s \sin sr}{k^2 - s^2} ds = - \int_{-\infty}^{+\infty} s \frac{e^{isr} - e^{-isr}}{2i} \frac{1}{(s-k)(s+k)} ds$$


We will use a certain way to shift poles as shown above. It turns out this way will give the so-called retarded Green's function that propagates wave function forward in time.

$$I = - \frac{1}{2i} \int_{-\infty}^{+\infty} \frac{s e^{isr}}{(s-k)(s+k)} ds + \frac{1}{2i} \int_{-\infty}^{+\infty} \frac{s e^{-isr}}{(s-k)(s+k)} ds$$

To evaluate these two integrals we can integrate over closed contours and use the residue theorem, which says that an integral over closed contour γ (counterclockwise) is equal to the sum of residues within the contour:

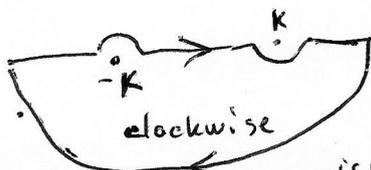
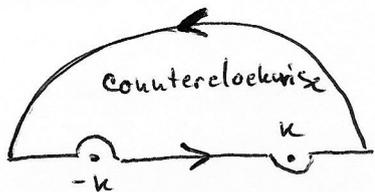
$$\int_{\gamma} f(z) dz = 2\pi i \sum_a \text{Res}[f, a]$$

where $\text{Res}[f, a] = \lim_{z \rightarrow a} (z-a) f(z)$ - for a simple pole (order 1)

$$\text{Res}[f, a] = \frac{1}{(n-1)!} \frac{d^{n-1}}{dz^{n-1}} (z-a)^n f(z)$$
 - for a pole of order n

We chose the contours for the above two integrals in such a way that the semicircle at infinity contributes nothing:

With this we have:



$$I = 2\pi i \left(-\frac{1}{2i} \text{Res} \left[\frac{s e^{isr}}{(s+k)(s-k)}, +k \right] + \frac{1}{2i} \text{Res} \left[\frac{s e^{-isr}}{(s+k)(s-k)}, -k \right] \right) = -\pi \left[\frac{k}{2k} e^{ikr} + \frac{k}{2k} e^{ikr} \right] = -\pi e^{ikr}$$

Note that we can add any $G_0(\vec{r})$ to $G(\vec{r})$ that satisfies the homogeneous Helmholtz equation:

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

The general solution of the Schrödinger equation then can be written as

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

where ψ_0 satisfies the free-particle SE:

$$(\nabla^2 + k^2)\psi_0 = 0$$

Note that the above equation is not really a solution but an integral form of the Schrödinger equation. It is called the Lippmann-Schwinger equation.

In more advanced courses it is often written as:

$$|\psi^\pm\rangle = |\phi\rangle + \frac{1}{E - H_0 \pm i\epsilon} V |\psi^\pm\rangle$$

The advantage of the Lippmann-Schwinger equation for scattering problems comes from two things: i) it incorporates the boundary conditions ii) it can be solved iteratively.

In the first Born approximation we just plug the free-particle solution into the integral and get $\psi(\vec{r})$. The physical motivation is as follows. Suppose $V(\vec{r}_0)$ is localized around $\vec{r}_0 = 0$. Then when $|\vec{r}| \gg |\vec{r}_0|$ we can write

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

$$|\vec{r} - \vec{r}_0| \approx r - \frac{\vec{r} \cdot \vec{r}_0}{r} = r - \hat{r} \cdot \vec{r}_0$$

Let $\vec{k} \equiv k \hat{r}$ then $e^{ik|\vec{r} - \vec{r}_0|} \approx e^{ikr} e^{-i\vec{k} \cdot \vec{r}_0}$

and $\frac{e^{ik|\vec{r} - \vec{r}_0|}}{|\vec{r} - \vec{r}_0|} \approx \frac{e^{ikr}}{r} e^{-i\vec{k} \cdot \vec{r}_0}$

For scattering $\psi_0(\vec{r}) = A e^{ikz}$. In the case of large r then

$$\psi(\vec{r}) \approx A e^{ikz} - \frac{m}{2\pi\hbar^2} \frac{e^{ikr}}{r} \int e^{-i\vec{k}' \cdot \vec{r}_0} V(\vec{r}_0) \psi(\vec{r}_0) d\vec{r}_0$$

From here it is easy to deduce what $f(\theta, \varphi)$ is (scattering amplitude):

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

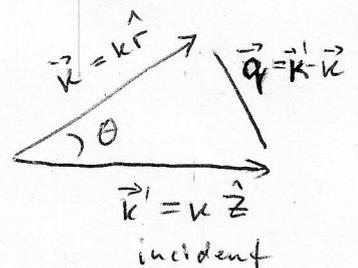
The first Born approximation makes an assumption that the incoming plane wave is not altered substantially:

$$\psi(\vec{r}_0) \approx \psi_0(\vec{r}_0) = A e^{ikz_0} = A e^{i\vec{k}' \cdot \vec{r}_0} \quad \text{where } \vec{k}' \equiv k \hat{z}$$

Then

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

$$= -\frac{m}{2\pi\hbar^2} \int e^{i\vec{q} \cdot \vec{r}_0} V(\vec{r}_0) d\vec{r}_0$$



In particular for low energy scattering ($e^{i\vec{q} \cdot \vec{r}_0} \approx 1$)

$$f(\theta, \varphi) \approx -\frac{m}{2\pi\hbar^2} \int V(\vec{r}_0) d\vec{r}_0$$

For a spherically symmetric potential $V(\vec{r}) = V(r)$

$\vec{q} = \vec{k}' - \vec{k}$ assume $(\vec{k}' - \vec{k}) \cdot \vec{r}_0 = q r_0 \cos \theta_0$

Then $f(\theta) = -\frac{m}{2\pi\hbar^2} \int e^{iq r_0 \cos \theta_0} V(r_0) r_0^2 \sin \theta_0 dr_0 d\theta_0 d\phi_0 =$

$$= -\frac{2m}{\hbar^2 q} \int_0^{\infty} r V(r) \sin(qr) dr \quad \text{where } q = 2k \sin \frac{\theta}{2}$$

Example: Yukawa potential

$$V(r) = \beta \frac{e^{-\mu r}}{r} \quad \text{In the first Born approximation}$$

$$f(\theta) \approx -\frac{2m\beta}{\hbar^2 q} \int_0^{\infty} e^{-\mu r} \sin(qr) dr = -\frac{2m\beta}{\hbar^2 (\mu^2 + q^2)}$$

here we used :

$$\int_0^{\infty} e^{-\mu r} \sin(qr) dr = \text{Im} \left[\int_0^{\infty} e^{-\mu r} e^{iqr} dr \right] = \text{Im} \left[\frac{1}{\mu - iq} \right] = \frac{q}{\mu^2 + q^2}$$