

PARTIAL WAVE ANALYSIS OF SCATTERING

These are my notes from the Electromagnetic Theory (387 K) class. Here I discuss scattering of the scalar waves — such as wave-functions in quantum mechanics — as a prelude to scattering of the vector EM waves. In particular, in these notes I focus on the partial-wave analysis of scattering.

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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 free wave equation

$$(\nabla^2 + k^2)\psi(\mathbf{x}) = 0, \quad (1)$$

and we are looking for solutions of the form

$$\psi(\mathbf{x}) = \psi_{\text{incident}}(\mathbf{x}) + \psi_{\text{scattered}}(\mathbf{x}) \xrightarrow{r \rightarrow \infty} \exp(ikz) + f(\theta) \frac{\exp(ikr)}{r}. \quad (2)$$

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

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

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

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

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

$$\psi_\ell''(r) + \frac{2}{r}\psi_\ell'(r) - \frac{\ell(\ell + 1)}{r^2}\psi_\ell(r) + k^2\psi_\ell(r) = \left(\begin{array}{c} \text{perturbation by} \\ \text{the scatterer} \end{array} \right) \xrightarrow{r \rightarrow \infty} 0. \quad (5)$$

Consequently, outside the scatterer the radial waves become 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

$$\psi_\ell(r) = \cos \delta_\ell \times j_\ell(kr) - \sin \delta_\ell \times n_\ell(kr) \quad (6)$$

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

$$j_\ell(kr) \xrightarrow{kr \gg 1} \frac{\sin(kr - \ell\frac{\pi}{2})}{kr}, \quad n_\ell(kr) \xrightarrow{kr \gg 1} -\frac{\cos(kr - \ell\frac{\pi}{2})}{kr}, \quad (7)$$

hence for large radii

$$\psi_\ell(r) \xrightarrow{r \rightarrow \infty} \cos \delta \frac{\sin(kr - \ell\frac{\pi}{2})}{kr} + \sin \delta \frac{\cos(kr - \ell\frac{\pi}{2})}{kr} = \frac{\sin(kr - \ell\frac{\pi}{2} + \delta_\ell)}{kr}. \quad (8)$$

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

$$\begin{aligned} \psi_\ell^{\text{free}}(r) &= j_\ell(kr) \text{ @ all } r \quad \langle\langle \text{because } \psi_\ell^{\text{free}}(r) \text{ should stay finite for } r \rightarrow 0 \rangle\rangle \\ &\xrightarrow{kr \gg 1} \frac{\sin(kr - \ell\frac{\pi}{2})}{kr}. \end{aligned} \quad (9)$$

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

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

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

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

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

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

so for each partial wave we should have

$$\psi_{\ell}^{\text{sc}}(r) \xrightarrow{r \rightarrow \infty} A_{\ell} \times \frac{e^{+ikr}}{r}\tag{14}$$

for some overall complex coefficient A_{ℓ} , or in terms of the spherical Bessel functions

$$\psi_{\ell}^{\text{sc}}(r) = A_{\ell} \times ki^{\ell+1} h_{\ell}(kr) = A_{\ell} ki^{\ell+1} \times (j_{\ell}(kr) + in_{\ell}(kr)) \xrightarrow{kr \gg 1} A_{\ell} \times \frac{e^{+ikr}}{r}.\tag{15}$$

Altogether, the scattered wave should have form

$$\psi_{\text{sc}}(r, \theta) = \sum_{\ell=0}^{\infty} (2\ell + 1) i^{\ell} A_{\ell} P_{\ell}(\cos \theta) \times (ih_{\ell}(kr) = ij_{\ell}(kr) - n_{\ell}(kr)),\tag{16}$$

hence adding the incident wave (12) we build

$$\psi^{\text{net}}(r, \theta) = \sum_{\ell=0}^{\infty} (2\ell + 1) i^\ell P_\ell(\cos \theta) \times \left((1 + iA_\ell) \times j_\ell(kr) - A_\ell \times n_\ell(kr) \right). \quad (17)$$

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

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

Solving these equations gives us

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

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

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

for the *scattering amplitude*

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

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

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

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

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

where

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

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

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

On the last line here

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

hence

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

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

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

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

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

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

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

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

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

where the radial ψ_{ℓ} are solutions of the free radial wave equations and hence linear combinations of the spherical Bessel functions. Specifically,

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

for some phase shift δ_{ℓ} , which obtains from the Dirichlet boundary condition

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

hence

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

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,

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

so eq. (34) for the phase shifts yields

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

In particular,

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

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

$$\delta_0 \approx -kR, \quad \text{other } \delta_\ell \approx 0. \quad (39)$$

In this approximation, the scattering amplitude becomes

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

hence isotropic scattering cross-section

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

and the total scattering cross-section is

$$\sigma_{\text{tot}} = 4\pi R^2. \quad (42)$$

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

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

and the long-distance regime

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

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

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

so we may approximate

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

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

$$\tan \delta_\ell \approx -\tan(kR - \ell\frac{\pi}{2}) \quad (46)$$

and hence

$$\delta_\ell = \frac{\ell\pi}{2} - kR. \quad (47)$$

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

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

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

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

Consequently, the total scattering cross-section is

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

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

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

thus isotropic scattering with the total cross-section $\sigma_{\text{geom}} = \pi R^2$. 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,

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

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 $\sigma_{\text{tot}} = 2 \times \pi R^2$.