PHY 742 Quantum Mechanics II
12-12:50 PM MWF Olin 103

Plan for Lecture 8

1. Continue reading Chapter 14 – Analysis of scattering phenomena

   a. Notion of scattering phase shifts
   b. Relationship of scattering phase shifts to differential and total scattering cross sections
   c. Examples

Course schedule for Spring 2022

(Preliminary schedule -- subject to frequent adjustment.)

	Lecture date	Reading	Topic	HW	Due date
1	Mon: 01/10/2022	Chap. 12	Approximate solutions for stationary states -- The variational approach	#1	01/14/2022
2	Wed: 01/12/2022	Chap. 12 C	Approximate solutions for stationary states -- Perturbation theory	#2	01/19/2022
3	Fri: 01/14/2022	Chap. 12 D	Approximate solutions for stationary states -- Degenerate perturbation theory	#3	01/21/2022
	Mon: 01/17/2022		MLK Holiday -- no class		
4	Wed: 01/19/2022	Chap. 12 C & D	Approximate solutions for stationary states -- Additional tricks	#4	01/24/2022
5	Fri: 01/21/2022	Chap. 13	Examples of of the use of perturbation theory	#5	01/26/2022
6	Mon: 01/24/2022	Chap. 13 & 12 B	Hyperfine perturbation and also the WKB approximation	#6	01/28/2022
7	Wed: 01/26/2022	Chap. 14	Scattering theory		
8	Fri: 01/28/2022	Chap. 14	Scattering theory	#7	02/04/2022
9	Mon: 01/31/2022	Chap. 14	Scattering theory		

PHY 742 -- Assignment #6

January 28, 2022

Continue reading Chapter 14 in **Carlson's** textbook.

1. Consider the function e^{ix} , where x is a positive quantity.
   a. Write the function as an expansion in terms of spherical bessel functions.
   b. Using Maple or Mathematica or other software, plot the real and imaginary parts of the function as a function for x in the range of 0 and 5, both for the function itself and a finite number of expansion terms
   c. Comment on the accuracy of the expansion.

Introduction to scattering theory for quantum particles -- Chap. 14 of textbook;

Geometry of ideal scattering measurement

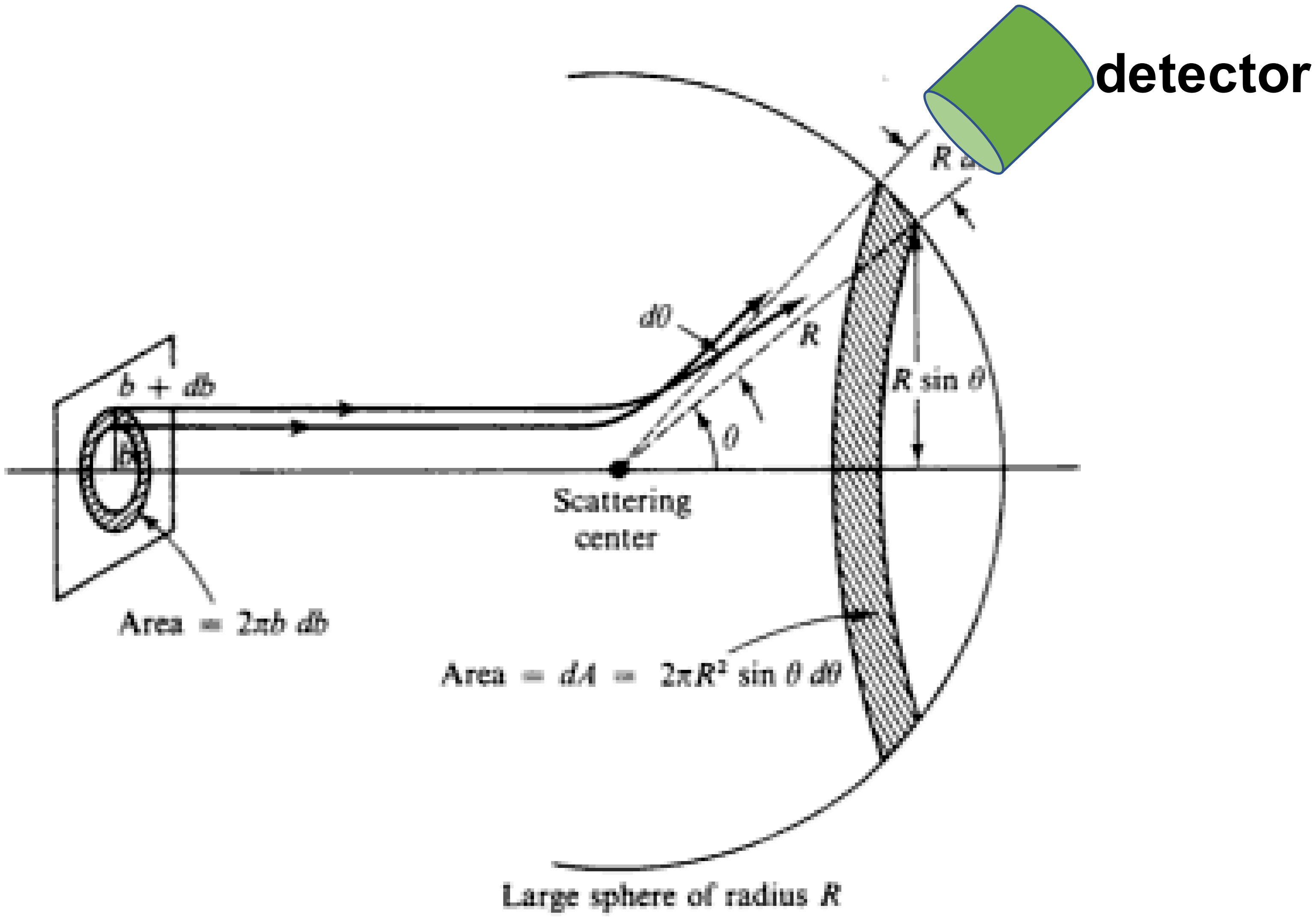
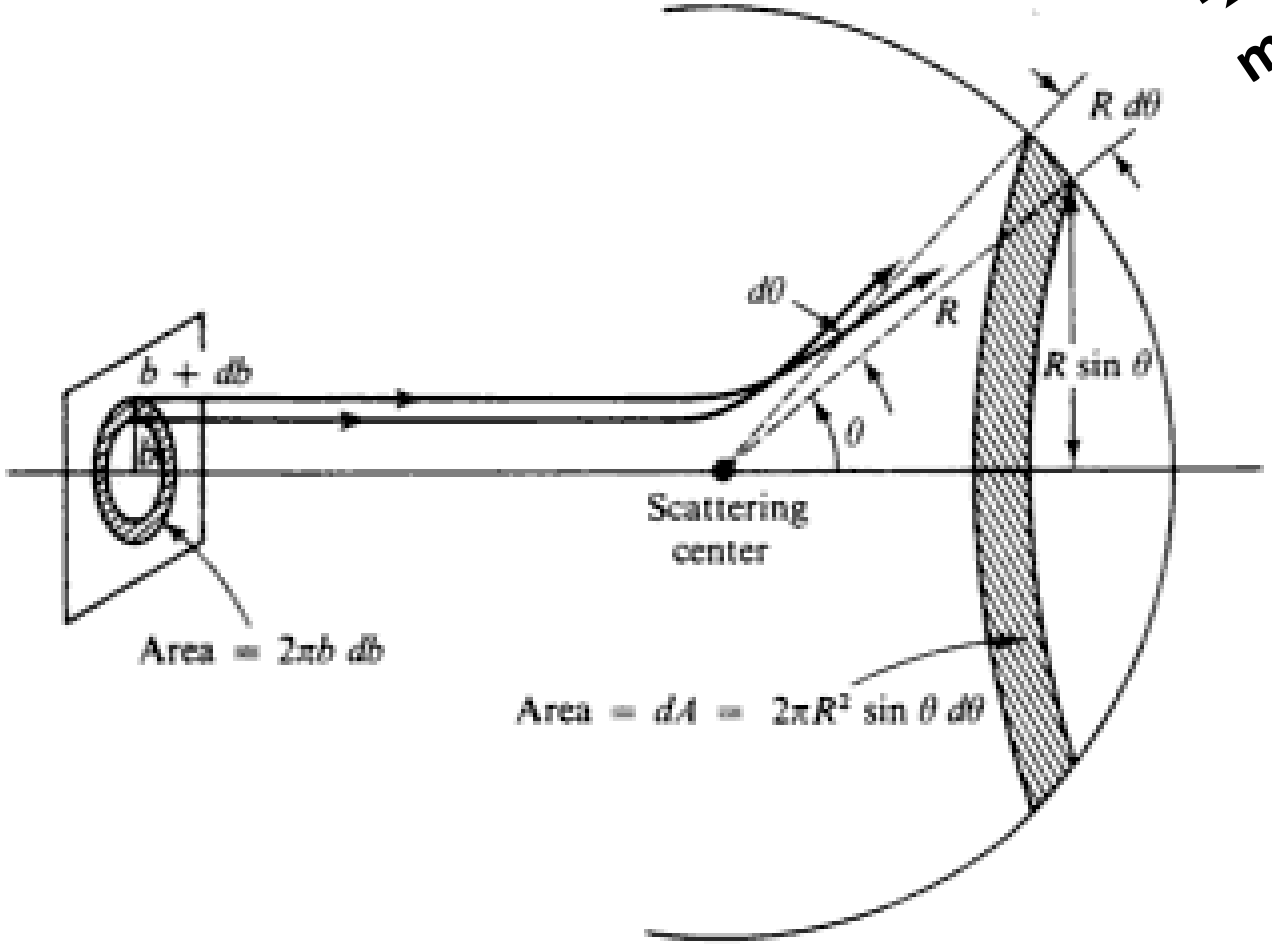


Figure 5.5 The scattering problem and relation of cross section to impact parameter.

Basic idea of scattering theory

➔ **Output measured at angle** θ

➔ **Well defined input; beam of independent particles of energy *E* moving toward target**



Quantitative measure – assumed to give information about the interaction between particle and target systems.

Differential cross section

$$\left(\frac{d\sigma}{d\Omega}\right) = \frac{\text{Number of detected particles at } \theta \text{ per target particle}}{\text{Number of incident particles per unit area}}$$

$$= \text{Area of incident beam that is scattered into detector at angle } \theta$$

In quantum mechanics, the beam of incident particles can be characterized in terms of its probability current:

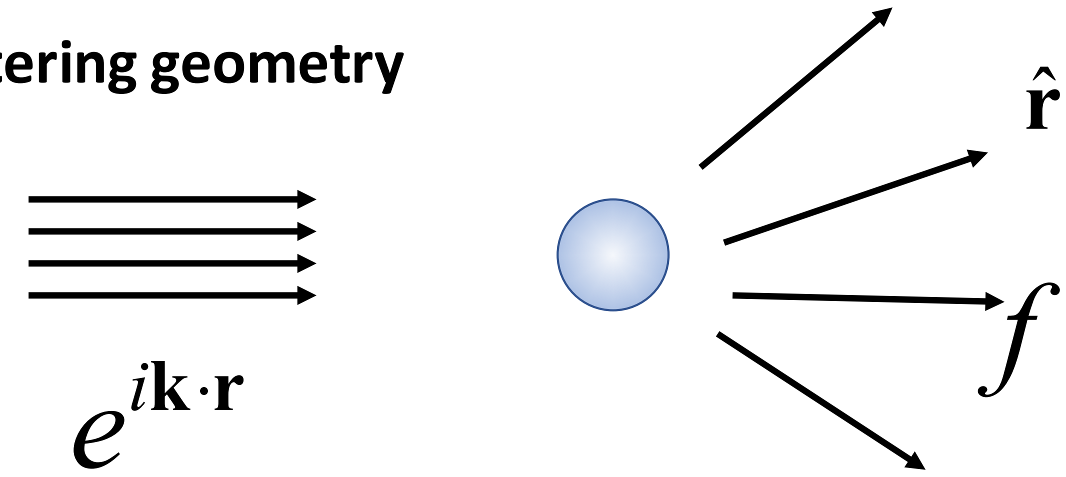
$$\mathbf{j}(\mathbf{r},t) \equiv \frac{\hbar}{2mi}\left[\Psi^*(\mathbf{r},t)\nabla\Psi(\mathbf{r},t) - \Psi(\mathbf{r},t)\nabla\Psi^*(\mathbf{r},t)\right]$$

Wave function of incident particle:

$$\Psi(\mathbf{r},t) = \frac{1}{\sqrt{\Omega}} e^{i\mathbf{k}\cdot\mathbf{r} - iEt/\hbar} \qquad \mathbf{j}(\mathbf{r},t) = \frac{1}{\Omega}\frac{\hbar\mathbf{k}}{m}$$

Representation of scattering in terms of probability amplitude

Scattering geometry



$$e^{i\mathbf{k}\cdot\mathbf{r}}$$

$$f(\hat{\mathbf{k}},\hat{\mathbf{r}})\frac{e^{ikr}}{r}$$

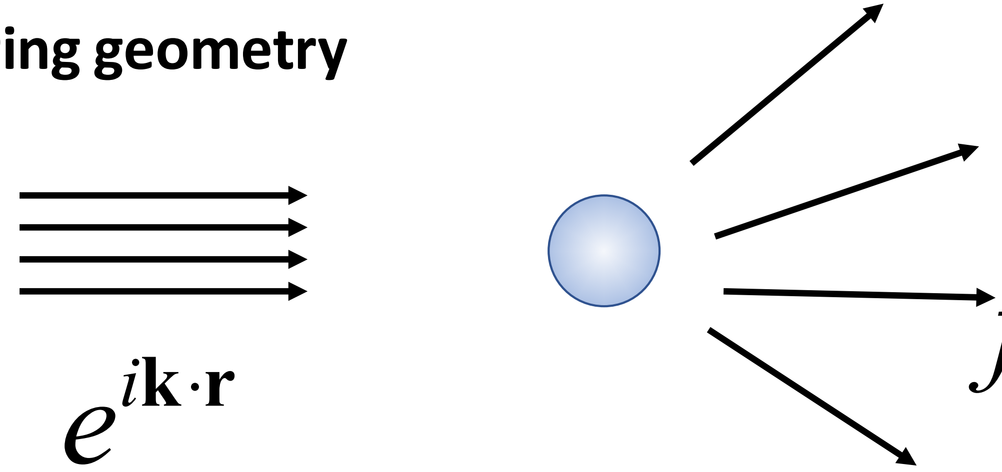
Incident plane wave with

wavevector $\mathbf{k}$ and energy $E = \dfrac{\hbar^2 k^2}{2m}$

Scattered spherical wave with

scattering amplitude $f(\hat{\mathbf{k}},\hat{\mathbf{r}})$

Scattering geometry



$$e^{i\mathbf{k}\cdot\mathbf{r}} \qquad f(\hat{\mathbf{k}},\hat{\mathbf{r}})\frac{e^{ikr}}{r}$$

Differential scattering cross section

$$\frac{d\sigma}{d\Omega}=\frac{\text{Probability of particle scattering}}{\text{Incident flux of particles}}$$

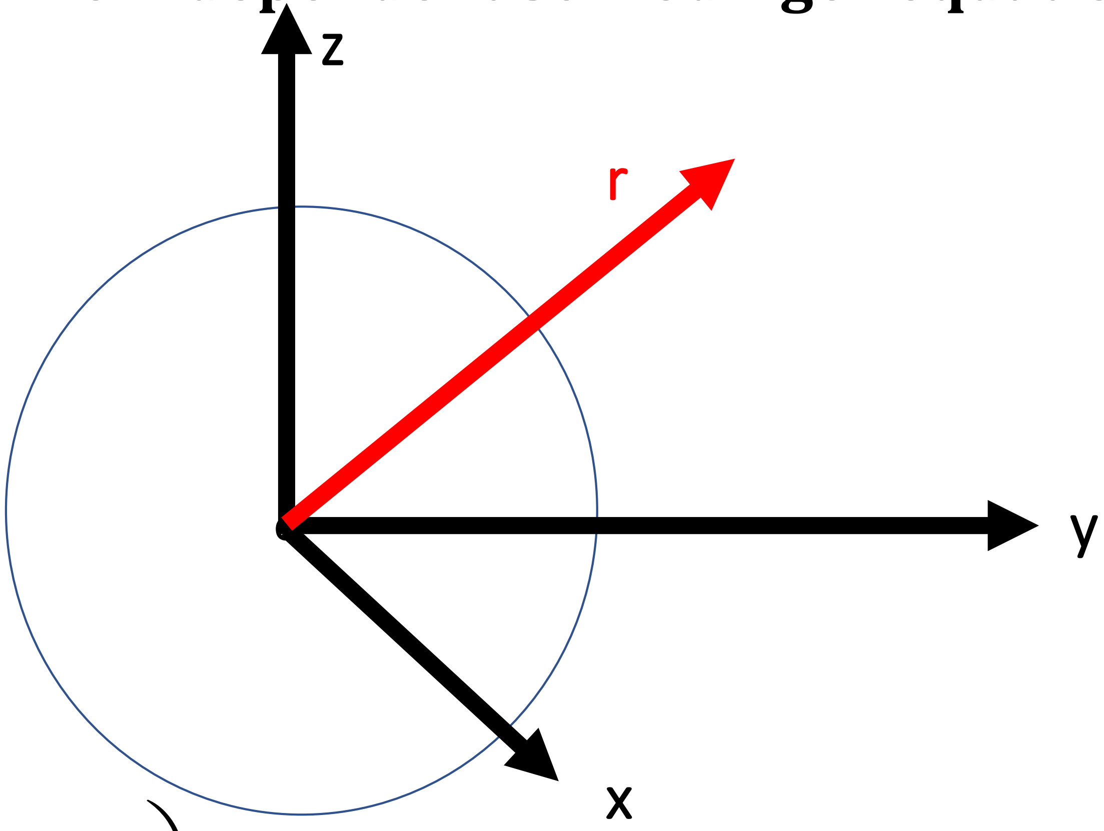
$$=\left|f(\hat{\mathbf{k}},\hat{\mathbf{r}})\right|^2$$

$$=\left(\frac{4\pi}{k}\right)^2\left|\sum_{lm} e^{i\delta_l(E)}\sin(\delta_l(E))Y^*_{lm}(\hat{\mathbf{k}})Y_{lm}(\hat{\mathbf{r}})\right|^2$$

What we will show for spherical target

Representation of a free particle in quantum mechanics --

Continuum solutions of the time independent Schrödinger equation.



$$\left(-\frac{\hbar^2}{2m}\nabla^2 + V(r)\right)\Psi_E(\mathbf{r}) = E\Psi_E(\mathbf{r})$$

Potential interaction due to spherical target for $0 \leq r \leq D$

If the system has spherical symmetry about a given origin, it is then convenient to expand the eigenfunctions into spherical harmonic functions:

$$\Psi_E(\mathbf{r}) = \sum_{lm} R_{El}(r) Y_{lm}(\hat{\mathbf{r}})$$

Differential equation for radial function

$$\left(-\frac{\hbar^2}{2m}\left(\frac{d^2}{dr^2} + \frac{2}{r}\frac{d}{dr} - \frac{l(l+1)}{r^2} \right) + V(r) - E \right) R_{El}(r) = 0$$

For many cases, $\quad V(r \to \infty) \approx 0$

In the range that $V(r)$ sufficiently small,

the radial equation satisfies:

$$\left(\frac{d^2}{dr^2} + \frac{2}{r}\frac{d}{dr} - \frac{l(l+1)}{r^2} + \frac{2mE}{\hbar^2} \right) R^0_{El}(r) = 0 \qquad \text{for } E > 0$$

In the range for $V(r) \approx 0$:

$$R_{El}(r) = A_l j_l(kr) + B_l y_l(kr) = \mathcal{N}\left(\cos\delta_l j_l(kr) - \sin\delta_l y_l(kr)\right)$$

Note that if $V(r) \equiv 0$, we expect $\delta_l = 0$.

How to determine phase shifts $\delta_l(E)$:

Suppose the range of the scattering potential is D:

For $r < D$, solve differential equation:

$$\left(-\frac{\hbar^2}{2m}\left(\frac{d^2}{dr^2} + \frac{2}{r}\frac{d}{dr} - \frac{l(l+1)}{r^2}\right) + V(r) - E\right) R_{El}(r) = 0$$

Continuity conditions at $r = D$:

$$R_{El}(D) = \mathcal{N}\left(\cos\delta_l j_l(kD) - \sin\delta_l y_l(kD)\right)$$

$$\frac{dR_{El}(D)}{dr} = \mathcal{N}\left(\cos\delta_l \frac{dj_l(kD)}{dr} - \sin\delta_l \frac{dy_l(kD)}{dr}\right)$$

Note that in Professor Carlson's text:

$y_l(z) \Leftrightarrow n_l(z)$

Continuity conditions at $r = D$ -- continued:

$$R_{El}(D) = \mathcal{N}\left(\cos\delta_l\, j_l(kD) - \sin\delta_l\, y_l(kD)\right)$$

$$\frac{dR_{El}(D)}{dr} = \mathcal{N}\left(\cos\delta_l \frac{dj_l(kD)}{dr} - \sin\delta_l \frac{dy_l(kD)}{dr}\right)$$

Some identities:

$$j_l(z)\frac{dy_l(z)}{dz} - y_l(z)\frac{dj_l(z)}{dz} = \frac{1}{z^2}$$

$$\frac{d\ln\left(R_{El}(r)\right)}{dr} = \left.\frac{\frac{dR_{El}(r)}{dr}}{R_{El}(r)}\right|_{r=D} \equiv L_l(E)$$

$$\tan\delta_l(E) = \frac{L_l(E)\, j_l(kD) - k j_l'(kD)}{L_l(E)\, y_l(kD) - k y_l'(kD)}$$

What we want to show, is that the scattering phase shift is a measure of the quantum mechanical scattering cross section:

Differential scattering cross section

$$\frac{d\sigma}{d\Omega} = \frac{\text{Probability of particle scattering}}{\text{Incident flux of particles}}$$

$$= \left| f(\hat{\mathbf{k}}, \hat{\mathbf{r}}) \right|^2$$

$$= \left(\frac{4\pi}{k}\right)^2 \left| \sum_{lm} e^{i\delta_l(E)} \sin(\delta_l(E)) Y^*_{lm}(\hat{\mathbf{k}}) Y_{lm}(\hat{\mathbf{r}}) \right|^2$$

Some details: Note that this is also covered in Jackson in Sec. 10.3

It can be shown that: $$e^{i\mathbf{k}\cdot\mathbf{r}} = \sum_l i^l \left(2l+1\right) j_l(kr) P_l(\hat{\mathbf{k}}\cdot\hat{\mathbf{r}}) = 4\pi \sum_{lm} i^l j_l(kr) Y_{lm}{}^*(\hat{\mathbf{k}}) Y_{lm}(\hat{\mathbf{r}})$$

Note that: $$e^{i\mathbf{k}\cdot\mathbf{r}} = e^{ikr\cos\theta} = 1 + ikr\cos\theta + \frac{1}{2}\left(ikr\cos\theta\right)^2 + \frac{1}{3!}\left(ikr\cos\theta\right)^3 \ldots$$

Legendre polynomials $P_l(\cos\theta)$: $$P_0(\cos\theta) = 1$$
$$P_1(\cos\theta) = \cos\theta$$
$$P_2(\cos\theta) = \tfrac{1}{2}(3\cos^2\theta - 1)$$

Note that by design:
$$P_l(1) = 1$$

Spherical Bessel functions $j_l(kr)$: $$j_0(kr) = 1 - \tfrac{1}{6}(kr)^2 \ldots$$
$$j_1(kr) = \tfrac{1}{3}kr - \tfrac{1}{30}(kr)^3 \ldots$$

Legendre polynomials vs spherical harmonics --

$$P_l(\hat{\mathbf{x}}\cdot\hat{\mathbf{y}}) = \frac{4\pi}{2l+1}\sum_{m=-l}^{l} Y_{lm}^*(\hat{\mathbf{x}}) Y_{lm}(\hat{\mathbf{y}})$$

More details:

Probability amplitude for free particle of wave vector $\mathbf{k}$ and energy $E = \frac{\hbar^2 k^2}{2m}$

$$\Psi_E^0(\mathbf{r}) = e^{i\mathbf{k}\cdot\mathbf{r}} = 4\pi \sum_{lm} i^l j_l(kr) Y_{lm}^*(\hat{\mathbf{k}}) Y_{lm}(\hat{\mathbf{r}}) \qquad \Rightarrow R_{El}^0(r) = 4\pi i^l j_l(kr) Y_{lm}^*(\hat{\mathbf{k}})$$

$$= \sum_{lm} R_{El}^0(r) Y_{lm}(\hat{\mathbf{r}})$$

In presence of spherically symmetric interaction potential $V(r)$:

$\Psi_E(\mathbf{r}) = \sum_{lm} R_{El}(r) Y_{lm}(\hat{\mathbf{r}})$, where $R_{El}(r)$ is a solution to differential equation:

$$\left(-\frac{\hbar^2}{2m} \left(\frac{d^2}{dr^2} + \frac{2}{r}\frac{d}{dr} - \frac{l(l+1)}{r^2} \right) + V(r) - E \right) R_{El}(r) = 0$$

We want to show that for $r \to \infty$: $\quad \Psi_E(\mathbf{r}) = e^{i\mathbf{k}\cdot\mathbf{r}} + f(\hat{\mathbf{k}}, \hat{\mathbf{r}}) \frac{e^{ikr}}{r}$

More details:

In presence of spherically symmetric interaction potential $V(r)$:

$$\Psi_E(\mathbf{r}) = \sum_{lm} R_{El}(r) Y_{lm}(\hat{\mathbf{r}})$$

$$\left(-\frac{\hbar^2}{2m}\left(\frac{d^2}{dr^2} + \frac{2}{r}\frac{d}{dr} - \frac{l(l+1)}{r^2}\right) + V(r) - E\right) R_{El}(r) = 0$$

Outside the range of $V(r)$; when $V(r) \approx 0$:

$$R_{El}(r) = A_l j_l(kr) + B_l y_l(kr) = \mathcal{N}_l\left(\cos\delta_l j_l(kr) - \sin\delta_l y_l(kr)\right)$$

Even further from the target, the asymptotic forms of the spherical Bessel functions are relevant:

$$j_l(kr) \underset{kr \to \infty}{=} \frac{\sin(kr - \frac{l\pi}{2})}{kr} \qquad y_l(kr) \underset{kr \to \infty}{=} -\frac{\cos(kr - \frac{l\pi}{2})}{kr}$$

More details:

For $r \to \infty$

$$R_{El}(r) = A_l j_l(kr) + B_l y_l(kr) = \mathcal{N}_l \left(\cos\delta_l \, j_l(kr) - \sin\delta_l \, y_l(kr) \right)$$

$$\to \mathcal{N}_l \frac{\sin(kr - \frac{l\pi}{2} + \delta_l(E))}{kr}$$

$$\to R^0_{El}(r) + R^{scatt}_{El}(r)$$

$$R^0_{El}(r) = 4\pi i^l j_l(kr) Y_{lm}{}^*(\hat{\mathbf{k}}) \underset{kr \to \infty}{=} 4\pi i^l Y_{lm}{}^*(\hat{\mathbf{k}}) \frac{\sin(kr - \frac{l\pi}{2})}{kr}$$

Can show that the appropriate choice is $\mathcal{N}_l = 4\pi i^l Y_{lm}{}^*(\hat{\mathbf{k}}) e^{i\delta_l(E)}$

$$R_{El}(r) \to 4\pi i^l Y_{lm}{}^*(\hat{\mathbf{k}}) \left(e^{i\delta_l(E)} \frac{\sin(kr - \frac{l\pi}{2} + \delta_l(E))}{kr} \right)$$

More details:

$$R_{El}(r) \to 4\pi i^l Y_{lm}{}^*(\hat{\mathbf{k}})\left(e^{i\delta_l(E)} \frac{\sin(kr - \frac{l\pi}{2} + \delta_l(E))}{kr} \right)$$

$$= 4\pi i^l Y_{lm}{}^*(\hat{\mathbf{k}})\left(\frac{e^{i\left(kr - \frac{l\pi}{2} + 2\delta_l(E)\right)} - e^{-i\left(kr - \frac{l\pi}{2}\right)}}{2ikr} \right)$$

$$= 4\pi i^l Y_{lm}{}^*(\hat{\mathbf{k}})\left(\frac{e^{i\left(kr - \frac{l\pi}{2}\right)} - e^{-i\left(kr - \frac{l\pi}{2}\right)}}{2ikr} + \left(e^{i2\delta_l(E)} - 1\right)\frac{e^{i\left(kr - \frac{l\pi}{2}\right)}}{2ikr} \right)$$

$$= 4\pi i^l Y_{lm}{}^*(\hat{\mathbf{k}})\left(\frac{\sin(kr - \frac{l\pi}{2})}{kr} + \left(e^{i2\delta_l(E)} - 1\right) i^{-l} \frac{e^{ikr}}{2ikr} \right)$$

$$= R^0_{El}(r) + R^{scatt}_{El}(r)$$

When the dust clears:

$$f(\hat{\mathbf{k}},\hat{\mathbf{r}}) = \frac{4\pi}{k}\sum_{lm} e^{i\delta_l(E)} \sin(\delta_l(E)) Y^*_{lm}(\hat{\mathbf{k}}) Y_{lm}(\hat{\mathbf{r}})$$

Differential cross section: $\frac{d\sigma}{d\Omega} = \left| f(\hat{\mathbf{k}},\hat{\mathbf{r}}) \right|^2$

Total cross section: $\int d\Omega \frac{d\sigma}{d\Omega} = \sigma(E) = \frac{4\pi}{k^2}\sum_l (2l+1)\sin^2(\delta_l(E))$

Note that:

$$\Im\left(f\left(\hat{\mathbf{k}} = \hat{\mathbf{r}}\right)\right) = \frac{k}{4\pi}\sigma(E)$$

Imaginary part of forward scattering is proportional to the total scattering cross section.

Example – scattering from an impenetrable spherical hard wall of radius *a*

$$V(r) = \begin{cases} \infty & r \le a \\ 0 & r > a \end{cases}$$

$$\left(-\frac{\hbar^2}{2m}\left(\frac{d^2}{dr^2} + \frac{2}{r}\frac{d}{dr} - \frac{l(l+1)}{r^2} \right) + V(r) - E \right) R_{El}(r) = 0$$

$$R_{El}(r) = \begin{cases} 0 & r \le a \\ \mathcal{N}_l\left(\cos\delta_l j_l(kr) - \sin\delta_l y_l(kr)\right) & r > a \end{cases}$$

$$R_{El}(r) = 0 = \mathcal{N}_l\left(\cos\delta_l j_l(ka) - \sin\delta_l y_l(ka)\right)$$

$$\Rightarrow \tan\delta_l(E) = \frac{j_l(ka)}{y_l(ka)}$$

For $k \ll 1, \quad l = 0$ dominates with $\delta_0 \approx -ka$

Example – scattering from an impenetrable spherical hard wall of radius *a*

$$\tan\delta_l(E) = \frac{j_l(ka)}{y_l(ka)}$$

Differential cross section: $\dfrac{d\sigma}{d\Omega} = \left| f(\hat{\mathbf{k}},\hat{\mathbf{r}}) \right|^2$

Total cross section: $\int d\Omega \dfrac{d\sigma}{d\Omega} = \sigma(E) = \dfrac{4\pi}{k^2}\sum_l (2l+1)\sin^2(\delta_l(E))$

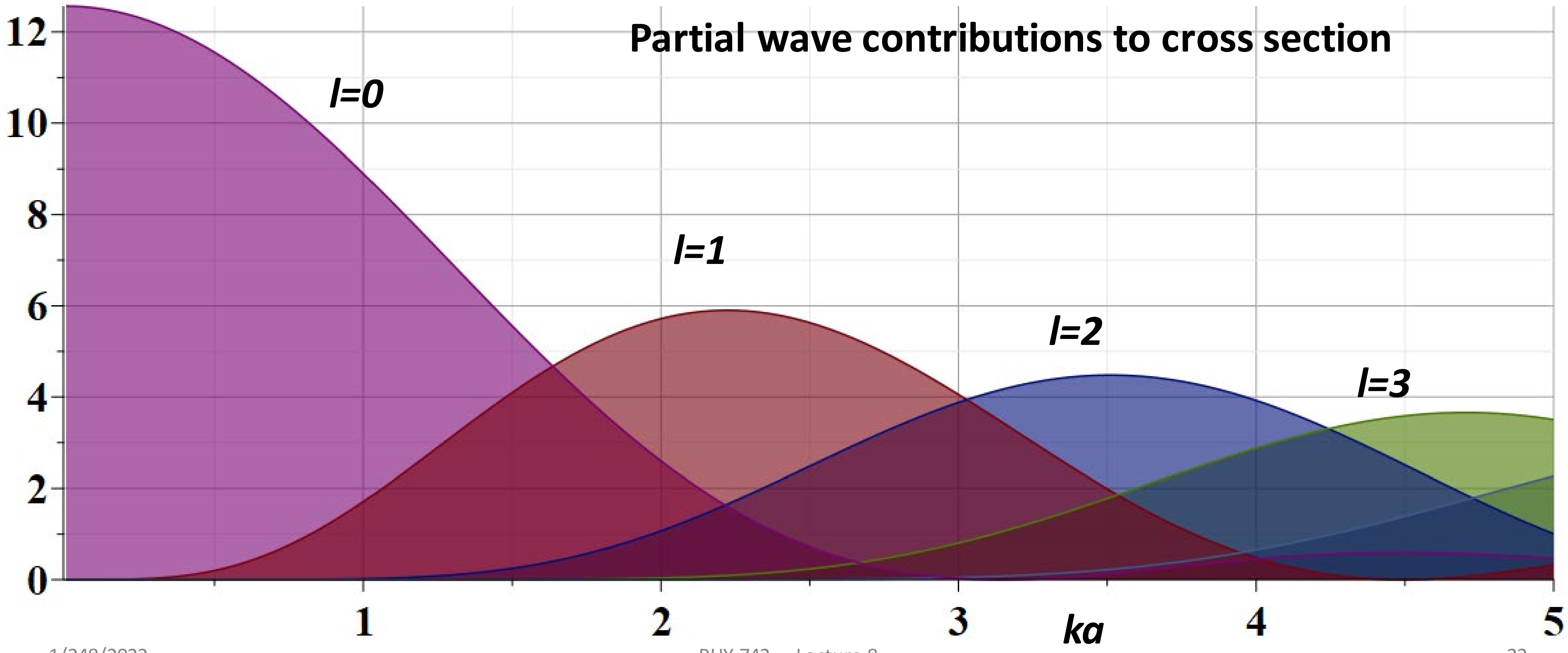
For $k \ll 1$, $l = 0$ dominates with $\delta_0 \approx -ka$

$$\Rightarrow \sigma(E) \approx 4\pi a^2$$

Different from classical case!

Example – scattering from an impenetrable spherical hard wall of radius *a*

$$\tan\delta_l(E) = \frac{j_l(ka)}{y_l(ka)} \qquad \sigma(E) = \frac{4\pi}{k^2}\sum_l \left(2l+1\right)\sin^2(\delta_l(E))$$



Total cross section as a function of *ka*