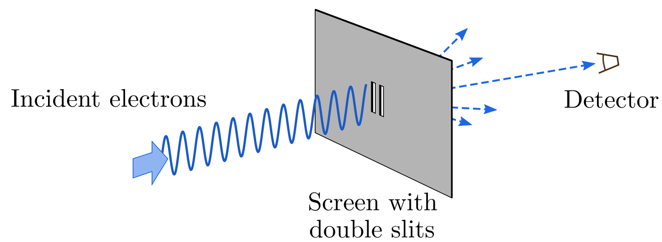
Chapter 1: Scattering Theory

1.1. SCATTERING EXPERIMENTS ON QUANTUM PARTICLES

Quantum particles exhibit a feature known as **wave-particle duality**, which can be summarized in the **quantum double-slit thought experiment**. As illustrated below, a source emits electrons of energy E toward a screen with a pair of slits. A movable detector, placed on the far side, measures the arrival rates at different positions.



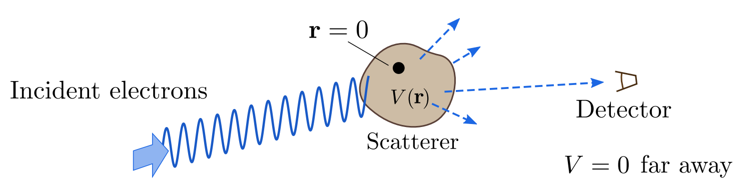
The experiment reveals the following: (i) the electrons arrive in discrete units, like classical particles; (ii) the *statistical* distribution of electron arrivals forms an interference pattern, like a diffracted wave. In the non-relativistic limit, the inferred wavelength λ is related to the electron energy E by

$$\lambda = \frac{2\pi}{k}, \quad E = \frac{\hbar^2 k^2}{2m}, \tag{1.1}$$

where $\hbar = h/2\pi$ is Dirac's constant, and m is the electron mass. (Thus, if E is known, we can deduce the spacing of the slits from the diffraction pattern.)

In this chapter, we will study a generalization of the double-slit experiment called a **scattering experiment**. The idea is to shoot quantum particles at a target, called a **scatterer**, and measure the distribution of scattered particles. Just as the double-slit interference pattern can be used to deduce the slit spacing, a scattering experiment can be used to deduce various facts about the scatterer. Scattering experiments constitute a large proportion of the methods used to probe the quantum world, from electron- and photon-based microscopy to accelerator experiments in high-energy physics.

We will focus on the non-relativistic scattering experiment depicted below:



An unbounded d-dimensional space is described by coordinates $\mathbf{r}$, with a scatterer near $\mathbf{r} = 0$. An incoming quantum particle, with energy E, is governed by the Hamiltonian

$$\hat{H} = \hat{H}_0 + V(\hat{\mathbf{r}}), \tag{1.2}$$

where

$$\hat{H}_0 = \frac{\hat{\mathbf{p}}^2}{2m} \tag{1.3}$$

describes the particle's kinetic energy, m is the particle's mass, $\hat{\mathbf{r}}$ and $\hat{\mathbf{p}}$ are the position and momentum operators, and V is a **scattering potential** describing how the scatterer acts upon the particle. We assume this potential vanishes far from the scatterer:

$$V(\mathbf{r}) \overset{|\mathbf{r}|\to\infty}{\longrightarrow} 0. \tag{1.4}$$

How is the particle scattered by the potential? In order to study this, we formulate the above description as the following mathematical problem:

1. A particle state $|\psi\rangle$ obeys the time-independent Schrödinger equation

   $$\hat{H}|\psi\rangle = E|\psi\rangle, \tag{1.5}$$

   where E is the incoming particle energy.

2. The state $|\psi\rangle$ can be decomposed into two pieces,

   $$|\psi\rangle \;=\; |\psi_i\rangle \,+\, |\psi_s\rangle, \tag{1.6}$$

   where $|\psi_i\rangle$ is called the **incident state** and $|\psi_s\rangle$ is called the **scattered state**.

3. The incident state is described by a plane wave, which is a simultaneous eigenstate of $\hat{H}_0$ (with energy E) and $\hat{\mathbf{p}}$ (with momentum $\mathbf{p}_i$):

   $$\begin{cases} \hat{H}_0|\psi_i\rangle &= E|\psi_i\rangle, \\ \hat{\mathbf{p}}|\psi_i\rangle &= \mathbf{p}_i|\psi_i\rangle, \end{cases} \quad \text{where} \quad E = \frac{|\mathbf{p}_i|^2}{2m}. \tag{1.7}$$

4. The scattered state is an "outgoing" state. What this means will be explained later.

We can interpret the above statements as follows. Statement 1 says the scattering is elastic: the scatterer is described by a potential $V(\mathbf{r})$, so its interaction with the particle is conservative and E is fixed. Statement 2 says that the wavefunction $\psi(\mathbf{r}) = \langle \mathbf{r}|\psi\rangle$ is a superposition of an incoming wave and a scattered wave. Statement 3 defines the incoming wave as a plane wave with wavelength determined by E. Statement 4 says the scattered wave moves outward to infinity, away from the scatterer.

Note that Statements 1–4 do *not* define an eigenproblem! Usually, we deal with the time-independent Schrödinger equation by finding eigenvalues and eigenstates. But here we are given $|\psi_i\rangle$, E, and $V(\mathbf{r})$, and want $|\psi_s\rangle$. In particular, E is an input to the calculation (a continuously variable parameter), not an output (an eigenvalue).

1.2. RECAP: POSITION AND MOMENTUM STATES

Before proceeding, let us review the properties of a quantum particle in free space. In a d-dimensional space, a coordinate vector $\mathbf{r}$ is a real vector with d components. We suppose there is a uncountably infinite set of position eigenstates, $\{|\mathbf{r}\rangle\}$, where each $|\mathbf{r}\rangle$ describes a particle with a definite position $\mathbf{r}$. The position eigenstates are assumed to span the state space, such that the identity operator can be resolved as

$$\hat{I} = \int d^d r\, |\mathbf{r}\rangle\langle\mathbf{r}|, \tag{1.8}$$

with the integral is taken over all allowed $\mathbf{r}$ (e.g., $\mathbf{r} \in \mathbb{R}^d$). It follows that

$$\langle \mathbf{r}|\mathbf{r}'\rangle = \delta^d(\mathbf{r} - \mathbf{r}'). \tag{1.9}$$

Thus, we say that the position eigenstates are **delta-normalized**, rather than being normalized to unity. Here $\delta^d(\cdots)$ denotes the d-dimensional delta function; e.g., in 2D,

$$\langle x, y \,|\, x', y'\rangle = \delta(x - x')\,\delta(y - y').$$

Moreover, the position operator $\hat{\mathbf{r}}$ is defined such that $\hat{\mathbf{r}}|\mathbf{r}\rangle = \mathbf{r}\,|\mathbf{r}\rangle$.

Momentum eigenstates are constructed from position eigenstates via Fourier transforms. First, let us suppose $\mathbf{r}$ runs over a finite box of length L on each side, with periodic boundary conditions. For plane waves of the form $\exp(i\mathbf{k}\cdot\mathbf{r})$, where $\mathbf{k} = (k_1, \ldots, k_d)$ is the wave-vector, the periodic boundary conditions are satisfied if and only if

$$k_j = 2\pi m/L \;\; \text{for } m \in \mathbb{Z}. \tag{1.10}$$

Note that the set of allowed wave-vectors is discrete (i.e., countable), with a discretization of $\Delta k = 2\pi/L$ in each direction. Next, define

$$|\mathbf{k}\rangle = \frac{1}{L^{d/2}} \int d^d r \; e^{i\mathbf{k}\cdot\mathbf{r}} |\mathbf{r}\rangle, \tag{1.11}$$

where the integral is taken over the box. We identify $|\mathbf{k}\rangle$ as a momentum eigenstate, i.e., a state with definite momentum $\hbar\mathbf{k}$. Using Eqs. (1.8)–(1.9) and Eq. (1.11), we can show that

$$\langle \mathbf{k}|\mathbf{k}'\rangle = \delta_{\mathbf{k},\mathbf{k}'}, \quad \langle \mathbf{r}|\mathbf{k}\rangle = \frac{1}{L^{d/2}} e^{i\mathbf{k}\cdot\mathbf{r}}, \quad I = \sum_{\mathbf{k}} |\mathbf{k}\rangle\,\langle\mathbf{k}|. \tag{1.12}$$

In particular, note that each momentum eigenstate is normalizable to unity.

Now let us take $L \to \infty$. In this limit, the wave-vector discretization $\Delta k = 2\pi/L$ goes to zero, so the momentum eigenvalues coalesce into a continuum. To handle this, we redefine the momentum eigenstates as

$$|\mathbf{k}\rangle^{(\text{new})} = \left(\frac{L}{2\pi}\right)^{d/2} |\mathbf{k}\rangle^{(\text{old})}. \tag{1.13}$$

Then, by using the formula

$$\int_{-\infty}^{\infty} dx \;\, \exp(ikx) \;=\; 2\pi\,\delta(k), \tag{1.14}$$

we can show that the new momentum eigenstates are related to the position eigenstates by

$$|\mathbf{k}\rangle = \frac{1}{(2\pi)^{d/2}} \int d^d r \; e^{i\mathbf{k}\cdot\mathbf{r}} |\mathbf{r}\rangle, \tag{1.15}$$

$$|\mathbf{r}\rangle = \frac{1}{(2\pi)^{d/2}} \int d^d k \; e^{-i\mathbf{k}\cdot\mathbf{r}} |\mathbf{k}\rangle. \tag{1.16}$$

Position and momentum are now treated on similar footing, with the integrals over $\mathbf{r}$ and $\mathbf{k}$ both taken over infinite spaces. Moreover, the momentum eigenstates now satisfy

$$I = \int d^dk \; |\mathbf{k}\rangle \langle \mathbf{k}|, \tag{1.17}$$

$$\langle \mathbf{k}|\mathbf{k}'\rangle = \delta^d(\mathbf{k}-\mathbf{k}'), \tag{1.18}$$

$$\langle \mathbf{r}|\mathbf{k}\rangle = \frac{e^{i\mathbf{k}\cdot\mathbf{r}}}{(2\pi)^{d/2}}. \tag{1.19}$$

The first two equations are analogous to their position eigenstate counterparts, Eq. (1.8) and (1.9). In particular, Eq. (1.18) says the new $|\mathbf{k}\rangle$'s are delta-normalized. The last equation, (1.19), can be interpreted as the wavefunction of the delta-normalized momentum eigenstate.

The momentum operator $\hat{\mathbf{p}}$ is defined using the $|\mathbf{k}\rangle$'s as the eigenbasis:

$$\hat{\mathbf{p}}|\mathbf{k}\rangle \;=\; \hbar\mathbf{k}\,|\mathbf{k}\rangle. \tag{1.20}$$

For any quantum state $|\psi\rangle$, whose wavefunction is $\psi(\mathbf{r}) = \langle \mathbf{r}|\psi\rangle$, we can use Eqs. (1.16) and (1.20) to show that the momentum operator acts on wavefunctions in the following way:

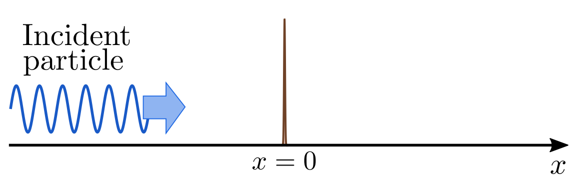
$$\begin{aligned}\langle \mathbf{r}|\hat{\mathbf{p}}|\psi\rangle &= \frac{1}{(2\pi)^{d/2}} \int d^dk \; e^{i\mathbf{k}\cdot\mathbf{r}} \langle \mathbf{k}|\hat{\mathbf{p}}|\psi\rangle \\ &= \frac{1}{(2\pi)^{d/2}} \int d^dk \; \hbar\mathbf{k}\, e^{i\mathbf{k}\cdot\mathbf{r}} \langle \mathbf{k}|\psi\rangle \\ &= -i\hbar\nabla \left[\frac{1}{(2\pi)^{d/2}} \int d^dk \, e^{i\mathbf{k}\cdot\mathbf{r}} \langle \mathbf{k}|\psi\rangle\right] \\ &= -i\hbar\nabla\psi(\mathbf{r}).\end{aligned} \tag{1.21}$$

1.3. SCATTERING FROM A 1D DELTA FUNCTION POTENTIAL

We are now ready to solve a simple scattering problem. Consider a 1D space with spatial coordinate x, and a scattering potential consisting of a "spike" at $x = 0$:

$$V(x) = \frac{\hbar^2\gamma}{2m}\,\delta(x). \tag{1.22}$$

The form of the prefactor $\hbar^2\gamma/2m$ is chosen for later convenience; the parameter γ, which has units of $[1/x]$, controls the strength of the scattering potential.



The particle wavefunction $\psi(x)$ satisfies the 1D Schrödinger wave equation

$$\left[-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V(x)\right]\psi(x) = E\psi(x). \tag{1.23}$$

As this is a second-order differential equation, we normally require $\psi(x)$ to be continuous and to have well-defined first and second derivatives. However, the delta function potential (1.22) relaxes these requirements in a peculiar way: at $x = 0$, $\psi(x)$ must still be continuous, but its first derivative may now be discontinuous (and hence, its second derivative is singular). To see this, integrate Eq. (1.23) over an infinitesimal range around $x = 0$:

$$\begin{aligned}\lim_{\varepsilon\rightarrow 0^+}\int_{-\varepsilon}^{+\varepsilon} dx\,\left[-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}+\frac{\hbar^2\gamma}{2m}\delta(x)\right]\psi(x) &= \lim_{\varepsilon\rightarrow 0^+}\int_{-\varepsilon}^{+\varepsilon} dx\; E\psi(x) \\ = \lim_{\varepsilon\rightarrow 0^+}\left(-\frac{\hbar^2}{2m}\left[\frac{d\psi}{dx}\right]_{-\varepsilon}^{+\varepsilon}\right) + \frac{\hbar^2\gamma}{2m}\psi(0) &= 0.\end{aligned} \tag{1.24}$$

Therefore,

$$\lim_{\varepsilon\rightarrow 0^+}\left(\left.\frac{d\psi}{dx}\right|_{x=+\varepsilon} - \left.\frac{d\psi}{dx}\right|_{x=-\varepsilon}\right) = \gamma\,\psi(0). \tag{1.25}$$

In accordance our previously-discussed formulation of the scattering problem, and specifically Eq. (1.6), the total wavefunction is split into

$$\psi(x) = \psi_i(x) + \psi_s(x). \tag{1.26}$$

Moreover, the incident state should be a momentum eigenstate. But we will *not* let it be delta-normalized, as momentum eigenstates normally are (see Sec. 1.2). Instead, we write

$$\psi_i(x) = \Psi_i\, e^{ikx}, \quad k = \sqrt{\frac{2mE}{\hbar^2}} > 0. \tag{1.27}$$

The complex coefficient Ψ_i is called the **incident amplitude**. Introducing Ψ_i in this way emphasizes that the magnitude and phase of the incident wavefunction are, in principle, adjustable parameters in the scattering experiment. In terms of the usual delta-normalized momentum eigenstates,

$$|\psi_i\rangle = \sqrt{2\pi}\,\Psi_i|k\rangle. \tag{1.28}$$

With this, Eq. (1.23) becomes

$$\left[-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}+\frac{\hbar^2\gamma}{2m}\delta(x)\right]\Big(\Psi_i\,e^{ikx}+\psi_s(x)\Big) = E\Big(\Psi_i\,e^{ikx}+\psi_s(x)\Big). \tag{1.29}$$

Taking $E = \hbar^2k^2/2m$, and doing a bit of algebra, simplifies this to

$$\left[\frac{d^2}{dx^2}+k^2\right]\psi_s(x) = \gamma\delta(x)\Big(\Psi_i\,e^{ikx}+\psi_s(x)\Big). \tag{1.30}$$

We can construct the solution by separately considering the regions $x < 0$ and $x > 0$. Within each half-space, $\delta(x)$ vanishes so Eq. (1.30) reduces to the Helmholtz equation

$$\left[\frac{d^2}{dx^2}+k^2\right]\psi_s(x) = 0. \tag{1.31}$$

This has the general solution

$$\psi_s(x) = \Psi_i\left(f_R\,e^{ikx} + f_L\,e^{-ikx}\right), \tag{1.32}$$

which is a superposition of right-moving (e^{ikx}) and left-moving (e^{-ikx}) waves. The complex parameters f_1 and f_2 can have different values in the $x < 0$ and $x > 0$ regions.

We want the scattered wave to be an outgoing wave. Thus, for $x < 0$, ψ_s is purely left-moving, so $f_R = 0$; and for $x > 0$, ψ_s is purely right-moving, so $f_L = 0$. Therefore,

$$\psi_s(x) = \Psi_i \times \begin{cases} f_-\, e^{-ikx}, & x < 0 \\ f_+\, e^{ikx}, & x > 0. \end{cases} \tag{1.33}$$

The complex numbers f_- and f_+ are called **scattering amplitudes**. They parameterize the magnitude and phase of the scattered wavefunction moving outward from the scatterer.

Recall from the discussion at the beginning of this section that $\psi(x)$ must be continuous at $x = 0$. This implies that $\psi_s(x)$ is also continuous, and therefore that

$$f_- = f_+ \quad \Rightarrow \quad \psi_s(x) = \Psi_i\, f_\pm\, e^{ik|x|}. \tag{1.34}$$

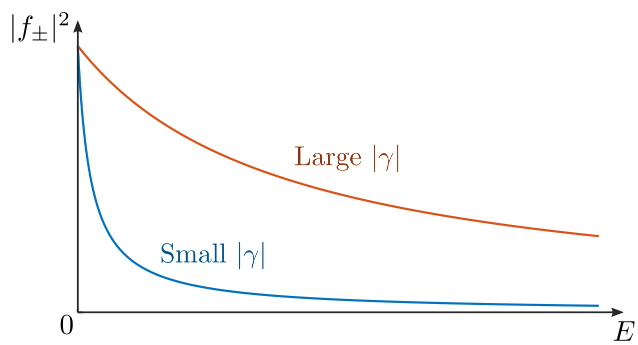
Plugging Eqs. (1.27) and (1.34) into Eq. (1.25) yields

$$f_\pm = -\frac{\gamma}{\gamma - 2ik}. \tag{1.35}$$

For now, let us focus on the magnitude of the scattering amplitude (in the next chapter, we will see that the phase also contains useful information). The quantity $|f_\pm|^2$ describes the overall strength of the scattering process:

$$|f_\pm|^2 = \left[1 + \frac{8mE}{(\hbar\gamma)^2}\right]^{-1}. \tag{1.36}$$

Its dependence on E is plotted below:



The behavior matches our intuition. For a given particle energy E, the scattering grows stronger as the potential strength parameter $|\gamma|$ increases. On the other hand, for fixed γ, a higher-energy particle undergoes less scattering. Note also that attractive potentials ($\gamma < 0$) and repulsive potentials ($\gamma > 0$) are equally effective at scattering.

1.4. SCATTERING AMPLITUDE AND SCATTERING CROSS SECTION

In the 1D scattering problem of the previous section, the particle can only scatter in two directions: forward or backward. In 2D and higher spatial dimensions, there is an important complication: the particle can also go "sideways", and in fact there is a continuous set of directions for it to scatter into. To deal with this, physicists have developed a systematic formalism for expressing the outcomes of scattering experiments using direction-dependent "scattering amplitudes", which we will now describe.

To begin, let us define the incident wavefunction as a plane wave in d dimensions, by analogy with the 1D case [Eq. (1.27)]:

$$\psi_i(\mathbf{r}) = \Psi_i \, e^{i\mathbf{k}_i\cdot\mathbf{r}}, \quad |\mathbf{k}_i| = k = \sqrt{\frac{2mE}{\hbar^2}}, \tag{1.37}$$

where $\mathbf{k}_i$ is the incident wave-vector and $\Psi_i \in \mathbb{C}$ is the incident amplitude.

The incident wavefunction generates a scattered wavefunction $\psi_s(\mathbf{r})$. We can express the $\mathbf{r}$-dependence of this wavefunction using a coordinate system of the form (r, Ω), where r is the distance from the origin and Ω denotes the other "directional" coordinates. Specifically,

- For $d = 2$, we use polar coordinates (r, ϕ), i.e. $\Omega \equiv \phi$.
- For $d = 3$, we use spherical coordinates (r, θ, ϕ), i.e. $\Omega \equiv (\theta, \phi)$.

We can also wrangle the $d = 1$ case into this framework by letting $\Omega \in \{+, -\}$, where $+$ denotes the forward $(+x)$ direction and $-$ denotes the backward $(-x)$ direction.

In a typical scattering experiment, the scattered wavefunction is detected at $r \to \infty$; i.e., at distances much longer than the size of the scatterer, the free-space wavelength, and any other relevant length scales. In this regime, we assert that the scattered wavefunction must reduce to the form

$$\psi_s(\mathbf{r}) \overset{r\rightarrow\infty}{\longrightarrow} \Psi_i \, r^{\frac{1-d}{2}} \, e^{ikr} \, f(\Omega). \tag{1.38}$$

To understand the reasoning behind this, let us go through the individual multiplicative factors on the right side of Eq. (1.38).

The first factor Ψ_i accounts for the fact that the Schrödinger wave equation is linear. If we vary the incident amplitude, the scattered wavefunction must vary proportionally.

The next two factors, $r^{\frac{1-d}{2}} \, e^{ikr}$, give the r-dependence of a wave expanding radially from the origin in d dimensions. The e^{ikr} factor captures its outgoing nature (the wavefunction's phase increases along the direction of propagation, i.e., the direction of increasing r). The other factor provides the r-scaling needed for probability conservation. Note that the probability current density associated with the scattered wavefunction is

$$\mathbf{J}_s = \frac{\hbar}{m} \mathrm{Im}\big[\psi_s^* \nabla \psi_s\big]. \tag{1.39}$$

Thus, its radial component is

$$\begin{aligned} J_s^r &= \frac{\hbar}{m} \, \mathrm{Im}\left[\psi_s^* \frac{\partial}{\partial r}\psi_s\right] \\ &\overset{r\rightarrow\infty}{\longrightarrow} \;\; (\cdots)\mathrm{Im}\left[\left(r^{\frac{1-d}{2}} \, e^{ikr}\right)^* \frac{\partial}{\partial r}\left(r^{\frac{1-d}{2}} \, e^{ikr}\right)\right] \\ &= (\cdots) \, \mathrm{Im}\left[\left(r^{\frac{1-d}{2}} \, e^{ikr}\right)^* \left(ikr^{\frac{1-d}{2}} \, e^{ikr} + \frac{1-d}{2} \, r^{\frac{-1-d}{2}} \, e^{ikr}\right)\right] \\ &= (\cdots) \, r^{-(d-1)} + O(r^{-d}), \end{aligned} \tag{1.40}$$

where $(\cdots)$ denotes r-independent terms. In d dimensions, the area of the surface at distance r from the origin scales as r^{d-1}. Hence, J_s^r scales inversely with area, and the total flux obtained by integrating J_s^r over the area is independent of r.

The final factor in Eq. (1.38), $f(\Omega)$, is called the **scattering amplitude**. This complex function is typically the main avenue by which a scattering experiment reveals information about the scatterer. As noted in the previous paragraphs, in the large-r limit, the other factors are determined by linearity, outgoing-ness, and flux conservation. Hence, only f is sensitive to the details of the scattering potential.

Note that the scattering amplitude is a function of Ω, i.e., the direction of $\mathbf{r}$. Sometimes, it is written using the alternative notation

$$f(\mathbf{k}_i \rightarrow \mathbf{k}_f), \qquad \mathbf{k}_f = k\,\frac{\mathbf{r}}{|\mathbf{r}|}. \tag{1.41}$$

This emphasizes that the particle is initially incident with wave-vector $\mathbf{k}_i$, then gets scattered elastically into a wave-vector $\mathbf{k}_f$ pointing in the direction of $\mathbf{r}$.

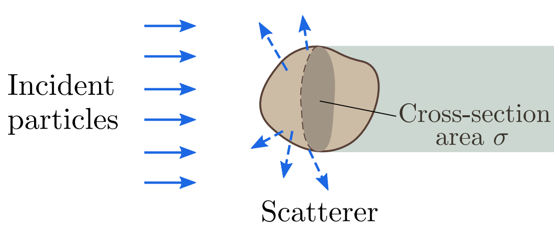
From the scattering amplitude, we can define two other important quantities:

$$\frac{d\sigma}{d\Omega} = \big|f(\Omega)\big|^2 \qquad \text{(the \textbf{differential scattering cross section})} \tag{1.42}$$

$$\sigma = \int d\Omega\,\big|f(\Omega)\big|^2 \qquad \text{(the \textbf{total scattering cross section})}. \tag{1.43}$$

In Eq. (1.43), $\int d\Omega$ denotes the integral(s) over all the angle coordinates. For 1D, this is replaced by a discrete sum over the forward and backward directions (see above).

The term "cross section" comes from an analogy with the scattering of classical particles. Imagine a stream of classical particles incident on a "hard-body" scatterer:



Let the incident classical particles have the same flux as the incident wavefunction (1.37),

$$J_i = \frac{\hbar k}{m}\,|\Psi_i|^2. \tag{1.44}$$

Note that this has units of $[x^{1-d}t^{-1}]$ (i.e., number per unit time per unit area in d dimensions). We assume the scatterer only interacts with the particles striking it directly, and the rate at which these strikes occur is

$$I_s = J_i\,\sigma, \tag{1.45}$$

where σ is the exposed cross-sectional area of the scatterer, as shown in the figure. This is the *total* rate at which scattering occurs, regardless of where the particles scatter to.

Let us compare this to the quantum mechanical scattering rate. Using Eq. (1.38), we can repeat the calculation in (1.40) for the radial component of the probability current density:

$$J_s^r \xrightarrow{r\rightarrow\infty} \frac{\hbar\, k}{m}\, |\Psi_i|^2\, |f(\Omega)|^2\, r^{1-d} + O(r^{-d}). \tag{1.46}$$

Hence, the total flux of outgoing probability is

$$I_s = \int d\Omega\; r^{d-1}\, J_{s,r} = \left(\frac{\hbar k}{m}\, |\Psi_i|^2\right) \int d\Omega\, \big|f(\Omega)\big|^2. \tag{1.47}$$

On the right side, the quantity in parentheses is the incident flux, Eq. (1.44). Comparing Eq. (1.47) to Eq. (1.45), we see that

$$\sigma \equiv \int d\Omega\, \big|f(\Omega)\big|^2$$

is the quantity analogous to the exposed cross-sectional area of the classical hard-body. We therefore call this the **total scattering cross section**.

Moreover, the integrand $|f|^2$ represents the rate, per unit of solid angle, at which particles are scattered in a given direction. We call this the **differential scattering cross section**. The total and differential scattering cross sections are the principal observable quantities typically obtained in scattering experiments.

1.5. 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:

$$\begin{aligned} \hat{H} &= \hat{H}_0 + \hat{V} \\ \hat{H}|\psi\rangle &= E|\psi\rangle \\ |\psi\rangle &= |\psi_i\rangle \,+\, |\psi_s\rangle \\ \hat{H}_0|\psi_i\rangle &= E|\psi_i\rangle. \end{aligned} \tag{1.48}$$

These equations can be combined as follows:

$$\left(\hat{H}_0 + \hat{V}\right)|\psi_i\rangle + \hat{H}|\psi_s\rangle = E\left(|\psi_i\rangle + |\psi_s\rangle\right) \tag{1.49}$$

$$\Rightarrow \quad \hat{V}|\psi_i\rangle + \hat{H}|\psi_s\rangle = E|\psi_s\rangle \tag{1.50}$$

$$\Rightarrow \quad \left(E - \hat{H}\right)|\psi_s\rangle = \hat{V}|\psi_i\rangle \tag{1.51}$$

To proceed, we define an operator called the **Green's function**, which is the inverse of the operator on the left side of Eq. (1.51):

$$\hat{G}(E) = \big(E - \hat{H}\big)^{-1}. \tag{1.52}$$

Note that $\hat{G}(E)$ depends parametrically on E. We can now convert Eq. (1.51) into

$$|\psi_s\rangle = \hat{G}\hat{V}|\psi_i\rangle. \tag{1.53}$$

It will also be useful to define the Green's function for a free particle,

$$\hat{G}_0(E) = \left(E - \hat{H}_0\right)^{-1}. \tag{1.54}$$

As we shall see, $\hat{G}_0$ often can be calculated exactly, whereas $\hat{G}$ typically has no closed-form analytic expression. Moreover, we can relate G and G_0 as follows:

$$\begin{aligned} &\hat{G}(E - \hat{H}_0 - \hat{V}) &= I \quad \text{and} \quad (E - \hat{H}_0 - \hat{V})\hat{G} = I \\ \Leftrightarrow \qquad &\hat{G}\hat{G}_0^{-1} - \hat{G}\hat{V} = I \quad \text{and} \quad \hat{G}_0^{-1}\hat{G} - \hat{V}\hat{G} &= I. \end{aligned} \tag{1.55}$$

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**:

$$\hat{G} = \hat{G}_0 + \hat{G}\hat{V}\hat{G}_0 \tag{1.56}$$

$$\hat{G} = \hat{G}_0 + \hat{G}_0\hat{V}\hat{G} \tag{1.57}$$

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

Applying the second Dyson equation, Eq. (1.57), to the scattering problem (1.53) gives

$$|\psi_s\rangle = \left(\hat{G}_0 + \hat{G}_0\hat{V}\hat{G}\right)\hat{V}\,|\psi_i\rangle \tag{1.58}$$

$$= \hat{G}_0\hat{V}\left(\hat{I} + \hat{G}\hat{V}\right)|\psi_i\rangle. \tag{1.59}$$

Using Eq. (1.53) again, we get

$$|\psi_s\rangle = \hat{G}_0\hat{V}|\psi\rangle. \tag{1.60}$$

This remains an implicit equation, but the unknown is $|\psi\rangle$ rather than $\hat{G}$. Note that the results up to this point have been approximation-free.

One approach to solving Eq. (1.60) is to repeatedly plug its right side back into itself:

$$\begin{aligned} |\psi_s\rangle &= \hat{G}_0\hat{V}\left(|\psi_i\rangle + \hat{G}_0\hat{V}|\psi\rangle\right) \\ &= \quad \vdots \\ &= \left[\hat{G}_0\hat{V} + (\hat{G}_0\hat{V})^2 + (\hat{G}_0\hat{V})^3 + \cdots\right]|\psi_i\rangle. \end{aligned} \tag{1.61}$$

Or, equivalently,

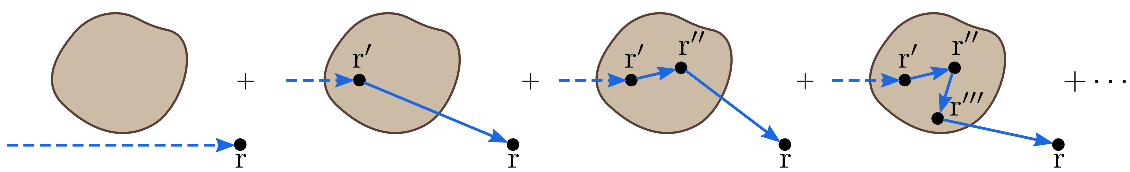
$$|\psi\rangle = \left[\hat{I} + \hat{G}_0\hat{V} + (\hat{G}_0\hat{V})^2 + (\hat{G}_0\hat{V})^3 + \cdots\right]|\psi_i\rangle. \tag{1.62}$$

This infinite series is called the **Born series**.

To interpret this result, let us go to the position basis:

$$\begin{aligned}\psi(\mathbf{r}) = \psi_i(\mathbf{r}) &+ \int d^d r' \langle \mathbf{r}|\hat{G}_0|\mathbf{r}'\rangle\, V(\mathbf{r}')\psi_i(\mathbf{r}') \\ &+ \int d^d r' d^d r'' \langle \mathbf{r}|\hat{G}_0|\mathbf{r}'\rangle\, V(\mathbf{r}')\, \langle \mathbf{r}'|\hat{G}_0|\mathbf{r}''\rangle\, V(\mathbf{r}'')\psi_i(\mathbf{r}'') \;+\; \cdots\end{aligned} \tag{1.63}$$

This can be regarded as a description of **multiple scattering**. The wavefunction is a superposition of terms involving zero, one, two, or more scattering events, as shown below:



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

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

which describes the particle undergoing (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 $\mathbf{r}$. Note that $\mathbf{r}'$ and $\mathbf{r}''$ are integrated over all possible positions. Since the integrals are weighted by V, the positions with the strongest scattering potential contribute the most.

For a sufficiently weak scatterer, it is often a good approximation to retain just the first few terms in the Born series. The question of when $\hat{V}$ is "sufficiently weak"—i.e., when the Born series converges—is a complex topic beyond the scope of our present discussion.

1.6. GREEN'S FUNCTION FOR A FREE PARTICLE

In the position basis representation of the Born series, Eq. (1.63), a crucial role is played by the matrix elements $\langle \mathbf{r}|\hat{G}_0|\mathbf{r}'\rangle$. We call this the **propagator**, as it describes how the particle propagates between discrete scattering events.

Starting from the definition of $\hat{G}_0$ in Eq. (1.54), we can evaluate it in the position basis:

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

Hence,

$$\left(\nabla^2 + k^2\right)\langle \mathbf{r}|\hat{G}_0|\mathbf{r}'\rangle = \frac{2m}{\hbar^2}\delta^d(\mathbf{r}-\mathbf{r}'), \tag{1.64}$$

where

$$k^2 = \frac{2mE}{\hbar^2}. \tag{1.65}$$

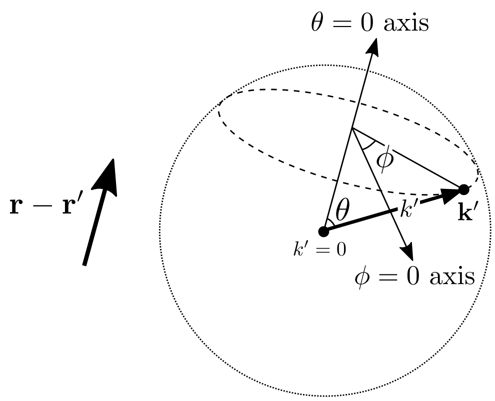
The left side of this equation is the same as the d-dimensional Helmholtz equation, with the ∇^2 acting on the $\mathbf{r}$ coordinates (not $\mathbf{r}'$). On the right side, we have a term proportional to a d-dimensional delta function at $\mathbf{r} = \mathbf{r}'$. The propagator thus describes a wave at each position $\mathbf{r}$, emitted from a point source at $\mathbf{r}'$.

Eq. (1.64) can be solved analytically for different values of the spatial dimension d. In the following, we will work through the derivation for $d = 3$. The derivations for $d = 1$ and $d = 2$ are left as exercises.

To derive the 3D propagator, we first re-express it using the momentum eigenbasis:

$$\begin{aligned}\langle \mathbf{r}|\hat{G}_0|\mathbf{r}'\rangle &= \langle \mathbf{r}|\hat{G}_0\Big(\int d^3k'\; |\mathbf{k}'\rangle\langle\mathbf{k}'|\Big)|\mathbf{r}'\rangle \\ &= \int d^3k'\; \langle \mathbf{r}|\mathbf{k}'\rangle\, \frac{1}{E - \frac{\hbar^2|\mathbf{k}'|^2}{2m}}\, \langle \mathbf{k}'|\mathbf{r}'\rangle \\ &= \frac{2m}{\hbar^2}\frac{1}{(2\pi)^3}\int d^3k'\; \frac{\exp\left[i\mathbf{k}'\cdot(\mathbf{r}-\mathbf{r}')\right]}{k^2 - |\mathbf{k}'|^2}. \end{aligned} \tag{1.66}$$

Next, we express $\mathbf{k}'$ using spherical coordinates (k', θ, ϕ). We are free to choose the $\theta = 0$ axis so that it points in the direction of $\mathbf{r} - \mathbf{r}'$, as illustrated below:

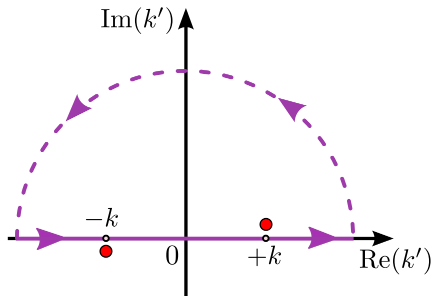


Then,

$$\begin{aligned}\langle \mathbf{r}|\hat{G}_0|\mathbf{r}'\rangle &= \frac{2m}{\hbar^2}\frac{1}{(2\pi)^3}\int d^3k'\; \frac{\exp\left[i\mathbf{k}'\cdot(\mathbf{r}-\mathbf{r}')\right]}{k^2 - |\mathbf{k}'|^2} \\ &= \frac{2m}{\hbar^2}\frac{1}{(2\pi)^3}\int_0^\infty dk' \int_0^\pi d\theta \int_0^{2\pi} d\phi\; k'^2 \sin\theta\; \frac{\exp\left(ik'|\mathbf{r}-\mathbf{r}'|\cos\theta\right)}{k^2 - k'^2} \\ &= \frac{2m}{\hbar^2}\frac{1}{(2\pi)^2}\int_0^\infty dk' \int_{-1}^{1} d\mu\; k'^2\; \frac{\exp\left(ik'|\mathbf{r}-\mathbf{r}'|\mu\right)}{k^2 - k'^2} \qquad (\text{letting } \mu = \cos\theta) \\ &= \frac{2m}{\hbar^2}\frac{1}{(2\pi)^2}\int_0^\infty dk'\; \frac{k'^2}{k^2 - k'^2}\; \frac{\exp\left(ik'|\mathbf{r}-\mathbf{r}'|\right) - \exp\left(-ik'|\mathbf{r}-\mathbf{r}'|\right)}{ik'|\mathbf{r}-\mathbf{r}'|} \\ &= \frac{2m}{\hbar^2}\frac{1}{(2\pi)^2}\frac{i}{|\mathbf{r}-\mathbf{r}'|}\int_{-\infty}^{\infty} dk'\; \frac{k'\,\exp\left(ik'|\mathbf{r}-\mathbf{r}'|\right)}{(k'-k)(k'+k)}. \end{aligned} \tag{1.67}$$

This looks like something we can handle via contour integration. But there's a snag: the integration contour runs over the real k' line, but since $k \in \mathbb{R}^+$ the poles at $\pm k$ lie on the contour. The integral, as currently defined, is singular.

To get a finite result, we must "regularize" the integral by adjusting its definition. One way is to perturb the integrand and shift its poles infinitesimally in the complex plane, moving them off the contour. We have a choice of whether to move each pole infinitesimally up or down. It turns out that the appropriate choice is to shift the pole at $-k$ down, and shift the pole at $+k$ up, as illustrated by the red dots in the following figure:



This alters the denominator in the integrand of Eq. (1.67) as follows:

$$(k'-k)(k'+k) \;\rightarrow\; (k'-k-i\epsilon)(k'+k+i\epsilon) = {k'}^2 - (k+i\epsilon)^2, \tag{1.68}$$

where ϵ is a positive infinitesimal. The implications of this adjustment will be discussed further below. For now, let us proceed to do the integral, which is no longer divergent:

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

Finally, plugging this into Eq. (1.67) gives the result

$$\langle \mathbf{r}|\hat{G}_0|\mathbf{r}'\rangle = -\frac{2m}{\hbar^2}\cdot\frac{\exp\left(ik|\mathbf{r}-\mathbf{r}'|\right)}{4\pi|\mathbf{r}-\mathbf{r}'|}. \tag{1.69}$$

The 3D propagator (1.69) describes a spherical wave centered at the source $\mathbf{r}'$. The wave is isotropic (i.e., independent of the direction of $\mathbf{r}-\mathbf{r}'$), consistent with the fact that the source, a delta function, has no preferred direction. The amplitude of the wave decreases inversely with $\Delta r = |\mathbf{r}-\mathbf{r}'|$, consistent with flux conservation in 3D (see Sec. 1.4).

Most importantly, the wave propagates *outward* from $\mathbf{r}'$ (since the phase of the wavefunction increases with Δr). Such a propagator is said to be **causal**, a word based on the term "cause and effect"—the wave travels from the source at $\mathbf{r}'$ (the *cause*) to $\mathbf{r}$ (the *effect*). We can trace this behavior back to the regularization in Eq. (1.68); other regularization choices can be shown to yield propagators with different properties (see exercises). Our regularization (1.68) can also be expressed as an infinitesimal shift in E, via Eq. (1.65):

$$\frac{\hbar^2 k^2}{2m} = E \quad\Rightarrow\quad \frac{\hbar^2 (k+i\epsilon)^2}{2m} = \frac{\hbar^2}{2m}\left(k^2 + 2ik\epsilon + \cdots\right) = E + i\varepsilon. \tag{1.70}$$

In other words, we have swapped the original definition of the Green's function, Eq. (1.54), for a **causal Green's function**

$$\hat{G}_0 = \lim_{\varepsilon\rightarrow 0^+} \left(E - \hat{H}_0 + i\varepsilon\right)^{-1}. \tag{1.71}$$

Based on Eq. (1.71), causal propagators can also be derived for other dimensions (see exercises). The results for $d = 1, 2,$ and 3 are summarized below:

$$\langle \mathbf{r}|\hat{G}_0|\mathbf{r}'\rangle = \frac{2m}{\hbar^2} \times \begin{cases} \dfrac{1}{2ik} \exp\left(ik|x-x'|\right), & d = 1 \\ \dfrac{1}{4i} H_0^+(k|\mathbf{r}-\mathbf{r}'|), & d = 2 \\ -\dfrac{\exp\left(ik|\mathbf{r}-\mathbf{r}'|\right)}{4\pi|\mathbf{r}-\mathbf{r}'|}, & d = 3. \end{cases} \tag{1.72}$$

For each d, the causal propagator describes a wave propagating outward isotropically from $\mathbf{r}'$. In 1D, this has the form of a plane wave on each side. In 2D, it is a circular wave (H_0^+ denotes a Hankel function; see Appendix A), and in 3D it is a spherical wave.

1.7. SCATTERING AMPLITUDES IN 3D

We are now in a position to generate explicit solutions for the scattering problem by combining the results of Sections 1.4–1.6. For ease of presentation, we will focus on the 3D case; the 1D and 2D cases are handled in a similar way.

Using Eqs. (1.38) and (1.59), we can write the scattered wavefunction as

$$\psi_s(\mathbf{r}) = \langle \mathbf{r}|\hat{G}_0\hat{V}\underbrace{\left(\hat{I}+\hat{G}\hat{V}\right)|\psi_i\rangle}_{=|\psi\rangle} \;\overset{r\rightarrow\infty}{\longrightarrow}\; \Psi_i\,\frac{e^{ikr}}{r}\,f(\mathbf{k}_i \rightarrow k\hat{\mathbf{r}}). \tag{1.73}$$

We want to use this to find the scattering amplitude f, which encodes the results of the scattering experiment in the large-r limit (see Sec. 1.4).

Let us work on the expression on the left first. Using the position representation,

$$\psi_s(\mathbf{r}) = \int d^3r'\; \langle \mathbf{r}|\hat{G}_0|\mathbf{r}'\rangle\, V(\mathbf{r}')\, \langle \mathbf{r}'|\left(\hat{I}+\hat{G}\hat{V}\right)|\psi_i\rangle. \tag{1.74}$$

From Eq. (1.72), the causal propagator in 3D is

$$\langle \mathbf{r}|\hat{G}_0|\mathbf{r}'\rangle = -\frac{2m}{\hbar^2}\frac{\exp\left(ik|\mathbf{r}-\mathbf{r}'|\right)}{4\pi|\mathbf{r}-\mathbf{r}'|}. \tag{1.75}$$

In the $r \to \infty$ limit, this can be simplified using the Taylor expansion

$$|\mathbf{r} - \mathbf{r}'| = r - \hat{\mathbf{r}} \cdot \mathbf{r}' + \cdots, \tag{1.76}$$

where $\hat{\mathbf{r}}$ is the unit vector pointing parallel to $\mathbf{r}$. (This is the same large-r expansion used to derive the electric dipole moment in classical electromagnetism.) Hence, to lowest order,

$$\langle \mathbf{r}|\hat{G}_0|\mathbf{r}'\rangle \overset{r\to\infty}{\longrightarrow} -\frac{2m}{\hbar^2}\frac{e^{ikr}}{4\pi r}\,\exp\left(-ik\,\hat{\mathbf{r}}\cdot\mathbf{r}'\right). \tag{1.77}$$

Applying this to Eq. (1.74) gives

$$\begin{aligned}\psi_s(\mathbf{r}) &\overset{r\to\infty}{\longrightarrow} -\frac{2m}{\hbar^2}\frac{e^{ikr}}{4\pi r}\int d^3r'\,\exp\left(-ik\,\hat{\mathbf{r}}\cdot\mathbf{r}'\right)\,V(\mathbf{r}')\,\langle\mathbf{r}'|\big(\hat{I}+\hat{G}\hat{V}\big)|\psi_i\rangle \\ &= -\frac{2m}{\hbar^2}\frac{e^{ikr}}{r}\sqrt{\frac{\pi}{2}}\,\big\langle\mathbf{k}_f\big|\hat{V}+\hat{V}\hat{G}\hat{V}\big|\psi_i\big\rangle.\end{aligned} \tag{1.78}$$

On the second line, we simplified the expression by introducing the momentum eigenstate with $\mathbf{k}_f \equiv k\hat{\mathbf{r}}$. This corresponds to the "final" momentum of the scattered particle, measured when the particle is picked up by a detector placed in the $\hat{\mathbf{r}}$ direction relative to the origin. Note that $|\mathbf{k}_f| = |\mathbf{k}_i| = k$, consistent with elastic scattering. Similarly, we can express the incident state in terms of a momentum eigenstate, by comparing Eqs. (1.19) to (1.37):

$$|\psi_i\rangle = \Psi_i(2\pi)^{3/2}|\mathbf{k}_i\rangle. \tag{1.79}$$

Thus, Eq. (1.78) becomes

$$\psi_s(\mathbf{r}) \overset{r\to\infty}{\longrightarrow} -\frac{2m}{\hbar^2}\,\Psi_i\,\frac{e^{ikr}}{r}\,2\pi^2\,\big\langle\mathbf{k}_f\big|\hat{V}+\hat{V}\hat{G}\hat{V}\big|\mathbf{k}_i\big\rangle. \tag{1.80}$$

Comparing this to the right side of Eq. (1.73), we can read off the scattering amplitude:

$$\begin{aligned}f(\mathbf{k}_i \to \mathbf{k}_f) &= -\frac{2m}{\hbar^2}\cdot 2\pi^2\,\big\langle\mathbf{k}_f\big|\hat{V}+\hat{V}\hat{G}\hat{V}\big|\mathbf{k}_i\big\rangle \\ &= -\frac{2m}{\hbar^2}\cdot 2\pi^2\,\big\langle\mathbf{k}_f\big|\hat{V}+\hat{V}\hat{G}_0\hat{V}+\hat{V}\hat{G}_0\hat{V}\hat{G}_0\hat{V}+\cdots\big|\mathbf{k}_i\big\rangle.\end{aligned} \tag{1.81}$$

As noted above, this result is subject to the elasticity constraint $|\mathbf{k}_i| = |\mathbf{k}_f|$. To get the infinite series on the second line of Eq. (1.81), we have used Eq. (1.62).

Eq. (1.81) is the culmination of numerous definitions and derivations from the preceding sections. On the left side is the scattering amplitude, the fundamental quantity of interest in a scattering experiment. The right side contains the various inputs to the scattering problem: the initial and final momenta, the scattering potential, and the Green's function. Although this result was derived for the 3D case, very similar formulas hold for other dimensions, with the $2\pi^2$ factor replaced with other numerical factors.

1.8. EXAMPLE: UNIFORM SPHERICAL WELL IN 3D

Let us test the Born series with a simple scatterer. Consider a scattering potential that consists of a uniform spherical well of depth $U > 0$ and radius R:

$$V(\mathbf{r}) = \begin{cases} -U, & |\mathbf{r}| \le R \\ 0, & |\mathbf{r}| > 0. \end{cases} \tag{1.82}$$

As it turns out, this particular scattering problem can be solved exactly by exploiting the spherical symmetry of $V(\mathbf{r})$. The solution method, called **partial wave analysis**, is explained in **Appendix A**. Its result is

$$\begin{aligned} f(\mathbf{k}_i \rightarrow \mathbf{k}_f) &= \frac{1}{2ik} \sum_{\ell=0}^{\infty} \left(e^{2i\delta_\ell} - 1\right)\left(2\ell+1\right) P_\ell(\hat{\mathbf{k}}_i \cdot \hat{\mathbf{k}}_f), \\ \text{where } \;\delta_\ell &= \frac{\pi}{2} + \arg\Big[k h_\ell^{+\prime}(kR)\, j_\ell(qR) - q h_\ell^{+}(kR)\, j_\ell'(qR)\Big], \\ q &= \sqrt{2m(E+U)/\hbar^2} \\ k &\equiv |\mathbf{k}_i| = |\mathbf{k}_f|. \end{aligned} \tag{1.83}$$

The solution is expressed in terms of the special functions j_ℓ (spherical Bessel function of the first kind), h_ℓ^+ (spherical Hankel function of the first kind), and P_ℓ (Legendre polynomial).

We will pit this against the Born series, which can be regarded as a more general method since it does not assume spherical symmetry. According to Eq. (1.81), the Born series gives

$$f(\mathbf{k}_i \rightarrow \mathbf{k}_f) = -\frac{2m}{\hbar^2} \cdot 2\pi^2 \Big[\langle \mathbf{k}_f|\hat{V}|\mathbf{k}_i\rangle + \langle \mathbf{k}_f|\hat{V}\hat{G}_0\hat{V}|\mathbf{k}_i\rangle + \cdots\Big]. \tag{1.84}$$

Evaluating the full infinite Born series is generally an intractable problem, but we can truncate it to get an approximation for f. For example, if we keep only the first term, the result is called the **first Born approximation**; if we keep only the first two terms, we obtain the **second Born approximation**. To evaluate the various bra-kets, we can use the position representation to express them as explicit integrals. For example,

$$\begin{aligned} \langle \mathbf{k}_f|\hat{V}|\mathbf{k}_i\rangle &= \int d^3r_1\, \frac{\exp(-i\mathbf{k}_f\cdot\mathbf{r}_1)}{(2\pi)^{3/2}}\, V(\mathbf{r}_1)\, \frac{\exp(i\mathbf{k}_i\cdot\mathbf{r}_1)}{(2\pi)^{3/2}} \\ &= -\frac{U}{8\pi^3} \int_{|\mathbf{r}_1|\le R} d^3r_1\; \exp\left[i(\mathbf{k}_i - \mathbf{k}_f)\cdot\mathbf{r}_1\right] \end{aligned} \tag{1.85}$$

$$\begin{aligned} \langle \mathbf{k}_f|\hat{V}\hat{G}_0\hat{V}|\mathbf{k}_i\rangle &= \int d^3r_1 \int d^3r_2\, \frac{\exp(-i\mathbf{k}_f\cdot\mathbf{r}_2)}{(2\pi)^{3/2}}\, V(\mathbf{r}_2)\, \langle \mathbf{r}_2|\hat{G}_0|\mathbf{r}_1\rangle\, V(\mathbf{r}_1)\, \frac{\exp(i\mathbf{k}_i\cdot\mathbf{r}_1)}{(2\pi)^{3/2}} \\ &= -\frac{U^2}{32\pi^4}\frac{2m}{\hbar^2} \int_{|\mathbf{r}_1|<R} d^3r_1 \int_{|\mathbf{r}_2|<R} d^3r_2\, \frac{\exp\left[i(k|\mathbf{r}_1-\mathbf{r}_2| - \mathbf{k}_f\cdot\mathbf{r}_2 + \mathbf{k}_i\cdot\mathbf{r}_1)\right]}{|\mathbf{r}_1-\mathbf{r}_2|}. \end{aligned} \tag{1.86}$$

To evaluate the integrals, an expedient approach is Monte Carlo integration. For instance, the integral (1.85) has the form

$$I = \int_{|\mathbf{r}|<R} d^3r\, F(\mathbf{r}). \tag{1.87}$$

To compute this, we randomly sample N points within a cube of volume $(2R)^3$ centered at the origin. Note that this cube encloses the radius-R sphere over which is the integration region. For each sampled point, $\mathbf{r}^{(n)}$, we take

$$F_n = \begin{cases} F(\mathbf{r}^{(n)}), & |\mathbf{r}^{(n)}| < R \\ 0, & \text{otherwise}, \end{cases} \tag{1.88}$$

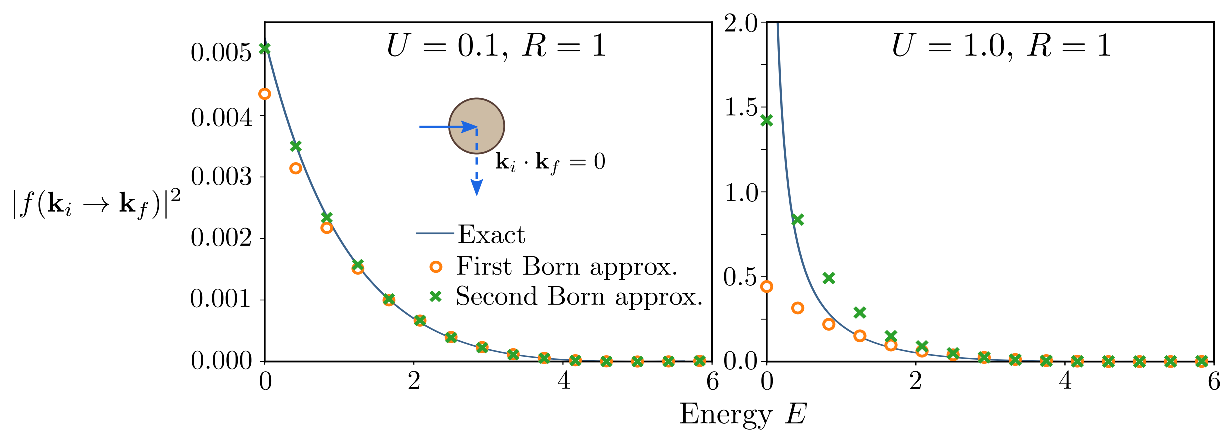
which drops contributions from points outside the sphere. Then our estimate for I is

$$I \;\approx\; (2R)^3 \, \langle F_n \rangle \;=\; \frac{(2R)^3}{N} \sum_{n=1}^{N} F_n. \tag{1.89}$$

The estimate converges to the true value as $N \to \infty$. In practice, $N \sim 10^4$ yields a good result for typical 3D integrals, and can be calculated in seconds on a modern computer.

Similarly, to calculate a double integral like Eq. (1.86), we sample *pairs* of points, $(\mathbf{r}_1^{(n)}, \mathbf{r}_2^{(n)})$, and replace the volume factor $(2R)^3$ in Eq. (1.89) with $(2R)^6$. The rest of the estimation procedure is the same.

In the figure below, we compare the Born approximation to the exact solution (1.83). We plot $|f|^2$ versus the energy E at a 90° scattering angle (i.e., $\mathbf{k}_f$ perpendicular to $\mathbf{k}_i$), for fixed well radius $R = 1$ and two well depths, $U = 0.1$ and $U = 1$. We adopt computational units $\hbar = m = 1$, and compute each Monte Carlo integral using 3×10^4 samples.



The first thing to notice is that $|f|^2$ diminishes to zero for large E. This makes sense: the scattering potential has some energy scale $\sim U$, so a particle with energy $E \gg U$ should simply zoom through, with little chance of being deflected.

Looking more closely, we see that for the shallower well ($U = 0.1$), the first Born approximation already agrees quite well with the exact results. However, the second Born approximation is significantly more accurate, particularly for small E.

For the deeper well ($U = 1$), neither the first nor second Born approximations do a good job. Roughly speaking, for the deep potential well, we cannot neglect multiple-scattering events represented by higher terms in the Born series, whereby the particle bounces around many times before leaving the scatterer (see Sec. 1.5).

In fact, for very strong scattering potentials, even taking the Born approximation to high orders may not work, as the Born series may become non-convergent. In such cases, different methods must be brought to bear. We will see an example in the next chapter.

EXERCISES

1. In Sec. 1.2, we derived the eigenstates of a particle in an empty infinite space by considering a box of length L on each side, applying periodic boundary conditions, and taking $L \to \infty$. Suppose we instead use Dirichlet boundary conditions (i.e., the wavefunction vanishes on the walls of the box). Show that this gives rise to the same set of momentum eigenstates in the $L \to \infty$ limit.

2. Using the results for the 1D delta-function scattering problem described in Section 1.3, calculate the probability current
$$J(x) = \frac{\hbar}{2mi} \left(\psi^* \frac{d\psi}{dx} - \psi \frac{d\psi^*}{dx} \right), \tag{1.90}$$
where $\psi(x)$ is the *total* (incident + scattered) wavefunction. Explain the relationship between the values of J on the left and right side of the scatterer.

3. Derive the causal 1D propagator:
$$\langle x|\hat{G}_0|x'\rangle = \frac{2m}{\hbar^2} \cdot \frac{1}{2ik_i} \exp\left(ik_i|x - x'|\right). \tag{1.91}$$

4. Derive the causal 2D propagator:
$$\langle \mathbf{r}|\hat{G}_0|\mathbf{r}'\rangle = \frac{2m}{\hbar^2} \frac{1}{4i} H_0^+(k|\mathbf{r} - \mathbf{r}'|). \tag{1.92}$$
You should be able to adapt many of the steps in the 3D propagator derivation from Section 1.6. When evaluating the polar integral, you may want to refer to the discussion of Bessel and Hankel functions in Appendix A. You may also need the following mathematical identity between the Hankel functions:
$$H_m^+(z) = -(-1)^m \, H_m^-(-z). \tag{1.93}$$

5. In place of the causal Green's function defined in Eq. (1.71), consider an infinitesimal shift of the opposite sign:
$$\hat{G}_0 = \lim_{\varepsilon \to 0^+} \left(E - \hat{H}_0 - i\varepsilon\right)^{-1}. \tag{1.94}$$
   (a) Whereas the causal propagators in Eq. (1.72) represent outgoing waves, explain why Eq. (1.94) will give rise to propagators representing incoming waves.
   (b) In the derivation of the 3D propagator, Eqs. (1.66)–(1.69), show mathematically how Eq. (1.94) changes the contour integration, resulting in an incoming-wave solution.

6. In Section 1.7, the scattering amplitude $f(\mathrm{k} \to \mathrm{k}')$ for the 3D scattering problem was derived using the Born series. Derive the corresponding expressions for 1D and 2D.

FURTHER READING

[1] Bransden & Joachain, §13.1—13.3 and §13.5—13.6.

[2] Sakurai, §7.1–7.3, 7.5–7.6