Appendix A: Circular and Spherical Waves

This Appendix describes the mathematics of circular waves and spherical waves, and their uses in 2D and 3D scattering problems.

A.1. THE HELMHOLTZ EQUATION

Consider a non-relativistic particle moving in d-dimensional space with zero potential. This is the case, for example, in a scattering problem at positions far from the scatterer (Chapter 1). The time-independent Schrödinger equation is

$$-\frac{\hbar^2}{2m}\nabla^2\psi(\mathbf{r}) = E\psi(\mathbf{r}), \tag{A.1}$$

where ∇^2 denotes the d-dimensional Laplacian and $E > 0$ is the particle's energy.

Eq. (A.1) can be re-written as a differential equation called the **Helmholtz equation**:

$$\Big(\nabla^2 + k^2\Big)\psi(\mathbf{r}) = 0, \tag{A.2}$$

where

$$k = \sqrt{\frac{2mE}{\hbar^2}} \;\in\; \mathbb{R}^+. \tag{A.3}$$

A well-known class of solutions consists of plane waves of the form

$$\psi(\mathbf{r}) = \psi_0\, \exp\left(i\mathbf{k}\cdot\mathbf{r}\right), \tag{A.4}$$

where $\psi_0 \in \mathbb{C}$ and $\mathbf{k}$ is a d-component wave-vector with $|\mathbf{k}| = k$.

When studying the scattering problem in Chapter 1, we saw that scattered wavefunctions should be "outgoing"—i.e., they should propagate outward from the scatterer, to infinity. However, a plane wave like (A.4) is neither outgoing, nor incoming. This indicates that we should look for a different type of solution to Eq. (A.2). In Sec. A.2–A.3, we will discuss the nature of these solutions for the $d = 2$ and $d = 3$ cases, and in Sec. A.4–A.5 we will talk about how they can used to solve scattering problems.

A.2. CIRCULAR WAVES IN 2D

In 2D, we can express $\mathbf{r}$ using polar coordinates (r, ϕ), and write the wavefunction as

$$\psi(\mathbf{r}) = \psi(r, \phi). \tag{A.5}$$

This should obey periodic boundary conditions in the azimuthal direction, $\psi(r, \phi + 2\pi) = \psi(r, \phi)$. Hence, we can express the ϕ-dependence via the Fourier basis, and focus on solutions of the form

$$\psi(r, \phi) = \Psi_m(r)\, e^{im\phi}, \quad m \in \mathbb{Z}. \tag{A.6}$$

These is called a **circular wave**, and the integer m describes its angular momentum. For example, for $m > 0$, the phase of ψ increases with ϕ, so the wave rotates in the $+\phi$ direction.

By plugging Eq. (A.6) into the Helmholtz equation (A.2), and expressing the 2D Laplacian in polar coordinates, we arrive at the following ordinary differential equation for $\Psi_m(r)$:

$$r\frac{d}{dr}\left(r\frac{d\Psi_m}{dr}\right) + \left(k^2r^2 - m^2\right)\Psi_m(r) = 0. \tag{A.7}$$

This is the **Bessel equation**, which supports the following solutions:

$$\Psi_m(r) \propto \begin{cases} J_m(kr) & \text{(Bessel function of the 1st kind)} \\ Y_m(kr) & \text{(Bessel function of the 2nd kind)} \\ H_m^+(kr) \equiv J_m(kr) + iY_m(kr) & \text{(Hankel function of the 1st kind)} \\ H_m^-(kr) \equiv J_m(kr) - iY_m(kr) & \text{(Hankel function of the 2nd kind).} \end{cases} \tag{A.8}$$

(Click on the links to refer to the implementations of these functions in Scientific Python.)

The Bessel functions J_m and Y_m are real-valued, whereas the Hankel functions H_m^+ and H_m^- are complex-valued. These two sets of functions are related by

$$\begin{cases} H_m^+ = J_m + iY_m \\ H_m^- = J_m - iY_m \end{cases} \Leftrightarrow \begin{cases} J_m = \frac{1}{2}\left(H_m^+ + H_m^-\right) \\ Y_m = \frac{1}{2i}\left(H_m^+ - H_m^-\right), \end{cases} \tag{A.9}$$

which is very similar to the relationship between the exponential and trigonometric functions:

$$\begin{cases} e^{iz} = \cos z + i\sin z \\ e^{-iz} = \cos z - i\sin z. \end{cases} \Leftrightarrow \begin{array}{l} \cos z = \frac{1}{2}\left(e^{iz} + e^{-iz}\right) \\ \sin z = \frac{1}{2i}\left(e^{iz} - e^{-iz}\right). \end{array} \tag{A.10}$$

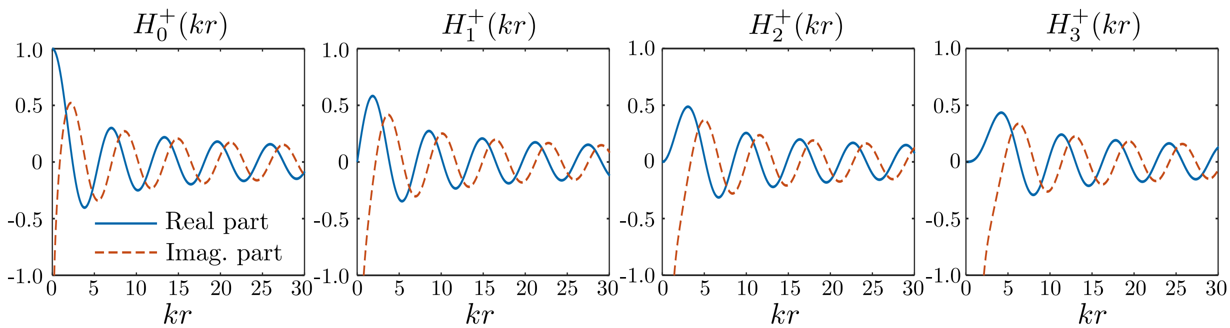
Importantly, the various Bessel and Hankel functions satisfy different boundary conditions:

- For $kr \to 0$, $J_m(kr)$ is finite, whereas Y_m, H_m^+, and H_m^- diverge.
- For $kr \to \infty$, they have the following asymptotic forms:

$$\left.\begin{array}{l} J_m(kr) \to \sqrt{\frac{2}{\pi kr}}\cos\left(kr - \frac{m\pi}{2} - \frac{\pi}{4}\right) \\ Y_m(kr) \to \sqrt{\frac{2}{\pi kr}}\sin\left(kr - \frac{m\pi}{2} - \frac{\pi}{4}\right) \\ H_m^\pm(kr) \to \sqrt{\frac{2}{\pi kr}}\exp\left[\pm i\left(kr - \frac{m\pi}{2} - \frac{\pi}{4}\right)\right] \end{array}\right\} \text{for } -\pi < \arg[kr] < \pi. \tag{A.11}$$

These further cement the analogy with Eq. (A.10). Moreover, from the last line in Eq. (A.11), we see that H_m^+ describes *outward* propagation (i.e., in the direction of increasing radial distance r), whereas H_m^- describes *inward* propagation. This indicates that using H_m^+ in Eq. (A.6) yields an outgoing circular wave—precisely what we need for describing scattered wavefunctions.

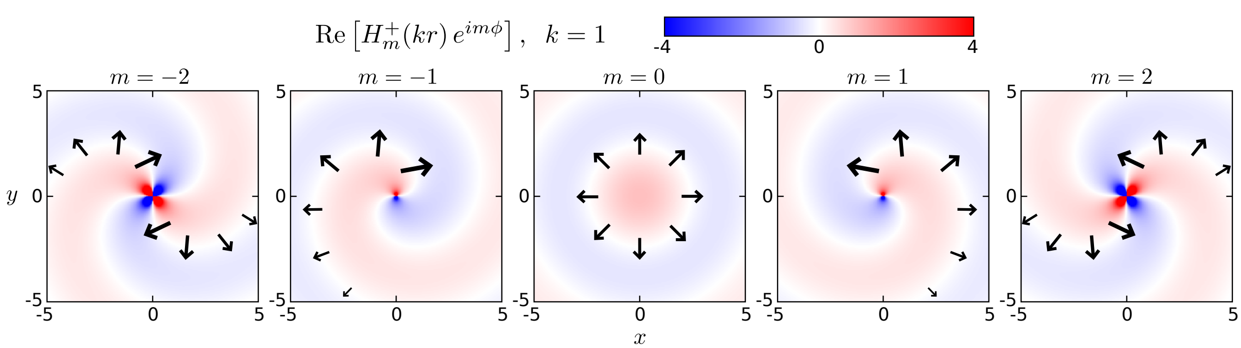
Let us examine the H_m^+ functions in more detail. (You are welcome to check the properties of the H_m^- counterparts.) Below, we plot the real and imaginary parts for $m = 0, 1, 2, 3$:



For large kr, the functions behave as decaying complex sinuoidals, in accordance with Eq. (A.11). In the asymptotic form Eq. (A.11), the decay factor of $1/\sqrt{r}$ satisfies the conservation of flux in the r direction in 2D (see Chapter 1, Sec. 1.4); moreover, the Hankel functions for different m's are all normalized to carry the same flux.

For small kr, the value of $H_m^+(kr)$ diverges (specifically, its imaginary part, which is Y_m). This is also consistent with flux conservation: as the circumference vanishes with r, the flux density must diverge as $1/r$ to keep the total flux constant.

The figure below shows 2D plots for a few outgoing circular waves. The real part of the wavefunction is plotted, using red and blue colors to represent positive and negative values, while black arrows indicate the direction of propagation of the wave at a few selected points:



We see that the wave travels outward in a clockwise spiral ($m < 0$), isotropically ($m = 0$), or in a counterclockwise spiral ($m > 0$).

Like plane waves, circular waves can be used as a basis for expressing arbitrary waveforms. However, when writing a waveform as a superposition of circular waves, we must choose the right set of circular waves by considering the boundary conditions. For example, for a purely outgoing wave like a scattered wavefunction, the decomposition naturally has the form

$$\psi_s(\mathbf{r}) = \sum_{m=-\infty}^{\infty} c_m^+ H_m^+(kr)\, e^{im\phi}, \quad c_m^+ \in \mathbb{C}, \tag{A.12}$$

involving only the H_m^+ functions.

Even a plane wave can be expressed as a superposition of circular waves. For a plane wave of wave-vector $\mathbf{k}_z = k\hat{z}$, one can show (using mathematical manipulations whose details we will skip) that

$$e^{i\mathbf{k}_z\cdot\mathbf{r}} = e^{ikr\cos\phi} = \sum_{m=-\infty}^{\infty} i^m\, J_m(kr)\, e^{im\phi}. \tag{A.13}$$

The sum involves J_m-type circular waves, consistent with our earlier assertion that plane waves are neither purely outgoing nor incoming.

A.3. SPHERICAL WAVES IN 3D

In 3D, we can express $\mathbf{r}$ using spherical coordinates (r, θ, ϕ). Proceeding by analogy with the 2D case of Sec. A.2, we look for solutions to the 3D Helmholtz equation of the form

$$\psi(r,\theta,\phi) = \Psi(r)\, f(\theta,\phi), \tag{A.14}$$

which exhibit a separation of variables between r and (θ, ϕ). Observing that θ and ϕ are angular variables, we can specialize further to solutions of definite angular momentum,

$$\psi(r,\theta,\phi) = \Psi_{\ell m}(r)\, Y_{\ell m}(\theta,\phi). \tag{A.15}$$

The spherical harmonic function $Y_{\ell m}(\theta,\phi)$ acts as a generalization of the $\exp(im\phi)$ factor in the 2D ansatz (A.6). It is indexed by two integers ℓ and m, which are the quantum numbers corresponding to the total angular momentum and the z-component of the angular momentum, respectively. If we take

$$\ell \ge 0 \;\; \text{and} \;\; -\ell \le m \le \ell, \tag{A.16}$$

it can be shown that $Y_{\ell m}(\theta,\phi)$ is a well-behaved function of the anglular coordinates θ and ϕ; i.e., periodic in ϕ and regular at the coordinate poles $\theta = \{0, \pi\}$.

By plugging Eq. (A.15) into the Helmholtz equation and expressing the 3D Laplacian in spherical coordinates, we arrive at the **spherical Bessel equation**

$$\frac{d}{dr}\left(r^2\frac{d\Psi_{\ell m}}{dr}\right) + \Big[k^2r^2 - \ell(\ell+1)\Big]\Psi_{\ell m}(r) = 0. \tag{A.17}$$

Remarkably, this turns out to involve only ℓ, not m. The solution thus only depends on ℓ, and we henceforth write it as $\Psi_\ell(r)$. Now, Eq. (A.17) has the following solutions:

$$\Psi_\ell(r) \propto \begin{cases} j_\ell(kr) & \text{(Spherical Bessel function of the 1st kind)}\\ y_\ell(kr) & \text{(Spherical Bessel function of the 2nd kind)}\\ h_\ell^+(kr) \equiv j_\ell(kr) + iy_\ell(kr) & \text{(Spherical Hankel function of the 1st kind)}\\ h_\ell^-(kr) \equiv j_\ell(kr) - iy_\ell(kr) & \text{(Spherical Hankel function of the 2nd kind).}\end{cases} \tag{A.18}$$

Their boundary conditions are closely analogous to the 2D circular waves from Section A.2:

- For $kr \to 0$, $j_\ell(kr)$ is finite, while y_ℓ, h_ℓ^+, and h_ℓ^- are divergent.
- For $kr \to \infty$, they have the following asymptotic forms:

$$\left.\begin{aligned} j_\ell(kr) &\rightarrow \frac{\sin(kr - \frac{\ell\pi}{2})}{kr} \\ y_\ell(kr) &\rightarrow -\frac{\cos(kr - \frac{\ell\pi}{2})}{kr} \\ h_\ell^\pm(kr) &\rightarrow \pm\frac{\exp\left[\pm i(kr - \frac{\ell\pi}{2})\right]}{ikr} \end{aligned}\right\} \text{for } -\pi < \arg[kr] < \pi. \tag{A.19}$$

Hence, the spherical Hankel functions of the first and second kind describe outgoing and incoming waves, respectively. The $1/r$ prefactors are consistent with flux conservation in 3D: spherical wavefronts are spread over an area $4\pi r^2$, so $|\Psi_{\ell m}(r)|^2 \cdot 4\pi r^2$ is r-independent. The spherical Hankel functions for different ℓ, m are normalized to carry the same flux.

Similar to the 2D case, we can express a plane wave as a superposition of spherical waves. This is accomplished via the identity

$$e^{i\mathbf{k}_i\cdot\mathbf{r}} = \sum_{\ell=0}^{\infty}\sum_{m=-\ell}^{\ell} 4\pi j_\ell(kr) e^{i\ell\pi/2}\, Y_{\ell m}^*(\hat{\mathbf{k}}_i)\, Y_{\ell m}(\hat{\mathbf{r}}), \tag{A.20}$$

where $\hat{\mathbf{k}}_i$ denotes the angular components (in spherical coordinates) of the incident wave-vector $\mathbf{k}_i$, and $\hat{\mathbf{r}}$ denotes the angular components of the position vector $\mathbf{r}$.

A.4. PARTIAL WAVE ANALYSIS

Circular waves (Section A.2) and spherical waves (Section A.3) play an important role in the analysis of scattering problems.

Let $\psi(\mathbf{r})$ be the wavefunction in the exterior region of a scattering experiment, where the scattering potential vanishes. It obeys the Helmholtz equation, so we can expand it as a superposition of incoming and outgoing circular waves (for 2D) or spherical waves (for 3D):

$$\psi(\mathbf{r}) = \begin{cases} \displaystyle\sum_{m=-\infty}^{\infty} \Big[c_m^+ H_m^+(kr) + c_m^- H_m^-(kr)\Big]\, e^{im\phi} & \text{(2D)} \\ \displaystyle\sum_{\ell=0}^{\infty}\sum_{m=-\ell}^{\ell} \Big[c_{\ell m}^+ h_\ell^+(kr) + c_{\ell m}^- h_\ell^-(kr)\Big]\, Y_{\ell m}(\theta,\phi). & \text{(3D)} \end{cases} \tag{A.21}$$

Since the individual circular or spherical waves satisfy the Helmholtz equation, which is linear, any such linear superposition automatically satisfies the Helmholtz equation. For simplicity, let us denote the coefficients by $\{c_\mu^\pm\}$, where $\mu \equiv m$ for 2D and $\mu \equiv (\ell, m)$ for 3D. Each μ is called a **scattering channel**. The approach of dividing a scattering problem into different scattering channels is called **partial wave analysis**.

The circular and spherical waves are appropriately normalized such that the energy flux in each scattering channel μ is directly proportional to $|c_\mu^\pm|^2$. This follows from the normalization choice in the definitions of the Hankel and spherical Hankel functions, as noted in Sections A.2 and A.3).

In a scattering problem, the incoming coefficients c_μ^- and the outgoing coefficients c_μ^+ are not independent. If we vary any individual c_μ^-, there should be a corresponding linear variation in every c_μ^+ (the variation is linear since the Schrödinger wave equation is linear). Hence, there exists a set of linear relations

$$c_\mu^+ = \sum_\nu S_{\mu\nu}\, c_\nu^-, \quad \text{for all } \mu. \tag{A.22}$$

Here, the outgoing wave coefficients are on the left, and the incoming coefficients on the right. The complex matrix S, called the **scattering matrix**, is determined by the scattering potential $V(\mathbf{r})$ and energy E. It specifies how the scatterer converts incoming waves into outgoing waves. Due to flux conservation, the scattering matrix must be unitary:

$$\left(S^{-1}\right)_{mm'} = S^*_{m'm}. \tag{A.23}$$

Do not confuse the "incoming" and "outgoing" waves of Eq. (A.21) with the "incident" and "scattered" waves defined in the scattering problem. As discussed in Chapter 1, a scattering experiment typically has an incident wave that is a plane wave, of the form

$$\psi_i(\mathbf{r}) = \Psi_i\, e^{i\mathbf{k}_i\cdot\mathbf{r}} \quad \text{where } |\mathbf{k}_i| = k. \tag{A.24}$$

However, relative to a given coordinate origin ($r = 0$), a plane wave is neither purely incoming nor outgoing! For 2D, we can use Eq. (A.13) to decompose the plane wave as

$$\psi_i(\mathbf{r}) = \frac{\Psi_i}{2} \sum_{m=-\infty}^{\infty} i^m e^{im\Delta\phi}\, \left[H_m^+(kr) + H_m^-(kr)\right], \tag{A.25}$$

where $r = |\mathbf{r}|$ and $\Delta\phi = \cos^{-1}\left[(\mathbf{k}_i\cdot\mathbf{r})/kr\right]$. Likewise, for 3D we can use Eq. (A.20) to write

$$\psi_i(\mathbf{r}) = 2\pi\Psi_i \sum_{\ell=0}^{\infty}\sum_{m=-\ell}^{\ell} \left[h_\ell^+(kr) + h_\ell^-(kr)\right]\, e^{i\ell\pi/2}\, Y^*_{\ell m}(\hat{\mathbf{k}}_i)\, Y_{\ell m}(\hat{\mathbf{r}}), \tag{A.26}$$

where $\hat{\mathbf{k}}_i$ and $\hat{\mathbf{r}}$ denote the angular components of $\mathbf{k}_i$ and $\mathbf{r}$ respectively. In both cases, the incident plane wave is evidently a superposition of incoming *and* outgoing waves.

Using Eqs. (A.25) and (A.26), we can relate the scattering matrix to the formulation of the scattering problem discussed in Chapter 1. Let us go through the details for 3D, leaving the 2D case as an exercise.

Focusing on 3D, a comparison of Eqs. (A.21) and (A.26) allows us to determine the spherical wave coefficients for the incident wave:

$$c^\pm_{i,\ell m} = 2\pi e^{i\ell\pi/2}\, Y^*_{\ell m}(\hat{\mathbf{k}}_i)\; \Psi_i. \tag{A.27}$$

The total wavefunction consists of $\psi_i(\mathbf{r})$ plus the scattered wavefunction $\psi_s(\mathbf{r})$. By assumption, the latter is a superposition of only outgoing waves, so denote its coefficients by $c^+_{s,\ell m}$. Next, re-express the scattering matrix equation (A.22) using these coefficients:

$$c^+_{i,\ell m} + c^+_{s,\ell m} = \sum_{\ell,m,\ell',m'} S_{\ell m,\ell' m'} c^-_{i,\ell' m'}. \tag{A.28}$$

Note that the scattered wave does not contribute to the right side because it has no incoming components. Moving $c^+_{i,\ell m}$ to the right side of the equation, and using Eq. (A.27), gives

$$c^+_{s,\ell m} = 2\pi \sum_{\ell' m'} \Big(S_{\ell m,\ell' m'} - \delta_{\ell\ell'}\delta_{mm'}\Big) e^{i\ell'\pi/2}\, Y^*_{\ell' m'}(\hat{\mathbf{k}}_i)\; \Psi_i. \tag{A.29}$$

Hence, the scattered wavefunction is

$$\begin{aligned}\psi_s(\mathbf{r}) &= \sum_{\ell m} c_{s,\ell m}^+ h_\ell^+(kr)\, Y_{\ell m}(\hat{\mathbf{r}}) \\ &= \Psi_i \sum_{\ell m}\sum_{\ell' m'} 2\pi \Big(S_{\ell m,\ell' m'} - \delta_{\ell\ell'}\delta_{mm'}\Big) e^{i\ell'\pi/2}\, Y^*_{\ell' m'}(\hat{\mathbf{k}}_i)\; h_\ell^+(kr)\, Y_{\ell m}(\hat{\mathbf{r}}).\end{aligned} \tag{A.30}$$

For large r, we can simplify the spherical Hankel functions using Eq. (A.19), obtaining

$$\psi_s(\mathbf{r}) \overset{r\rightarrow\infty}{\longrightarrow} \Psi_i \frac{e^{ikr}}{r} \left[\frac{2\pi}{ik} \sum_{\ell m}\sum_{\ell' m'} \Big(S_{\ell m,\ell' m'} - \delta_{\ell\ell'}\delta_{mm'}\Big)\, e^{-i(\ell-\ell')\pi/2}\, Y^*_{\ell' m'}(\hat{\mathbf{k}}_i)\; Y_{\ell m}(\hat{\mathbf{r}})\right]. \tag{A.31}$$

The quantity in square brackets is the scattering amplitude (Section 1.5):

$$f(\mathbf{k}_i \rightarrow k\hat{\mathbf{r}}) = \frac{2\pi}{ik} \sum_{\ell m}\sum_{\ell' m'} \Big(S_{\ell m,\ell' m'} - \delta_{\ell\ell'}\delta_{mm'}\Big)\, e^{-i(\ell-\ell')\pi/2}\, Y^*_{\ell' m'}(\hat{\mathbf{k}}_i)\; Y_{\ell m}(\hat{\mathbf{r}}). \tag{A.32}$$

A.5. SCATTERING FROM A UNIFORM SPHERE

As a concluding example, we will use the results from the preceding sections to derive the scattering amplitudes for a spatially uniform 3D sphere. The scattering potential is

$$V(\mathbf{r}) = \begin{cases} -U & \text{for } \;|\mathbf{r}| < R, \\ \;\;0 & \text{for } \;|\mathbf{r}| > R, \end{cases} \tag{A.33}$$

where R is the radius of the well and U is its depth. For simplicity, we assume an attractive potential, $U > 0$. (The interested reader can work through the repulsive case, $U < 0$, which is almost the same, except that the wavefunction inside the scatterer is an evanescent wave.)

This scattering potential is isotropic, so angular momentum is conserved. There must therefore exist solutions where both the incident and scattered wavefunctions have definite angular momentum ℓ, m. The total wavefunction takes the form

$$\psi(r,\theta,\phi) = A_{\ell m}(r)\, Y_{\ell m}(\theta,\phi) \tag{A.34}$$

everywhere (i.e., inside and outside the scatterer). The existence of such solutions implies that the scattering matrix is diagonal; in other words, the scattering channels can be considered independently of each other. Moreover, the diagonal entries turn out to depend on only the principal angular momentum quantum number ℓ (see below), so

$$S_{\ell m,\ell' m'} \;=\; s_\ell\, \delta_{\ell\ell'}\, \delta_{mm'}. \tag{A.35}$$

We also know from Eq. (A.23) that the scattering matrix is unitary. For a matrix that is both diagonal and unitary, each diagonal matrix element must have magnitude 1. Hence,

$$s_\ell = e^{i\Delta_\ell}, \tag{A.36}$$

for some real phase Δ_ℓ. This has a simple physical intepretation: since each scattering channel is independent and flux-conserving, the outgoing wave in that channel must have the same magnitude as the incoming wave. It can only vary by a phase shift.

Let us plug the ansatz (A.34) into the Schrödinger equation. This gives

$$\frac{d}{dr}\left(r^2\frac{dA_{\ell m}}{dr}\right) + \Big[K^2(r)\,r^2 - \ell(\ell+1)\Big]A_{\ell m}(r) = 0, \tag{A.37}$$

where $r = |\mathbf{r}|$ and

$$K^2(r) = \sqrt{\frac{2m\big[E - V(r)\big]}{\hbar^2}}. \tag{A.38}$$

Since the differential equation does not involve m, the solution only depends on ℓ. We therefore replace $A_{\ell m}(r)$ with $A_\ell(r)$ in Eq. (A.34):

$$\psi(r,\theta,\phi) = A_\ell(r)\,Y_{\ell m}(\theta,\phi). \tag{A.39}$$

In the exterior region $r > R$, Eq. (A.37) reduces to the spherical Bessel equation (A.17), with $K(r) \to k$, and we can write

$$A_\ell(r) = c_\ell^- h_\ell^-(kr) + c_\ell^+ h_\ell^+(kr), \tag{A.40}$$

for some coefficients c_ℓ^+ and c_ℓ^- obeying the scattering relation (A.22). The fact that A_ℓ does not depend on m justifies our prior assertion, in Eq. (A.35), that the scattering matrix entries do not depend on m. Using Eqs. (A.35)–(A.36), we can simplify this to

$$A_\ell(r) = c_\ell^-\Big(h_\ell^-(kr) + e^{i\Delta_\ell}\,h_\ell^+(kr)\Big), \quad \text{for } \; r > R. \tag{A.41}$$

Next, consider the region inside the scatterer, $r < R$. Here, the Schrödinger wave equation reduces to the Helmholtz equation, with k replaced by

$$q = \sqrt{\frac{2m(E+U)}{\hbar^2}}. \tag{A.42}$$

Given that $U > 0$, we have $q \in \mathbb{R}^+$ for all $E > 0$. As discussed in Section A.3, the solutions are spherical Bessel functions (of the first and second kind) or spherical Hankel functions (of the first and second kind). But the interior region includes the point $r = 0$, and the wavefunction must be finite, so we cannot use the y_ℓ or $h_\ell^\pm$ functions, which diverge at $r = 0$. This leaves only the spherical Bessel function of the first kind:

$$A_\ell(r) = \alpha_\ell\, j_\ell(qr) \quad \text{for } \; r < R. \tag{A.43}$$

To proceed, we compare the exterior solution (A.41) and the interior solution (A.43) at $r = R$. Matching both the wavefunction and its first derivative, we obtain two equations:

$$\begin{aligned} \alpha_\ell\, j_\ell(qR) &= \;\; c_\ell^-\Big(h_\ell^-(kR) \;+ e^{i\Delta_\ell} h_\ell^+(kR)\Big) \\ \alpha_\ell\, q j_\ell'(qR) &= c_\ell^-\, k\Big(h_\ell^{-\prime}(kR) + e^{i\Delta_\ell} h_\ell^{+\prime}(kR)\Big). \end{aligned} \tag{A.44}$$

Here, j_ℓ' denotes the derivative of the spherical Bessel function, and likewise for $h_\ell^{\pm\prime}$. Taking the ratio of these two equations eliminates α_ℓ and c_ℓ^-. Then a bit of rearrangement yields

$$e^{i\Delta_\ell} = -\frac{k h_\ell^{-\prime}(kR) j_\ell(qR) - q h_\ell^-(kR) j_\ell'(qR)}{k h_\ell^{+\prime}(kR) j_\ell(qR) - q h_\ell^+(kR) j_\ell'(qR)}. \tag{A.45}$$

On the right-hand side, the numerator and denominator are complex conjugates of one another, since j_ℓ is real and $(h_\ell^+)^* = h_\ell^-$; hence, the expression has magnitude 1, matching the left-hand side. We thus obtain

$$\Delta_\ell = \frac{\pi}{2} - \arg\Big[k h_\ell^{+\prime}(kR) j_\ell(qR) - q h_\ell^+(kR) j_\ell'(qR)\Big]. \tag{A.46}$$

This result can then be plugged into the scattering amplitude formula (A.32):

$$f(\mathbf{k}_i \rightarrow k\hat{\mathbf{r}}) = \frac{2\pi}{ik} \sum_{\ell=0}^{\infty} \left(e^{2i\Delta_\ell} - 1\right) \sum_{m=-\ell}^{\ell} Y_{\ell m}^*(\hat{\mathbf{k}}_i)\, Y_{\ell m}(\hat{\mathbf{r}}). \tag{A.47}$$

This can be further simplified with the aid of the following addition theorem for spherical harmonics:

$$P_\ell(\hat{\mathbf{r}}_1 \cdot \hat{\mathbf{r}}_2) = \frac{4\pi}{2\ell+1} \sum_{m=-\ell}^{\ell} Y_{\ell m}^*(\hat{\mathbf{r}}_1) Y_{\ell m}(\hat{\mathbf{r}}_2). \tag{A.48}$$

where $P_\ell(\cdots)$ denotes a Legendre polynomial. Finally, we obtain

$$\begin{aligned} f(\mathbf{k}_i \rightarrow k\hat{\mathbf{r}}) &= \frac{1}{2ik} \sum_{\ell=0}^{\infty} \left(e^{2i\Delta_\ell} - 1\right)\left(2\ell+1\right) P_\ell(\hat{\mathbf{k}}_i \cdot \hat{\mathbf{r}}) \\ \Delta_\ell &= \frac{\pi}{2} - \arg\Big[k h_\ell^{+\prime}(kR)\, j_\ell(qR) - q h_\ell^+(kR)\, j_\ell'(qR)\Big] \\ k = |\mathbf{k}_i| &= \sqrt{2mE/\hbar^2}, \quad q = \sqrt{2m(E+U)/\hbar^2}. \end{aligned} \tag{A.49}$$

Evidently, $f(\mathbf{k}_i \rightarrow k\hat{\mathbf{r}})$ depends on two variables: E, the conserved particle energy, and $\Delta\theta = \cos^{-1}(\hat{\mathbf{k}}_i \cdot \hat{\mathbf{r}})$, the deflection angle between the incident and scattered directions.

The formulas in (A.49) are used to generate the exact scattering amplitude plots shown in Chapter 1, Section 1.8.

EXERCISES

1. In Section A.4, we derived an expression for the 3D scattering amplitudes in terms of the scattering matrix S, Eq. (A.32). Starting from Eq. (A.25), derive the corresponding relation for the 2D scattering amplitudes.