1.6: The Green's Function

The scattering amplitude $f(\Omega)$ can be calculated using a variety of analytical and numerical methods. We will discuss one particularly important approach, based on a quantum variant of the Green's function technique for solving inhomogenous differential equations.

Let us return to the previously-discussed formulation of the scattering problem:

$$\begin{aligned}\hat{H} &= \hat{H}_0 + \hat{V} \\ \hat{H}|\psi\rangle &= E|\psi\rangle \\ |\psi\rangle &= |\psi_i\rangle + |\psi_s\rangle \\ \hat{H}_0|\psi_i\rangle &= E|\psi_i\rangle.\end{aligned} \tag{1.6.1}$$

These equations can be combined as follows:

$$\begin{aligned}\left(\hat{H}_0 + \hat{V}\right)|\psi_i\rangle + \hat{H}|\psi_s\rangle &= E\left(|\psi_i\rangle + |\psi_s\rangle\right) \\ \Rightarrow \quad \hat{V}|\psi_i\rangle + \hat{H}|\psi_s\rangle &= E|\psi_s\rangle \\ \Rightarrow \quad \left(E - \hat{H}\right)|\psi_s\rangle &= \hat{V}|\psi_i\rangle\end{aligned} \tag{1.6.2}$$

To proceed, we define the inverse of the operator on the left-hand side:

$$\hat{G} = \left(E - \hat{H}\right)^{-1}. \tag{1.6.3}$$

This operator is called the **Green's function**. Using it, we get

$$|\psi_s\rangle = \hat{G}\hat{V}|\psi_i\rangle. \tag{1.6.4}$$

Note that $\hat{G}$ depends on both the energy E and the scattering potential. To isolate the dependence on the scattering potential, let us define the Green's function for a free particle,

$$\hat{G}_0 = \left(E - \hat{H}_0\right)^{-1}. \tag{1.6.5}$$

This will be very useful for us, for $\hat{G}_0$ can be calculated exactly, whereas $\hat{G}$ often has no analytic expression. We can relate G and G_0 as follows:

$$\begin{aligned}\hat{G}(E - \hat{H}_0 - \hat{V}) &= I \quad \text{and} \quad (E - \hat{H}_0 - \hat{V})\hat{G} = I \\ \Rightarrow \quad \hat{G}\hat{G}_0^{-1} - \hat{G}\hat{V} &= I \quad \text{and} \quad \hat{G}_0^{-1}\hat{G} - \hat{V}\hat{G} = I.\end{aligned} \tag{1.6.6}$$

Upon respectively right-multiplying and left-multiplying these equations by $\hat{G}_0$, we arrive at the following pair of equations, called **Dyson's equations**:

Definition: Dyson's Equations

$$\hat{G} = \hat{G}_0 + \hat{G}\hat{V}\hat{G}_0 \tag{1.6.7}$$

$$\hat{G} = \hat{G}_0 + \hat{G}_0\hat{V}\hat{G} \tag{1.6.8}$$

These equations are "implicit", as the unknown $\hat{G}$ appears in both the left and right sides.

Applying the second Dyson equation, Equation (1.6.8), to the scattering problem (1.6.4) gives

$$\begin{aligned}|\psi_s\rangle &= \left(\hat{G}_0 + \hat{G}_0\hat{V}\hat{G}\right)\hat{V}|\psi_i\rangle \\ &= \hat{G}_0\hat{V}|\psi_i\rangle + \hat{G}_0\hat{V}\hat{G}\hat{V}|\psi_i\rangle \\ &= \hat{G}_0\hat{V}|\psi_i\rangle + \hat{G}_0\hat{V}|\psi_s\rangle \\ &= \hat{G}_0\hat{V}|\psi\rangle.\end{aligned} \tag{1.6.9}$$

This is a useful simplification, since it involves $\hat{G}_0$ rather than $\hat{G}$. The downside is that the equation is still implicit: the right-hand side involves the unknown total state $|\psi\rangle$, rather than the known incident state $|\psi_i\rangle$.

We can try to solve this implicit equation by using Equation (1.6.9) to get an expression for $|\psi\rangle$, then repeatedly plugging the result back into the right-hand side of Equation (1.6.9). This yields an infinite series formula:

$$\begin{aligned}|\psi_s\rangle &= \hat{G}_0\hat{V}\left(|\psi_i\rangle + \hat{G}_0\hat{V}|\psi\rangle\right) \\ &= \;\vdots \\ &= \left[\hat{G}_0\hat{V} + (\hat{G}_0\hat{V})^2 + (\hat{G}_0\hat{V})^3 + \cdots\right]|\psi_i\rangle.\end{aligned} \tag{1.6.10}$$

Or, equivalently,

$$|\psi\rangle = \left[\hat{I} + \hat{G}_0\hat{V} + (\hat{G}_0\hat{V})^2 + (\hat{G}_0\hat{V})^3 + \cdots\right]|\psi_i\rangle. \tag{1.6.11}$$

This is called the **Born series**.

To understand its meaning, let us go to the position basis:

$$\begin{aligned}\psi(\mathbf{r}) = \psi_i(\mathbf{r}) &+ \int d^dr' \,\langle\mathbf{r}|\hat{G}_0|\mathbf{r}'\rangle\, V(\mathbf{r}')\psi_i(\mathbf{r}') \\ &+ \int d^dr'd^dr''\langle\mathbf{r}|\hat{G}_0|\mathbf{r}'\rangle\, V(\mathbf{r}')\,\langle\mathbf{r}'|\hat{G}_0|\mathbf{r}''\rangle\, V(\mathbf{r}'')\psi_i(\mathbf{r}'') \\ &+ \;\cdots\end{aligned} \tag{1.6.12}$$

This formula can be regarded as a description of **multiple scattering**. Due to the presence of the scatterer, the particle wavefunction is a quantum superposition of terms describing zero, one, two, or more scattering events, as illustrated below:

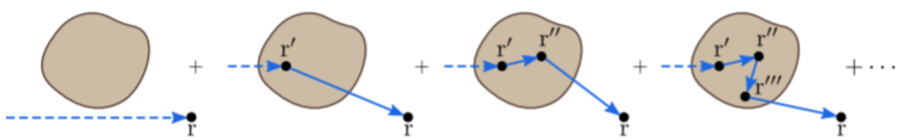

Figure 1.6.1

Each successive term in the Born series involves more scattering events, i.e., higher multiples of $\hat{V}$. For example, the second-order term is

$$\int d^dr'd^dr''\langle\mathbf{r}|\hat{G}_0|\mathbf{r}'\rangle\, V(\mathbf{r}')\,\langle\mathbf{r}'|\hat{G}_0|\mathbf{r}''\rangle\, V(\mathbf{r}'')\psi_i(\mathbf{r}''). \tag{1.6.13}$$

This describes the particle undergoing the following process: (i) scattering of the incident particle at point $\mathbf{r}''$, (ii) propagation from $\mathbf{r}''$ to $\mathbf{r}'$, (iii) scattering again at point $\mathbf{r}'$, and (iv) propagation from $\mathbf{r}'$ to $\mathbf{r}$. The scattering points $\mathbf{r}'$ and $\mathbf{r}''$ are integrated over, with all possible positions contributing to the result; since the integrals are weighted by V, those positions where the scattering potential are strongest will contribute the most.

For a sufficiently weak scatterer, it can be a good approximation to retain just the first few terms in the Born series. For the rest of this discussion, let us assume that such an approximation is valid. The question of what it means for $\hat{V}$ to be "sufficiently weak"—i.e., the exact requirements for the Born series to converge—is a complex topic beyond the scope of our present discussion.