Lecture 24 Highlights
Phys 402

We consider the integral version of the Schrodinger equation, and the Born series expansion for quantum scattering.

Start with the TISE in three dimensions: $-\frac{\hbar^2}{2m}\nabla^2\psi + V\psi = E\psi$, and re-write it in this form,

$(\nabla^2 + k^2)\psi = Q$, with $E = \frac{\hbar^2 k^2}{2m}$, and $Q \equiv \frac{2m}{\hbar^2} V\,\psi$.

Recall that the Helmholtz equation for a scalar wave is written as $(\nabla^2 + k^2)\psi = 0$, and it describes the waves on a drumhead, or [quantum waves in a billiard potential](), for example. How to deal with the inhomogeneous 'source term' term Q? We utilize the idea of a Green's function.

Define the Green's function as that which satisfies the Helmholtz equation for a delta-function source (sort of like the 'impulse response' of the wave field):

$$(\nabla^2 + k^2)G = \delta^3(\vec{r}) \tag{1}$$

Once we know $G(\vec{r})$ we can find the solution for any source term (i.e. any potential $V(\vec{r})$) as,

$$\psi(\vec{r}) = \int G(\vec{r} - \vec{r_0})\, Q(\vec{r_0})\, d^3\vec{r_0}$$

This is essentially a convolution of the Green's function with the source term Q.

The Green's function for the Helmholtz equation is derived in the textbook on pages 388-390. This Green's function is specific to the equation and the dimensionality of the system, and works just as well for classical waves, as well as for quantum waves. The result is:

$G(\vec{r}) = -\frac{e^{ikr}}{4\pi r}$, where the exponent is just $kr = |\vec{k}||\vec{r}| \neq \vec{k}\cdot\vec{r}$ (note that the dot product has an additional factor of the cosine of the angle between the two vectors). You will show in HW10 that this Green's function is a solution to the equation (1) above. Note that one can always add to $G(\vec{r})$ a solution to the homogeneous Helmholtz equation, $(\nabla^2 + k^2)G_0(\vec{r}) = 0$, and not change the solution to the Schrodinger equation. Hence the general solution is,

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

where $\psi_0(\vec{r})$ is a free-particle solution that satisfies the homogeneous Helmholtz equation (i.e. with $Q = 0$). This is called the Lippmann-Schwinger equation. It is the integral form of the Schrodinger equation. Note that ψ appears on both sides of the equation, so we need a strategy to solve the equation. It turns out that the Lippmann-Schwinger equation is especially well suited for quantum scattering problems.

Let's begin to attack the Lippmann-Schwinger equation in the context of quantum scattering. Imagine a plane wave (free particle) arriving from the left and scattering from a localized-in-space potential $V(\vec{r_0})$. We take the approximation that $V(\vec{r_0})$ only extends a few fm from the origin, while the observation point for the outgoing particle ($\vec{r}$) is 1 to 10 meters away from the potential (like the CMS detector at the Large Hadron Collider at CERN). In this case it is an excellent approximation to say that $|\vec{r}| \gg |\vec{r_0}|$, and the wave solution becomes:

$$\psi(\vec{r}) = A\, e^{ikz} - \frac{m}{2\pi\hbar^2}\frac{e^{ikr}}{r}\int e^{-i\vec{k}\cdot\vec{r_0}}\, V(\vec{r_0})\, \psi(\vec{r_0})\, d^3\vec{r_0}\ . \tag{3}$$

This is the standard form of a scattering problem that we have seen before (namely $\psi(r,\theta) = A\left\{e^{ikz} + f(\theta)\frac{e^{ikr}}{r}\right\}$), leading to this expression for the angular distribution function,

$$f(\theta) = -\frac{m}{2\pi\hbar^2 A}\int e^{-i\vec{k}\cdot\vec{r_0}}\, V(\vec{r_0})\, \psi(\vec{r_0})\, d^3\vec{r_0} \ . \qquad (4)$$

However, we still do not know $\psi(\vec{r_0})$ in the integrand of Eq. (4). Now we will make an approximation, called the **first Born approximation**. Assume that the incident plane wave $A\, e^{ikz}$ is not substantially altered by scattering from the potential, so that $\psi(\vec{r_0}) = \psi_0(\vec{r_0}) = A\, e^{ikz} = A\, e^{i\vec{k'}\cdot\vec{r_0}}$, where we have defined the wave-vector of the *incoming* particle as $\vec{k'} = k\hat{z}$. The first Born approximation results in this solution for the scattering structure factor,

$$f(\theta) \cong -\frac{m}{2\pi\hbar^2}\int e^{i(\vec{k'}-\vec{k})\cdot\vec{r_0}}\, V(\vec{r_0})\, d^3\vec{r_0} \ . \qquad (5)$$

Note that $\hbar\left(\vec{k'} - \vec{k}\right)$ is the momentum transfer that the particle gives to the scattering potential. The vectors $\vec{k}$, $\vec{k'}$, and $\vec{\kappa} \equiv \vec{k'} - \vec{k}$ make a triangle, with angle θ between $\vec{k}$, and $\vec{k'}$. The isosceles triangle has the relation $\kappa = 2k\sin\left(\frac{\theta}{2}\right)$, where k is the magnitude of the incident and outgoing wavevectors (we are assuming elastic scattering). One more point about Eq. (5) – it represents the Fourier transform of the scattering potential.

An example use of the first Born approximation is that of "low energy" scattering from a potential. In this case the deBroglie wavelength of the incident and scattered particle is much larger than the extent of the potential. Under this approximation, the phase factor in the integral of Eq. (5) satisfies $\left(\vec{k'} - \vec{k}\right)\cdot\vec{r_0} \ll 1$, hence the phase factor $e^{i(\vec{k'}-\vec{k})\cdot\vec{r_0}}$ is 1, to good approximation, and we have:

$f_{Low-Energy}(\theta) \approx -\frac{m}{2\pi\hbar^2}\int V(\vec{r_0})\, d^3\vec{r_0}$, which is basically just the average value of the potential. When this is applied to the soft-sphere potential,

$$V(r) = \begin{cases} V_0 \text{ for } r < a \\ 0 \text{ for } r > a \end{cases},$$

the result is $f_{Low-Energy}(\theta) \approx -\frac{mV_0}{\hbar^2}\frac{2}{3}a^3$, which you will note is independent of scattering angle θ (we will see this again below). The DSCS is $\frac{d\sigma}{d\Omega} = \left(\frac{2mV_0a^3}{3\hbar^2}\right)^2$, so the full scattering cross section is $\sigma = 4\pi\left(\frac{2mV_0a^3}{3\hbar^2}\right)^2$, is proportional to the volume squared of the soft sphere.

Another special situation is that of a spherically-symmetric potential $V(r)$. In this case the scattering amplitude in the first Born approximation simplifies to,

$$f_{spherically\ Symmetric}(\theta) = -\frac{2m}{\hbar^2\,\kappa}\int_0^\infty r_0\, V(r_0)\sin(\kappa\, r_0)\ dr_0. \qquad (6)$$

Note again that the momentum transfer is $\hbar\kappa$, where $\kappa = 2k\sin\left(\frac{\theta}{2}\right)$. We considered several examples of spherically-symmetric potentials. The first is the **Yukawa nuclear scattering potential**, $V(r) = \gamma\frac{e^{-\mu r}}{r}$, where $\gamma < 0$ typically. This is an attractive Coulomb-like potential that is cut off at a few times $1/\mu$ by the exponential term. This keeps the potential finite in extent and insures that the total scattering cross section is finite. The resulting scattering function is $f(\theta) = -\frac{2m\gamma}{\hbar^2\,(4k^2\sin^2\left(\frac{\theta}{2}\right)+\mu^2)}$, and the differential scattering cross section is $\frac{d\sigma}{d\Omega} = |f(\theta)|^2$. Example plots of $\frac{d\sigma}{d\Omega}$ vs. scattering angle θ are shown on the class [web site](). The angular dependence of $f(\theta)$ depends on the energy of the incoming/outgoing particle. At low energy, the DSCS is independent of scattering angle, similar to the soft sphere scattering case considered above. At higher energy the DSCS favors forward scattering. Note that one can transform these results into those for Coulomb scattering by making the substitution $\gamma = \frac{q_1 q_1}{4\pi\varepsilon_0}$ and $\mu = 0$. The result is exactly the same DSCS as for the (classical) Rutherford scattering problem!

Another example of a spherically-symmetric potential arises for electron scattering off of a Hydrogen atom in its ground state. The potential energy due to the Coulomb interaction of the electron and atom in this case is $V(r) = -e\int \frac{\rho(\vec{r'})}{|\vec{r}-\vec{r'}|}\, d^3r'$, where the charge density of the Hydrogen atom is $\rho(\vec{r}) = e\{\delta^3(\vec{r}) - |\psi_{100}(\vec{r})|^2\}$. The first term in the charge density is that of the nucleus, while the second is that of the electron in the spherically-symmetric $\psi_{100}(\vec{r})$ state. The result for the spherically-symmetric potential (after several pages of calculations) is $V(r) = -\frac{e^2}{a_0}\left(1+\frac{a_0}{r}\right)e^{-2r/a_0}$, where a_0 is the Bohr radius. Using Eq. (6) for $f_{spherically\ Symmetric}(\theta)$, the resulting scattering function is $f(\theta) \propto\ a_0^2\,\frac{(8+a_0^2\,\kappa^2)}{(4+a_0^2\,\kappa^2)^2}$, where $\kappa^2 = 4k^2\sin^2\left(\frac{\theta}{2}\right)$. It turns out that bare Hydrogen atoms are hard to come by, so the experiment is more easily done with Helium atoms. In this case the ground state has two electrons in the $\psi_{100}(\vec{r})$ state in a spin-singlet, giving rise to a spherically-symmetric scattering potential again. The [results of the experiment]() for $\frac{d\sigma}{d\Omega} = |f(\theta)|^2$ are in good agreement with a calculation similar to the one for Hydrogen.

Finally, we can go beyond the first Born approximation to carry out a series expansion for the scattered wavefunction. We can re-write the wavefunction in Eq. (2) as follows,

$$\psi(\vec{r}) = \psi_0(\vec{r}) + \int g(\vec{r}-\vec{r_0})\,V(\vec{r_0})\,\psi(\vec{r_0})\,d^3\vec{r_0}\ , \qquad (7)$$

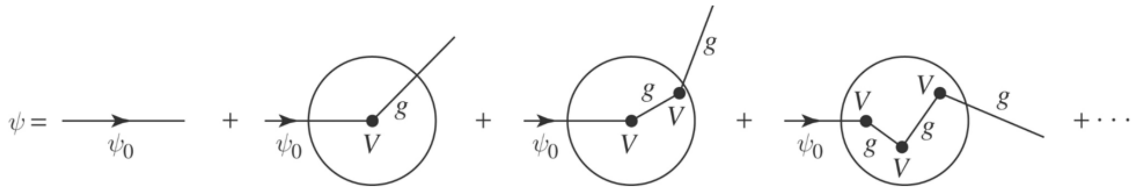
where we have simply defined the decorated version of the Green's function as $g(\vec{r}-\vec{r_0}) \equiv \frac{2m}{\hbar^2}G(\vec{r}-\vec{r_0}) = -\frac{m}{2\pi\hbar^2}\frac{e^{ik|\vec{r}-\vec{r_0}|}}{|\vec{r}-\vec{r_0}|}$. With this, we can write Eq. (7) schematically as "$\psi = \psi_0 + \int g\,V\,\psi$". The problem remains that the unknown wavefunction ψ still appears in two places in this integral equation. Here is an idea: substitute the full expression for ψ into the ψ that appears in the integral:

$$\psi = \psi_0 + \int g\,V\,(\psi_0 + \int g\,V\,\psi\,) = \psi_0 + \int g\,V\,\psi_0 + \iint g\,V\,g\,V\,\psi \qquad (8)$$

The first term ψ_0 is the incident particle, while the second term $\int g\,V\,\psi_0$ is the effect of the potential treated in the first Born approximation. The process of substituting Eq. (7) into Eq. (8) can continue to create an infinite series, called **the Born series**:

$$\psi = \psi_0 + \int g\,V\,\psi_0 + \iint g\,V\,g\,V\,\psi_0 + \iiint g\,V\,g\,V\,g\,V\,\psi_0 + \cdots$$

Each term in the series involves an additional interaction with the potential V, and can be thought of as a higher-order interaction between the projectile particle and the scattering force center. There is no guarantee that the series will converge, but for many interesting scattering problems, it does. The Born series can be visualized by the diagrams below:



Each diagram represents an integral in the Born series expansion. [Feynman diagrams](#) were developed as a means to keep track of integrals that appear in a perturbation series expansion. These diagrams show the evolution of the particle, and its interactions with the scattering potential, in a space-time diagram format.