# INTEGRAL FORM OF THE SCHRÖDINGER EQUATION

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As a prelude to the Born approximation in quantum scattering, we need to look at the integral form of the time-independent Schrödinger equation. The equation in its original differential equation form is

$$-\frac{\hbar^2}{2m}\nabla^2\psi+V\psi=E\psi \tag{1}$$

which can be written as

$$\left(\nabla^2+k^2\right)\psi=Q \tag{2}$$

$$k\equiv\frac{\sqrt{2mE}}{\hbar} \tag{3}$$

$$Q\equiv\frac{2m}{\hbar^2}V\psi \tag{4}$$

To convert this to an integral equation, we need to define a *Green's function* $G(\mathbf{r})$ which satisfies the differential equation

$$\left(\nabla^2+k^2\right)G(\mathbf{r})=\delta^3(\mathbf{r}) \tag{5}$$

Using this function we can write $\psi$ as an integral equation

$$\psi(\mathbf{r})=\int G(\mathbf{r}-\mathbf{r}_0)\,Q(\mathbf{r}_0)\,d^3\mathbf{r}_0 \tag{6}$$

We can show this works by plugging in $G$ from 5:

$$\left(\nabla^2+k^2\right)\psi(\mathbf{r})=\int\left(\nabla^2+k^2\right)G(\mathbf{r}-\mathbf{r}_0)\,Q(\mathbf{r}_0)\,d^3\mathbf{r}_0 \tag{7}$$

$$=\int\delta(\mathbf{r}-\mathbf{r}_0)\,Q(\mathbf{r}_0)\,d^3\mathbf{r}_0 \tag{8}$$

$$=Q(\mathbf{r}) \tag{9}$$

which gives us back 2.

This isn't a solution of the Schrödinger equation, of course, because $Q$ contains $\psi$, so we'd need to actually know $\psi$ in advance in order to work out the integral with the Green's function. Rather, it's just a different way of writing the Schrödinger equation which proves useful in scattering theory.

Because 5 doesn't depend on the potential $V$, we can work out the Green's function which is valid for every potential. The process is rather involved, but Griffiths goes through the details in section 11.4.1, so I won't reproduce them here, apart from noting that the solution uses what is, to me, one of the most beautiful theorems in mathematics: Cauchy's theorem on contour integration. Maybe I'll return to it later.

Anyway, the Green's function turns out to be

$$G(\mathbf{r}) = -\frac{e^{ikr}}{4\pi r} \tag{10}$$

We can verify this is in fact a solution by plugging it back into 5. We need the Laplacian of $G$ which we can get by calculating the divergence of the gradient. Taking the gradient first, we use the product rule for gradients:

$$\nabla(fg) = f\nabla g + g\nabla f \tag{11}$$

We get

$$\nabla G = -\frac{1}{4\pi}\left(\frac{1}{r}\nabla e^{ikr} + e^{ikr}\nabla\frac{1}{r}\right) \tag{12}$$

To calculate the divergence of the gradient, we use the identity for the divergence of the product of a scalar and a vector:

$$\nabla\cdot(f\mathbf{A}) = \mathbf{A}\cdot\nabla f + f\nabla\cdot\mathbf{A} \tag{13}$$

We therefore have

$$\nabla^2 G = -\frac{1}{4\pi}\left[\left(\nabla\frac{1}{r}\right)\cdot\left(\nabla e^{ikr}\right) + \frac{1}{r}\nabla^2 e^{ikr} + \left(\nabla e^{ikr}\right)\cdot\left(\nabla\frac{1}{r}\right) + e^{ikr}\nabla^2\frac{1}{r}\right] \tag{14}$$

The last term turns out to be a delta function:

$$\nabla^2\frac{1}{r} = \nabla\cdot\left(\nabla\frac{1}{r}\right) = -\nabla\cdot\left(\frac{\hat{\mathbf{r}}}{r^2}\right) = -4\pi\delta^3(\mathbf{r}) \tag{15}$$

To work out the second term, we use the formula for the Laplacian in spherical coordinates, for a function that depends only on $r$:

$$\nabla f(r) = \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial f}{\partial r}\right) \tag{16}$$

We get

$$\nabla^2 e^{ikr} = \frac{1}{r^2}\frac{\partial}{\partial r}\left(ikr^2 e^{ikr}\right) \tag{17}$$

$$= \frac{2ik}{r}e^{ikr} - k^2 e^{ikr} \tag{18}$$

Putting this back into 14 we get

$$\nabla^2 G = -\frac{1}{4\pi}\left[2\left(\nabla\frac{1}{r}\right)\cdot\left(\nabla e^{ikr}\right) + \frac{2ik}{r^2}e^{ikr} - \frac{k^2}{r}e^{ikr} - 4\pi\delta^3(\mathbf{r})\,e^{ikr}\right] \tag{19}$$

$$= -\frac{1}{4\pi}\left[-\frac{2ik}{r^2}e^{ikr} + \frac{2ik}{r^2}e^{ikr} - \frac{k^2}{r}e^{ikr} - 4\pi\delta^3(\mathbf{r})\,e^{ikr}\right] \tag{20}$$

$$= -\frac{1}{4\pi}\left[-\frac{k^2}{r}e^{ikr} - 4\pi\delta^3(\mathbf{r})\right] \tag{21}$$

$$= \frac{k^2}{4\pi r}e^{ikr} + \delta^3(\mathbf{r}) \tag{22}$$

$$= -k^2 G(\mathbf{r}) + \delta^3(\mathbf{r}) \tag{23}$$

$$\left(\nabla^2 + k^2\right) G(\mathbf{r}) = \delta^3(\mathbf{r}) \tag{24}$$

where we dropped the $e^{ikr}$ from the last term in the third line since the delta function is zero except when $\mathbf{r} = 0$.

Using this Green's function, the integral form of the Schrödinger equation is

$$\psi(\mathbf{r}) = \psi_0(\mathbf{r}) - \frac{m}{2\pi\hbar^2}\int \frac{e^{ik|\mathbf{r}-\mathbf{r}_0|}}{|\mathbf{r}-\mathbf{r}_0|}V(\mathbf{r}_0)\,\psi(\mathbf{r}_0)\,d^3\mathbf{r}_0 \tag{25}$$

where $\psi_0$ is a solution of the free particle Schrödinger equation

$$\left(\nabla^2 + k^2\right)\psi_0(\mathbf{r}) = 0 \tag{26}$$

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