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.

\[
\begin{align*}
\psi(x) &= \psi_{\text{incident}}(x) + \psi_{\text{scattered}}(x) \\
&\xrightarrow{r\to\infty} \exp(ikz) + f(\theta) \frac{\exp(iKr)}{r}.
\end{align*}
\]

Consider scattering of a scalar wave \(\psi(x)\) 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 \(\psi(x)\) obeys the free wave equation

\[
(\nabla^2 + k^2)\psi(x) = 0,
\]

and we are looking for solutions of the form

\[
\psi(x) = \psi_{\text{incident}}(x) + \psi_{\text{scattered}}(x) \xrightarrow{r\to\infty} \exp(ikz) + f(\theta) \frac{\exp(iKr)}{r}.
\]

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 \(f(n)\) depends only on the angle between the incident wave and the direction \(n\) 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

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

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

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

(4)

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

$$\psi''_\ell(r) + \frac{2}{r} \psi'_\ell(r) - \frac{\ell(\ell + 1)}{r^2} \psi_\ell(r) + k^2 \psi_\ell(r) = \left( \text{perturbation by the scatterer} \right) \xrightarrow{r \to \infty} 0.$$  

(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

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

(6)

for some angle $\delta_\ell$ 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

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

(7)

hence for large radii

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

(8)

In this formula, $\delta_\ell$ shifts the phase of the asymptotic sine wave from the no-scattering asymptotic behavior

$$\psi^\text{free}_\ell(r) = j_\ell(kr) \at \text{all } r \quad \llbracket \text{because } \psi^\text{free}_\ell(r) \text{ should stay finite for } r \to 0 \rrbracket$$

$$\xrightarrow{kr \gg 1} \frac{\sin(kr - \ell \frac{\pi}{2})}{kr}.$$  

(9)
Next, let’s assemble the partial waves for different $\ell$’s into the sum

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

$$= \sum_{\ell=0}^{\infty} C_\ell (2\ell + 1)P_\ell(\cos \theta) \times \left( \cos \delta_\ell \times j_\ell(kr) - \sin \delta_\ell \times n_\ell(kr) \right)$$

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

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

and hence

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

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

$$\psi_{\text{sc}}(r, \theta) = \frac{f(\theta)}{r} \times e^{ikr}$$

without an $e^{-ikr}$ term,

so for each partial wave we should have

$$\psi_{\text{sc}}^\ell(r) \xrightarrow{r \to \infty} A_\ell \times \frac{e^{ikr}}{r}$$

for some overall complex coefficient $A_\ell$, or in terms of the spherical Bessel functions

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

Altogether, the scattered wave should have form

$$\psi_{\text{sc}}(r, \theta) = \sum_{\ell=0}^{\infty} (2\ell + 1)i^\ell A_\ell P_\ell(\cos \theta) \times \left( ih_\ell(kr) + in_\ell(kr) \right),$$

\[3\]
hence adding the incident wave (12) we build

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

(17)

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

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

(18)

Solving these equations gives us

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

(19)

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

\[ \psi_{\text{sc}}(r, \theta) = \sum_{\ell=0}^{\infty} (2\ell + 1)A_\ell P_\ell(\cos \theta) \times i^\ell h_\ell(kr) \xrightarrow{kr \gg 1} \sum_{\ell=0}^{\infty} (2\ell + 1)A_\ell P_\ell(\cos \theta) \times \frac{e^{ikr}}{ikr} \]

\[ = \frac{e^{ikr}}{kr} \times \sum_{\ell=0}^{\infty} (2\ell + 1)A_\ell P_\ell(\cos \theta) \]

\[ = f(\theta) \times \frac{e^{ikr}}{r} \]

(20)

for the \textit{scattering amplitude}

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

(21)

The coefficients \( A_\ell \) here should be as in eq. (19), thus

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

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

\[
\frac{d\sigma}{d\Omega} = |f(\theta)|^2,
\]  

(23)

where

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

(24)

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

\[
\sigma_{\text{tot}} = \iint d^2\Omega |f|^2
\]

\[
= \int_0^\pi |f|^2 \times 2\pi \sin \theta d\theta
\]

\[
= \sum_{\ell,\ell'} \frac{(\exp(+2i\delta_\ell) - 1)(\exp(-2i\delta_{\ell'}) - 1)}{4k^2} \times
\]

\[
\times (2\ell + 1)(2\ell' + 1) \int_0^\pi P_\ell(\cos \theta) P_{\ell'}(\cos \theta) 2\pi \sin \theta d\theta
\]

(25)

On the last line here

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

(26)

hence

\[
\sigma_{\text{tot}} = \sum_{\ell} \left| \frac{\exp(2i\delta_\ell) - 1}{2k} \right|^2 \times 4\pi(2\ell + 1)
\]

\[
= \frac{4\pi}{k^2} \sum_{\ell=0}^\infty (2\ell + 1) \sin^2(\delta_\ell).
\]

(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

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

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

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

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

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

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

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

where the radial \( \psi_{\ell} \) are solutions of the free radial wave equations and hence linear combinations of the spherical Bessel functions. Specifically,

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

for some phase shift \( \delta_{\ell} \), which obtains from the Dirichlet boundary condition

\[ \psi_{\ell}(r = R) = 0, \] (33)

hence

\[ \tan \delta_{\ell} = \frac{j_{\ell}(kR)}{n_{\ell}(kR)}. \] (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,

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

so eq. (34) for the phase shifts yields

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

In particular,

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

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

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

In this approximation, the scattering amplitude becomes

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

hence isotropic scattering cross-section

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

and the total scattering cross-section is

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

Note: this total scattering cross-section 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 $R \ll \lambda$. 7
**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

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

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-$\ell$ modes with $\ell > kR$ obtain from the short-distance approximation to the Bessel functions despite $kR \gg 1$. Specifically, for these very-large-$\ell$ modes

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

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

$$
 \tan \delta_\ell \approx -\tan(kR - \ell\pi/2) \quad (46)
$$

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

\[ \delta_\ell \approx -\frac{\pi}{4} - \int_{(\ell + \frac{1}{2})}^{R} dr \sqrt{k^2 - \left(\frac{\ell + \frac{1}{2}}{r}\right)^2} \]

\[ = -\frac{\pi}{4} - \sqrt{(kR)^2 - (\ell + \frac{1}{2})^2} + (\ell + \frac{1}{2}) \arccos \left(\frac{\ell + \frac{1}{2}}{kR}\right). \] (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 \( \delta_\ell \) are large and change by a sizable fraction of \( \pi \) between adjacent values of \( \ell \). Consequently, \( \sin^2 \delta_\ell \) as a function of \( \ell \) jumps almost randomly between 0 and 1, and when we average its value over some range of \( \ell \), we end up with

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

Consequently, the total scattering cross-section is

\[ \sigma_{\text{tot}} = \frac{4\pi}{k^2} \sum_{\ell=0}^{\infty} (2\ell + 1) \sin^2 \delta_\ell \]

\[ \approx \frac{4\pi}{k^2} \times \sum_{\ell=0}^{kR} (2\ell + 1) \times \left( \langle \sin^2 \delta_\ell \rangle = \frac{1}{2} \right) \]

\[ = \frac{2\pi}{k^2} \times \sum_{\ell=0}^{kR} (2\ell + 1) \]

\[ \approx \frac{2\pi}{k^2} \times (kR)^2 \]

\[ = 2\pi R^2. \]

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

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

(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,

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

(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 $\pi R^2$, same as the net cross-section over larger angles outside the forward peak, and that’s why the total cross-section is $\sigma_{\text{tot}} = 2 \times \pi R^2$. 

10