

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


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

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:

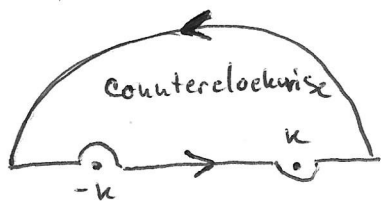
$$\int_{\gamma} f(z) dz = 2\pi i \sum_a \text{Res}[f, a]$$

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

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

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

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 $\psi_0(\vec{r}) = Ae^{ikz}$. In the case of

large r then

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

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

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

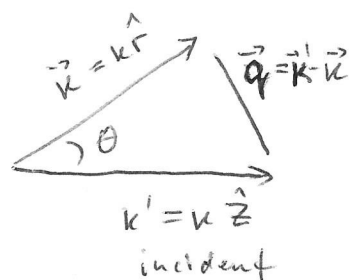
The first Born approximation makes an assumption that the incoming plane wave is not altered substantially:

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

Then

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

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



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

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

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

$\vec{q} = \vec{k}' - \vec{k}$ assume $(\vec{k}' - \vec{k}) \cdot \vec{r}_0 = qr_0 \cos\theta_0$

Then $f(\theta) = -\frac{m}{2\pi\hbar^2} \int e^{iqr_0 \cos\theta_0} V(r_0) r_0^2 \sin\theta_0 dr_0 d\theta_0 d\phi_0 =$

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

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 :

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