1.7: The Green's Function for a Free Particle

We have defined the free-particle Green's function as the operator $\hat{G}_0 = \left(E - \hat{H}_0\right)^{-1}$. Its representation in the position basis, $\langle \mathbf{r}|\hat{G}_0|\mathbf{r}'\rangle$, is called the **propagator**. As we have just seen, when the Born series is written in the position basis, the propagator appears in the integrand and describes how the particle "propagates" between discrete scattering events.

The propagator is a solution to a partial differential equation:

$$\begin{aligned} \langle\mathbf{r}|\left(E-\hat{H}_0\right)\hat{G}_0|\mathbf{r}'\rangle &= \langle\mathbf{r}|\hat{I}\,|\mathbf{r}'\rangle \\ =\left(E+\frac{\hbar^2}{2m}\nabla^2\right)\langle\mathbf{r}|\hat{G}_0|\mathbf{r}'\rangle &= \delta^d(\mathbf{r}-\mathbf{r}') \\ \Rightarrow \qquad \left(\nabla^2+k^2\right)\langle\mathbf{r}|\hat{G}_0|\mathbf{r}'\rangle &= \frac{2m}{\hbar^2}\delta^d(\mathbf{r}-\mathbf{r}'). \end{aligned} \tag{1.7.1}$$

As before, $k=\sqrt{2mE/\hbar^2}$ where E is the energy of the incident particle. Therefore, up to a factor of $2m/\hbar^2$, the propagator is the Green's function for the d-dimensional Helmholtz equation (see Section 1.4). Note that the ∇^2 acts upon the $\mathbf{r}$ coordinates, not $\mathbf{r}'$.

To solve for $\langle\mathbf{r}|\hat{G}_0|\mathbf{r}'\rangle$, we can use the momentum eigenstates:

$$\begin{aligned} \langle\mathbf{r}|\hat{G}_0|\mathbf{r}'\rangle &= \langle\mathbf{r}|\hat{G}_0\left(\int d^dk'\,|\mathbf{k}'\rangle\langle\mathbf{k}'|\right)|\mathbf{r}'\rangle \\ &= \int d^dk'\;\langle\mathbf{r}|\mathbf{k}'\rangle\;\frac{1}{E-\frac{\hbar^2|\mathbf{k}'|^2}{2m}}\;\langle\mathbf{k}'|\mathbf{r}'\rangle \\ &= \frac{2m}{\hbar^2}\frac{1}{(2\pi)^d}\int d^dk'\;\frac{\exp\left[i\mathbf{k}'\cdot(\mathbf{r}-\mathbf{r}')\right]}{k^2-|\mathbf{k}'|^2}. \end{aligned} \tag{1.7.2}$$

To proceed, we must specify the spatial dimension d. Let us set $d=3$; the calculations for other d are fairly similar. To calculate the integral over the 3D wave-vector space, we adopt spherical coordinates (k',θ,ϕ), with the coordinate axes aligned so that $\mathbf{r}-\mathbf{r}'$ points along the $\theta=0$ direction. We can now do the integral:

$$\begin{aligned} \langle\mathbf{r}|\hat{G}_0|\mathbf{r}'\rangle &= \frac{2m}{\hbar^2}\frac{1}{(2\pi)^3}\int d^3k'\;\frac{\exp\left[i\mathbf{k}'\cdot(\mathbf{r}-\mathbf{r}')\right]}{k^2-|\mathbf{k}'|^2} \\ &= \frac{2m}{\hbar^2}\frac{1}{(2\pi)^3}\int_0^\infty dk'\int_0^\pi d\theta\int_0^{2\pi}d\phi\;k'^2\sin\theta\;\frac{\exp(ik'|\mathbf{r}-\mathbf{r}'|\cos\theta)}{k^2-k'^2} \\ &= \frac{2m}{\hbar^2}\frac{1}{(2\pi)^2}\int_0^\infty dk'\int_{-1}^1 d\mu\;k'^2\;\frac{\exp(ik'|\mathbf{r}-\mathbf{r}'|\mu)}{k^2-k'^2} \qquad (\text{letting } \mu=\cos\theta) \\ &= \frac{2m}{\hbar^2}\frac{1}{(2\pi)^2}\int_0^\infty dk'\;\frac{k'^2}{k^2-k'^2}\;\frac{\exp(ik'|\mathbf{r}-\mathbf{r}'|)-\exp(-ik'|\mathbf{r}-\mathbf{r}'|)}{ik'|\mathbf{r}-\mathbf{r}'|} \\ &= \frac{2m}{\hbar^2}\frac{1}{(2\pi)^2}\frac{i}{|\mathbf{r}-\mathbf{r}'|}\int_{-\infty}^{\infty}dk'\;\frac{k'\,\exp(ik'|\mathbf{r}-\mathbf{r}'|)}{(k'-k)(k'+k)} \end{aligned} \tag{1.7.3}$$

This looks like something we can handle with contour integration techniques. But there's a snag: the integration contour runs over the real-k' line, and since $k\in\mathbb{R}^+$, there are two poles on the contour (at $\pm k$). Hence, the value of the integral, as written, is singular.

To make the integral non-singular, we must "regularize" it by tweaking its definition. One way is to displace the poles infinitesimally in the complex k' plane, shifting them off the contour. We have a choice of whether to move each pole upwards or downwards; this choice turns out to be linked to whether the waves described by $\hat{G}_0$ are incoming, outgoing, or behave some other way at infinity. It turns out that the right choice for us is to move the pole at $-k$ infinitesimally downwards, and the pole at $+k$ infinitesimally upwards:

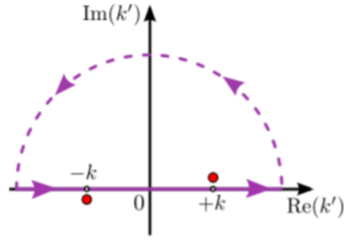

Figure 1.7.1

This means replacing the denominator of the integrand as follows:

$$(k'-k)(k'+k) \;\to\; (k'-k-i\varepsilon)(k'+k+i\varepsilon) = {k'}^2-(k+i\varepsilon)^2, \tag{1.7.4}$$

where ε is a positive infinitesimal. This is equivalent to replacing $E \to E + i\varepsilon$ in the definition of the Green's function. The integral can now be computed as follows:

$$\begin{aligned}\int_{-\infty}^{\infty} dk' \, \frac{k' \exp(ik'|\mathbf{r}-\mathbf{r}'|)}{(k'-k)(k'+k)} &\to \lim_{\varepsilon\to 0^+} \int_{-\infty}^{\infty} dk' \, \frac{k' \exp(ik'|\mathbf{r}-\mathbf{r}'|)}{(k'-k-i\varepsilon)(k'+k+i\varepsilon)} \quad \text{(regularize)} \\ &= \lim_{\varepsilon\to 0^+} \int_C dk' \, \frac{k' \exp(ik'|\mathbf{r}-\mathbf{r}'|)}{(k'-k-i\varepsilon)(k'+k+i\varepsilon)} \quad \text{(close contour above)} \\ &= 2\pi i \lim_{\varepsilon\to 0^+} \mathrm{Res}\left[\frac{k' \exp(ik'|\mathbf{r}-\mathbf{r}'|)}{(k'-k-i\varepsilon)(k'+k+i\varepsilon)}\right]_{k'=k+i\varepsilon^+} \\ &= \pi i \exp(ik|\mathbf{r}-\mathbf{r}'|).\end{aligned} \tag{1.7.5}$$

Plugging this into Equation (1.7.2) yields the propagator $\langle \mathbf{r}|\hat{G}_0|\mathbf{r}'\rangle$. The final result is given below, along with the results for $d=1$ and $d=2$ (which are obtained in a similar fashion):

Definition: Propagator

$$\langle \mathbf{r}|\hat{G}_0|\mathbf{r}'\rangle = \frac{2m}{\hbar^2} \times \begin{cases} \dfrac{1}{2ik}\exp(ik|x-x'|), & d=1 \\ \dfrac{1}{4i}H_0^+(k|\mathbf{r}-\mathbf{r}'|), & d=2 \\ -\dfrac{\exp(ik|\mathbf{r}-\mathbf{r}'|)}{4\pi|\mathbf{r}-\mathbf{r}'|}, & d=3. \end{cases} \tag{1.7.6}$$

The propagator can be regarded as a function of the position $\mathbf{r}$, describing a wave propagating outwards from a source point $\mathbf{r}'$. This outgoing behavior comes from our above choice of regularization, which tweaked the definition of the Green's function to be

Definition: Green's function

$$\hat{G}_0 = \lim_{\varepsilon\to 0^+} \left(E - \hat{H}_0 + i\varepsilon\right)^{-1}. \tag{1.7.7}$$

This is called an **outgoing** or **causal Green's function**. The word "causal" refers to the concept of "cause-and-effect": i.e., a source at one point of space (the "cause") leads to the emission of waves that move outwards (the "effect").

Different regularizations produce Green's functions with alternative features. For instance, we could flip the sign of $i\varepsilon$ in the Green's function redefinition, which displaces the k-space poles in the opposite direction. The resulting propagator $\langle \mathbf{r}|\hat{G}_0|\mathbf{r}'\rangle$ is complex-conjugated, and describes a wave moving inwards from infinity, "sinking" into the point $\mathbf{r}'$. Such a choice of regularization thus corresponds to an **incoming Green's function**. In the scattering problem, we will always deal with the outgoing/causal Green's function.