PARTIAL WAVE ANALYSIS OF SCATTERING

Scalar Waves

Consider scattering of a scalar wave $\psi(\mathbf{x})$ off some spherically symmetric obstacle. In quantum mechanics, this obstacle is usually a short-ranged central potential $V(r)$, although it can also be a reflective — or partially reflective — sphere with non-trivial boundary conditions. In any case, far away from the obstacle $\psi(\mathbf{x})$ obeys the wave equation

$$\left(\nabla^2 + k^2\right)\psi(\mathbf{x}) \;=\; 0, \tag{1}$$

and we are looking for solutions of the form

$$\psi(\mathbf{x}) \;=\; \psi_{\text{incident}}(\mathbf{x}) \;+\; \psi_{\text{scattered}}(\mathbf{x}) \;\xrightarrow[r\to\infty]{}\; \exp(ikz) \;+\; f(\theta)\,\frac{\exp(ikr)}{r}\,. \tag{2}$$

Note: by the spherical symmetry of the scattering object, the direction of the incident plane wave does not matter, so without loss of generality we make that direction the z axis. Likewise, the scattering amplitude $f(\mathbf{n})$ depends only on the angle between the incident wave and the direction $\mathbf{n}$ of the scattering, thus in the spherical coordinates $f(\theta)$ rather than $f(\theta,\phi)$.

We also use the spherical symmetry to separate the variables of the wave equation in spherical coordinates, thus

$$\psi(r,\theta,\phi) \;=\; \sum_{\ell,m} C_{\ell,m}\sqrt{4\pi(2\ell+1)}Y_{\ell,m}(\theta,\phi)\times\psi_\ell(r), \tag{3}$$

although thanks to the axial symmetry of the scattering solution (2) $C_{\ell,m}=0$ for $m\neq 0$. As to the $m=0$ modes, $Y_{\ell,0}(\theta,\phi)=\sqrt{(2\ell+1)/4\pi}\,P_\ell(\cos\theta)$, thus

$$\psi(r,\theta) \;=\; \sum_{\ell=0}^{\infty} C_\ell(2\ell+1)P_\ell(\cos\theta)\times\psi_\ell(r) \tag{4}$$

where $P_\ell(x)$ are the Legendre polynomials. The radial functions $\psi_\ell(r)$ in the sum (4) obey the radial wave equations

$$\psi_\ell''(r) \;+\; \frac{2}{r}\psi_\ell'(r) \;-\; \frac{\ell(\ell+1)}{r^2}\psi_\ell(r) \;+\; k^2\psi_\ell(r) \;=\; \begin{pmatrix}\text{perturbation by}\\ \text{the scatterer}\end{pmatrix} \;\xrightarrow[r\to\infty]{}\; 0. \tag{5}$$

Consequently, outside the scatterer the radial waves becomes linear combinations of the spherical Bessel functions $j_\ell(kr)$ and $n_\ell(kr)$, and if the perturbation potential or boundary condition (on the surface of some reflecting sphere) are real, then we should have a real linear combination

$$\psi_\ell(r) \;=\; \cos\delta_\ell\times j_\ell(kr) \;-\; \sin\delta_\ell\times n_\ell(kr) \tag{6}$$

for some angle δ_ℓ called *the phase shift*. The reason for this name is the asymptotic behavior of the radial solution at large r, — meaning both $r \gg R_{\text{scatterer}}$ and $kr \gg 1$. For $kr \gg 1$, the spherical Bessel functions asymptote to

$$j_\ell(kr) \;\xrightarrow[kr\gg 1]{}\; \frac{\sin\bigl(kr-\ell\frac{\pi}{2}\bigr)}{kr}\,, \qquad n_\ell(kr) \;\xrightarrow[kr\gg 1]{}\; -\frac{\cos\bigl(kr-\ell\frac{\pi}{2}\bigr)}{kr}\,, \tag{7}$$

hence for large radii

$$\psi_\ell(r) \;\xrightarrow[r\to\infty]{}\; \cos\delta\frac{\sin\bigl(kr-\ell\frac{\pi}{2}\bigr)}{kr} \;+\; \sin\delta\frac{\cos\bigl(kr-\ell\frac{\pi}{2}\bigr)}{kr} \;=\; \frac{\sin\bigl(kr-\ell\frac{\pi}{2}+\delta_\ell\bigr)}{kr}\,. \tag{8}$$

In this formula, δ_ℓ shifts the phase of the asymptotic sine wave from the no-scattering asymptotic behavior

$$\begin{aligned} \psi_\ell^{\text{free}}(r) \;&=\; j_\ell(kr) \text{ @ all } r \qquad \langle\!\langle\, \text{because } \psi_\ell^{\text{free}}(r) \text{ should stay finite for } r\to 0\,\rangle\!\rangle \\ &\xrightarrow[kr\gg 1]{}\; \frac{\sin\bigl(kr-\ell\frac{\pi}{2}\bigr)}{kr}\,. \end{aligned} \tag{9}$$

Next, let's assemble the partial waves for different ℓ's into the sum

$$\begin{aligned} \psi(r,\theta) \;&=\; \sum_{\ell=0}^{\infty} C_\ell(2\ell+1)P_\ell(\cos\theta)\times\psi_\ell(r) \\ &=\; \sum_{\ell=0}^{\infty} C_\ell(2\ell+1)P_\ell(\cos\theta)\times\Bigl(\cos\delta_\ell\times j_\ell(kr) \;-\; \sin\delta_\ell\times\; n_\ell(kr)\Bigr) \end{aligned} \tag{10}$$

and choose the coefficients C_ℓ such that the net wave has asymptotic behavior (2) at large distances. The key to this choice is the following **Lemma:**

$$\int_{-1}^{+1} e^{ikrc}\, P_\ell(c)\, dc \;=\; 2i^\ell j_\ell(kr) \tag{11}$$

and hence

$$\psi_{\rm inc} \;=\; \exp(ikz) \;=\; \exp(ikr\cos\theta) \;=\; \sum_{\ell=0}^{\infty}(2\ell+1)i^\ell P_\ell(\cos\theta)\times j_\ell(kr). \tag{12}$$

At the same time, the scattered wave is purely divergent: its asymptotic behavior is

$$\psi_{\rm sc}(r,\theta) \;=\; \frac{f(\theta)}{r}\times e^{+ikr} \qquad \text{without an } e^{-ikr} \text{ term,} \tag{13}$$

so for each partial wave we should have

$$\psi_\ell^{\rm sc}(r) \;\xrightarrow[r\to\infty]{}\; A_\ell\times\frac{e^{+ikr}}{r} \tag{14}$$

for some overall complex coefficient A_ℓ, or in terms of the spherical Bessel functions

$$\psi_\ell^{\rm sc}(r) \;=\; A_\ell k\times i^\ell h_\ell(kr) \;=\; A_\ell k i^\ell\times\big(j_\ell(kr)\,+\,in_\ell(kr)\big) \;\xrightarrow[kr\gg 1]{}\; A_\ell\times\frac{e^{+ikr}}{r}\,. \tag{15}$$

Altogether, the scattered wave should have form

$$\psi_{\rm sc}(r,\theta) \;=\; \sum_{\ell=0}^{\infty}(2\ell+1)i^\ell A_\ell P_\ell(\cos\theta)\times\big(h_\ell(kr)\;=\;j_\ell(kr)\,+\,in_\ell(kr)\big), \tag{16}$$

hence adding the incident wave (12) we build

$$\psi^{\rm net}(r,\theta) \;=\; \sum_{\ell=0}^{\infty}(2\ell+1)i^\ell P_\ell(\cos\theta)\times\Big((1+A_\ell)\times j_\ell(kr)\,+\,iA_\ell\times n_\ell(kr)\Big). \tag{17}$$

Comparing this formula to eq. (10), we find the same general behavior provided

$$C_\ell\times\cos\delta_\ell \;=\; A_\ell\,+\,1 \quad\text{and}\quad C_\ell\times(-\sin\delta_\ell) \;=\; iA_\ell\,. \tag{18}$$

Solving these equations gives us

$$C_\ell \;=\; \exp(i\delta_\ell), \qquad A_\ell \;=\; i\sin\delta_\ell \times \exp(i\delta_\ell) \;=\; \frac{e^{2i\delta_\ell}-1}{2}\,. \tag{19}$$

Coming back to the scattered wave, eq. (16) leads to

$$\begin{aligned}
\psi_{\rm sc}(r,\theta) &= \sum_{\ell=0}^{\infty}(2\ell+1)A_\ell P_\ell(\cos\theta)\times i^\ell h_\ell(kr) \\
&\xrightarrow[kr\gg1]{} \sum_{\ell=0}^{\infty}(2\ell+1)A_\ell P_\ell(\cos\theta)\times\frac{e^{+ikr}}{kr} \\
&= \frac{e^{+ikr}}{kr}\times\sum_{\ell=0}^{\infty}(2\ell+1)A_\ell P_\ell(\cos\theta) \\
&= f(\theta)\times\frac{e^{+ikr}}{r}
\end{aligned} \tag{20}$$

for the *scattering amplitude*

$$f(\theta) \;=\; \frac{1}{k}\sum_{\ell=0}^{\infty}(2\ell+1)A_\ell P_\ell(\cos\theta)\,. \tag{21}$$

The coefficients A_ℓ here should be as in eq. (19), thus

$$f(\theta) \;=\; \sum_{\ell=0}^{\infty}\frac{e^{2i\delta_\ell}-1}{2k}\times(2\ell+1)P_\ell(\cos\theta). \tag{22}$$

The partial scattering cross-section follows from the amplitude (22) as

$$\frac{d\sigma}{d\Omega} \;=\; |f(\theta)|^2\,, \tag{23}$$

where

$$|f(\theta)|^2 \;=\; \sum_{\ell,\ell'}\frac{(\exp(+2i\delta_\ell)-1)(\exp(-2i\delta_{\ell'})-1)}{4k^2}\times(2\ell+1)(2\ell'+1)P_\ell(\cos\theta)P_{\ell'}(\cos\theta). \tag{24}$$

Consequently, integrating this partial cross-section over the 4π directions to obtain the total cross-section, we obtain

$$\begin{aligned}\sigma_{\text{tot}} &= \oiint d^2\Omega\, |f|^2 \\ &= \int_0^\pi |f|^2 \times 2\pi \sin\theta\, d\theta \\ &= \sum_{\ell,\ell'} \frac{(\exp(+2i\delta_\ell)-1)(\exp(-2i\delta_{\ell'})-1)}{4k^2} \times \\ &\qquad \times (2\ell+1)(2\ell'+1) \int_0^\pi P_\ell(\cos\theta) P_{\ell'}(\cos\theta)\, 2\pi\sin\theta\, d\theta\end{aligned} \tag{25}$$

On the last line here

$$\int_0^\pi P_\ell(\cos\theta) P_{\ell'}(\cos\theta)\, 2\pi\sin\theta\, d\theta \;=\; 2\pi \int_{-1}^{+1} P_\ell(\cos\theta) P_{\ell'}(\cos\theta)\, d\cos\theta \;=\; \frac{4\pi}{2\ell+1} \times \delta_{\ell,\ell'}\,, \tag{26}$$

hence

$$\begin{aligned}\sigma_{\text{tot}} &= \sum_\ell \left| \frac{\exp(2i\delta_\ell)-1}{2k} \right|^2 \times 4\pi(2\ell+1) \\ &= \frac{4\pi}{k^2} \sum_{\ell=0}^\infty (2\ell+1)\sin^2(\delta_\ell).\end{aligned} \tag{27}$$

Scattering off a Hard Sphere

A hard sphere is a spherical surface which cannot be penetrated by a particle or a wave. In quantum mechanics, its implemented by the infinite-wall potential

$$V(r) \;=\; \begin{cases} 0 & \text{for } r > R, \\ +\infty & \text{for } r < R. \end{cases} \tag{28}$$

Consequently, the wave-function $\psi(r,\theta,\phi)$ obeys the un-perturbed wave equation outside the sphere,

$$(\nabla^2 + k^2)\psi(r, \theta, \phi) \;=\; 0 \quad \text{for } r \;>\; R, \tag{29}$$

but also the Dirichlet boundary conditions on the sphere's surface

$$\psi(r, \theta, \phi) \;=\; 0 \quad \text{for } r \;=\; r \text{ and any } \theta, \phi. \tag{30}$$

Separating the variables in the spherical coordinates, we see that outside the sphere we have the usual

$$\psi(r, \theta) \;=\; \sum_\ell C_\ell (2\ell + 1) P_\ell(\cos\theta) \times \psi_\ell(r) \tag{31}$$

where the radial ψ_ℓ are solutions of the free radial wave equations and hence linear combinations of the spherical Bessel functions. Specifically,

$$\psi_\ell(r) \;=\; \cos\delta_\ell \times j_\ell(kr) \;-\; \sin\delta_\ell \times n_\ell(kr) \tag{32}$$

for some phase shift δ_ℓ, which obtains from the Dirichlet boundary condition

$$\psi_\ell(r = R) \;=\; 0, \tag{33}$$

hence

$$\tan\delta_\ell \;=\; \frac{j_\ell(kR)}{n_\ell(kR)}\,. \tag{34}$$

Alas, this formula is not particularly transparent, so let us explore the two limiting cases: a small sphere of radius $R \ll (1/k)$, and a large sphere of radius $R \gg (1/k)$.

Small Sphere Limit

Let's start with a hard sphere of a small radius, $kR \ll 1$. In this limit,

$$j_\ell(kR) \approx \frac{(kR)^\ell}{(2\ell-1)!!}, \qquad n_\ell(kR) \approx -\frac{(2\ell+1)!!}{(kR)^{\ell+1}}, \tag{35}$$

so eq. (34) for the phase shifts yields

$$\tan\delta_\ell = -\frac{(kR)^{2\ell+1}}{(2\ell-1)!!\,(2\ell+1)!!}. \tag{36}$$

In particular,

$$\tan\delta_0 \approx -(kR), \qquad \tan\delta_1 \approx -\frac{(kR)^3}{3} \qquad \tan\delta_2 \approx -\frac{(kR)^5}{45}, \ \ldots. \qquad (37)(38)$$

Note that for $kR \ll 1$ all the phase shifts are negative and small, and their magnitudes rapidly decrease with ℓ. Thus, to the leading order in (kR) we may approximate

$$\delta_0 \approx -kR, \qquad \text{other } \delta_\ell \approx 0. \tag{39}$$

In this approximation, the scattering amplitude becomes

$$f(\theta) \approx \frac{e^{2i\delta_0}-1}{2k} \times P_0(\cos\theta) + 0 \approx \frac{2i\delta_0}{2k} \times 1 \approx -iR, \tag{40}$$

hence isotropic scattering cross-section

$$\frac{d\sigma}{d\Omega} = |f|^2 \approx R^2 \quad \text{in all directions}, \tag{41}$$

and the total scattering cross-section is

$$\sigma_{\text{tot}} = 4\pi R^2. \tag{42}$$

Note: this total scattering cross-sections is 4 times larger than the geometric cross-section $\sigma_{\text{geom}} = \pi R^2$ of the sphere in question. However, this discrepancy does not raise a paradox since one should not expect the geometric optics to work around objects of size $R \ll \lambda$.

Large Sphere Limit

Now consider the opposite limit of the hard sphere having a large radius $R \gg \lambda$, hence $kR \gg 1$. In this limit, the scattering is not dominated by a single mode $\ell = 0$; instead, it gets noticeable contributions from great many modes, from $\ell = 0$ to $\ell \sim kR \gg 1$. To see how this works, we see that for spherical Bessel functions with large $\ell \gg 1$, the transition between the short-distance regime

$$j_\ell(x) \approx \frac{x^\ell}{(2\ell-1)!!}, \qquad n_\ell(x) \approx -\frac{(2\ell+1)!!}{x^{\ell+1}}, \tag{35}$$

and the long-distance regime

$$j_\ell(x) \approx \frac{\sin(x - \ell\frac{\pi}{2})}{x}, \qquad n_\ell(x) \approx -\frac{\cos(x - \ell\frac{\pi}{2})}{x}, \tag{43}$$

happens at $x \approx (\ell + 1)$ rather than $x \approx 1$. Consequently, for a given $kR \gg 1$, the phase shifts of the very-large-ℓ modes with $\ell > kR$ obtain from the short-distance approximation to the Bessel functions despite $kR \gg 1$. Specifically, for these very-large-ℓ modes

$$\tan\delta_\ell = \frac{j_\ell(kR)}{n_\ell(kR)} \approx -\frac{(kR)^{2\ell+1}}{(2\ell+1)!!(2\ell-1)!!} \ll 1 \quad \text{for } \ell > kR, \tag{44}$$

so we may approximate

$$\delta_\ell \approx 0 \quad \text{for } \ell > kR. \tag{45}$$

On the other hand, for modes with $\ell \ll kR$ we have

$$\tan\delta_\ell \approx -\tan(kR - \ell\tfrac{\pi}{2}) \tag{46}$$

and hence

$$\delta_\ell = \frac{\ell\pi}{2} - kR. \tag{47}$$

Actually, this approximation is good for $\ell \ll kR$ but becomes rather crude for $\ell = O(kR)$ (but $\ell < kR$). In this case, a better approximation — based on the WKB approximation to the spherical Bessel functions — yields

$$\begin{aligned}\delta_\ell &\approx -\frac{\pi}{4} - \int\limits_{(\ell+\frac{1}{2})}^{R} dr\sqrt{k^2 - \frac{(\ell+\frac{1}{2})^2}{r^2}} \\ &= -\frac{\pi}{4} - \sqrt{(kR)^2 - (\ell+\tfrac{1}{2})^2} + (\ell+\tfrac{1}{2})\arccos\frac{(\ell+\frac{1}{2})}{kR}\,.\end{aligned} \tag{48}$$

But fortunately, we do not need the gory details of this formula. All we need to know is that for $\ell \leq kR$, the phase shifts δ_ℓ are large and change by a sizable fraction of π between adjacent values of ℓ. Consequently, $\sin^2\delta_\ell$ as a function of ℓ jumps almost randomly between 0 and 1, and when we average its value over some range of ℓ, we end up with

$$\left\langle\sin^2\delta_\ell\right\rangle_{\text{avg}} = \frac{1}{2} \qquad (\text{for } \ell \leq kR). \tag{49}$$

Consequently, the total scattering cross-section is

$$\begin{aligned}\sigma_{\text{tot}} &= \frac{4\pi}{k^2}\sum_{\ell=0}^{\infty}(2\ell+1)\sin^2\delta_\ell \\ &\approx \frac{4\pi}{k^2}\times\sum_{\ell=0}^{kR}(2\ell+1)\times\left(\left\langle\sin^2\delta_\ell\right\rangle = \frac{1}{2}\right) \\ &= \frac{2\pi}{k^2}\times\sum_{\ell=0}^{kR}(2\ell+1) \\ &\approx \frac{2\pi}{k^2}\times(kR)^2 \\ &= 2\pi R^2.\end{aligned}$$

Thus, the total scattering cross-section off a large hard sphere is twice the sphere's geometric cross-section, $\sigma_{\text{tot}} = 2\sigma_{\text{geom}}$.

For a large sphere of radius $R \gg \lambda$, we expect the geometric optics to be a good approximation to the wave optics. Geometrically, relating the scattering angle to the impact parameter $b = R\cos(\theta/2)$, we obtain the partial scattering cross-section as

$$\frac{d\sigma_{\rm geom}}{d\Omega} \;=\; \frac{1}{2\pi}\frac{d(\pi b^2)}{d\cos\theta} \;=\; \frac{R^2}{4} \tag{50}$$

thus isotropic scattering with the total cross-section $\sigma_{\rm geom} = \pi R^2$. In the wave optics, calculating the partial cross-section is a lot harder than the total cross-section, so let me simply give you the summary: For most angles,

$$\frac{d\sigma}{d\Omega} \;=\; |f(\theta)|^2 \;\approx\; \frac{R^2}{4}\,, \tag{51}$$

exactly as in the geometric optics. However, eq. (51) breaks down at small angles $\theta \lesssim (1/kR)$, where the cross-section has a narrow but very high forward peak due to diffraction of the wave around the sphere. The net cross-section over this forward peak is πR^2, same as the net cross-section over larger angles outside the forward peak, and that's why the total cross-section is $\sigma_{\rm tot} = 2 \times \pi R^2$.

Partial Analysis of EM Waves

For the EM waves there is a similar expansion of the scattering amplitudes into partial waves. However, for the EM waves there is no $\ell = 0$ mode, for each $\ell \geq 1$ there modes with $m = -1, 0, +1$ rather than just the $m = 0$, and for each combination of (ℓ, m) there are 2 distinct modes, one transverse-magnetic (TM) and the other transverse-electric.

In a perfect world, I would explain this partial wave expansion in detail, but alas we are running out of the semester. So instead of explaining this issue in class — and in these notes — I make this a reading assignment as a part of your last homework, specifically §10.3–4 of the Jackson's textbook.