

PHY 742 Quantum Mechanics II

12-12:50 PM MWF Olin 103

Plan for Lecture 7

Scattering theory (Chap. 14) –

- 1. Introduction and geometry**
- 2. Scattering from spherically symmetric target**
- 3. Scattering phase shifts**

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 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		

Introduction to scattering theory for quantum particles -- Chap. 14 of textbook;
also see other quantum textbooks

Geometry of ideal scattering measurement

This geometry can also be used for quantum
systems ..

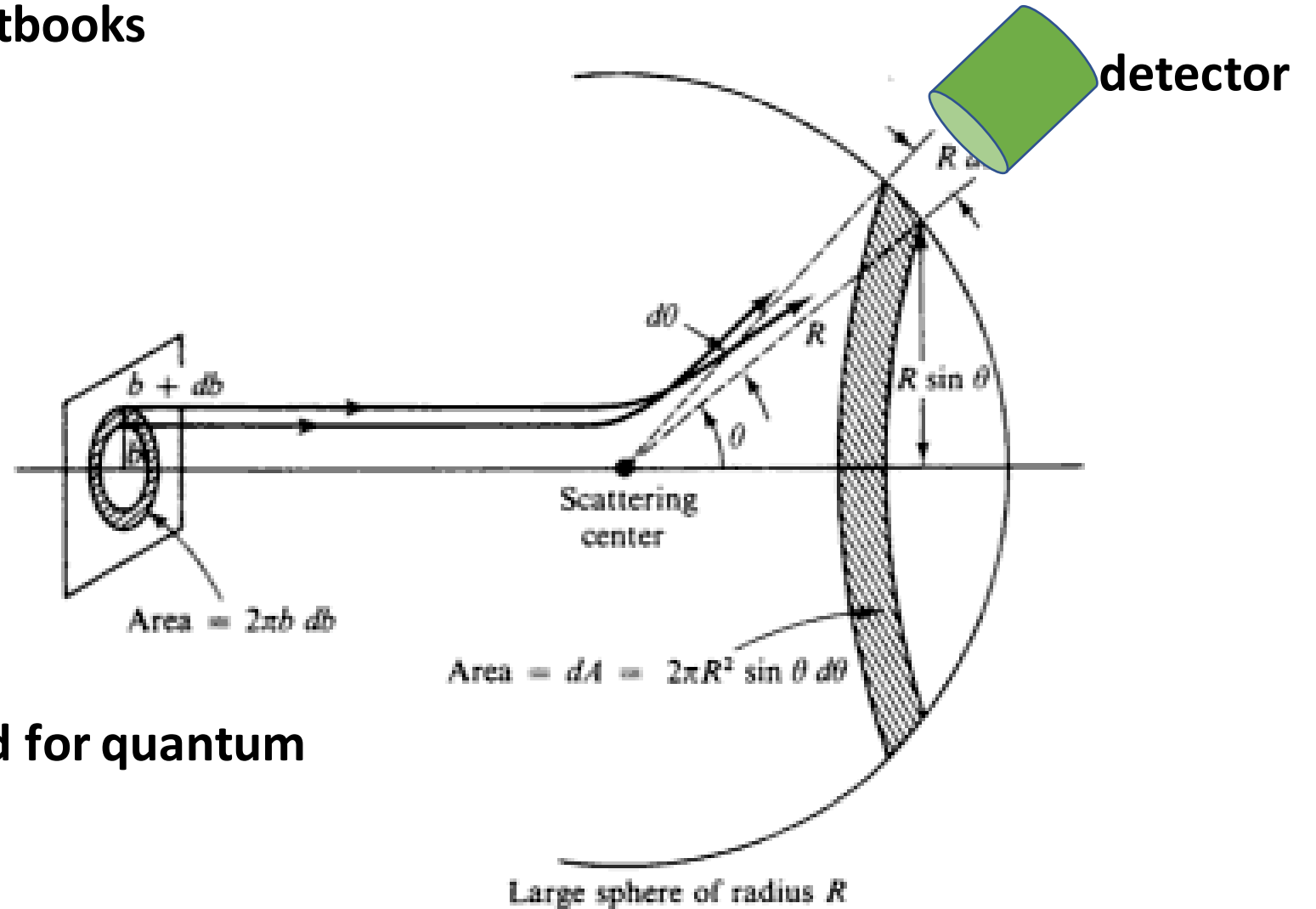


Figure 5.5 The scattering problem and relation of cross section to impact parameter.

Differential cross section

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

= Area of incident beam that is scattered into detector
at angle θ

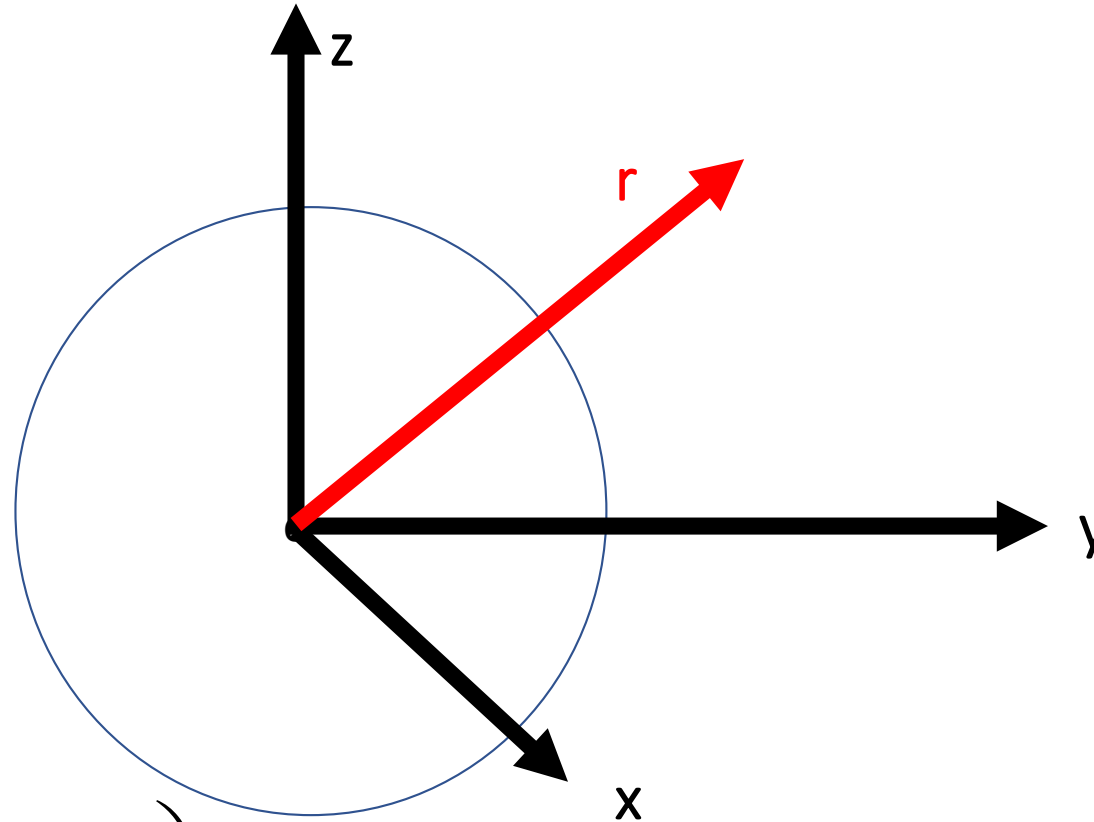
In classical mechanics, for an isotropic target, it is possible to calculate the cross section in terms of the impact parameter b :

$$\left(\frac{d\sigma}{d\Omega}\right) = \frac{d\phi \, b \, db}{d\phi \sin\theta \, d\theta} = \frac{b}{\sin\theta} \left| \frac{db}{d\theta} \right|$$

In quantum mechanics, the same phenomenon is formulated in terms of the probability amplitudes. We will specifically focus on free particles scattering from a spherically symmetric target.

Representation of a free particle in quantum mechanics --

Continuum solutions of the time independent Schrödinger equation.



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

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, $V(r \rightarrow \infty) \approx 0$

In the range that $V(r)$ sufficiently small, the radial equation satisfies:

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

Free particle partial waves -- continued

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

Define $k \equiv \sqrt{\frac{2mE}{\hbar^2}}$ $z \equiv kr$

$$\left(\frac{d^2}{dz^2} + \frac{2}{z} \frac{d}{dz} - \frac{l(l+1)}{z^2} + 1 \right) R_{El}^0(z) = 0$$

Properties of spherical Bessel functions

<http://dlmf.nist.gov/10.47>

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§10.47 Definitions and Basic Properties

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- [§10.47\(ii\) Standard Solutions](#)
- [§10.47\(iii\) Numerically Satisfactory Pairs of Solutions](#)
- [§10.47\(iv\) Interrelations](#)
- [§10.47\(v\) Reflection Formulas](#)

§10.47(i) Differential Equations

10.47.1
$$z^2 \frac{d^2 w}{dz^2} + 2z \frac{dw}{dz} + (z^2 - n(n+1))w = 0,$$

Spherical Bessel
functions of order n

Cylindrical Bessel
functions of order $n+1/2$

$$j_n(z) = \sqrt{\frac{1}{2} \pi / z} J_{n+\frac{1}{2}}(z)$$

$$y_n(z) = \sqrt{\frac{1}{2} \pi / z} Y_{n+\frac{1}{2}}(z) =$$

$$h_n^{(1)}(z) = \sqrt{\frac{1}{2} \pi / z} H_{n+\frac{1}{2}}^{(1)}(z) =$$

$$h_n^{(2)}(z) = \sqrt{\frac{1}{2} \pi / z} H_{n+\frac{1}{2}}^{(2)}(z)$$

$$h_n^{(1)}(z) = j_n(z) + i y_n(z)$$

Forms of spherical Bessel and Hankel functions: (also see Jackson $\geq$ 426)

$$j_0(x) = \frac{\sin(x)}{x}$$

$$h_0(x) = \frac{e^{ix}}{ix}$$

$$j_1(x) = \frac{\sin(x)}{x^2} - \frac{\cos(x)}{x}$$

$$h_1(x) = -\left(1 + \frac{i}{x}\right) \frac{e^{ix}}{x}$$

$$j_2(x) = \left(\frac{3}{x^3} - \frac{1}{x}\right) \sin(x) - \frac{3 \cos(x)}{x^2}$$

$$h_2(x) = i \left(1 + \frac{3i}{x} - \frac{3}{x^2}\right) \frac{e^{ix}}{x}$$

Asymptotic behavior :

$$x \ll 1 \quad \Rightarrow \quad j_l(x) \approx \frac{(x)^l}{(2l+1)!!}$$

$$x \gg 1 \quad \Rightarrow \quad h_l(x) \approx (-i)^{l+1} \frac{e^{ix}}{x}$$

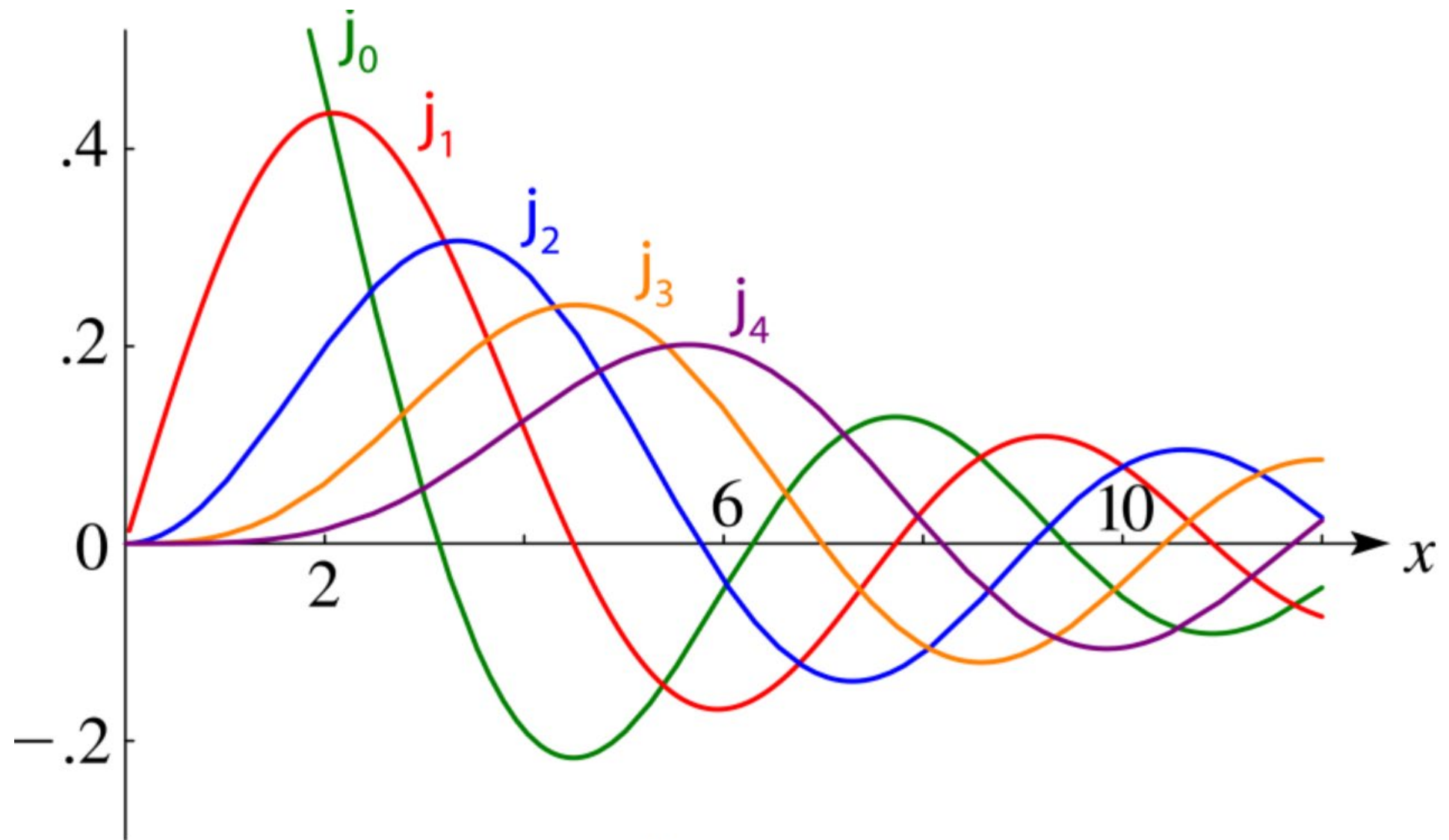


Figure 10.48.1: $j_n(x)$, $n = 0(1)4$, $0 \leq x \leq 12$. 

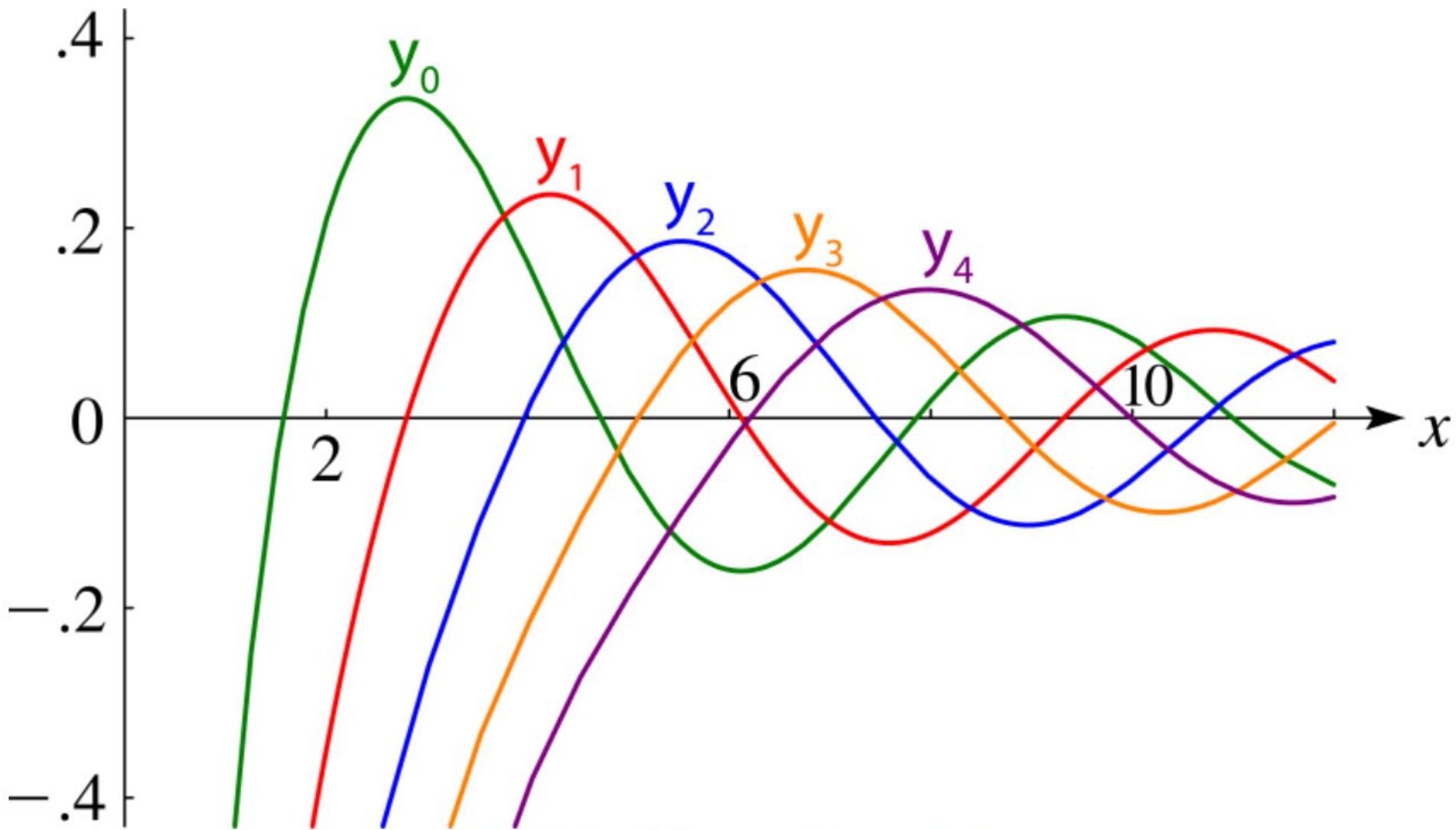


Figure 10.48.2: $y_n(x)$, $n = 0(1)4$, $0 < x \leq 12$. 

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

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

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 $r = D$:

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

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

Continuity conditions at $r = D$ – continued:

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

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

Some identities:

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

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

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

Why use term “phase shift”?

For free particle -- $V(r) = 0$

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

Define $k \equiv \sqrt{\frac{2mE}{\hbar^2}}$

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

Solution that is well-behaved for $r = 0$: $R_{El}^0(r) = j_l(kr)$

For hard sphere potential

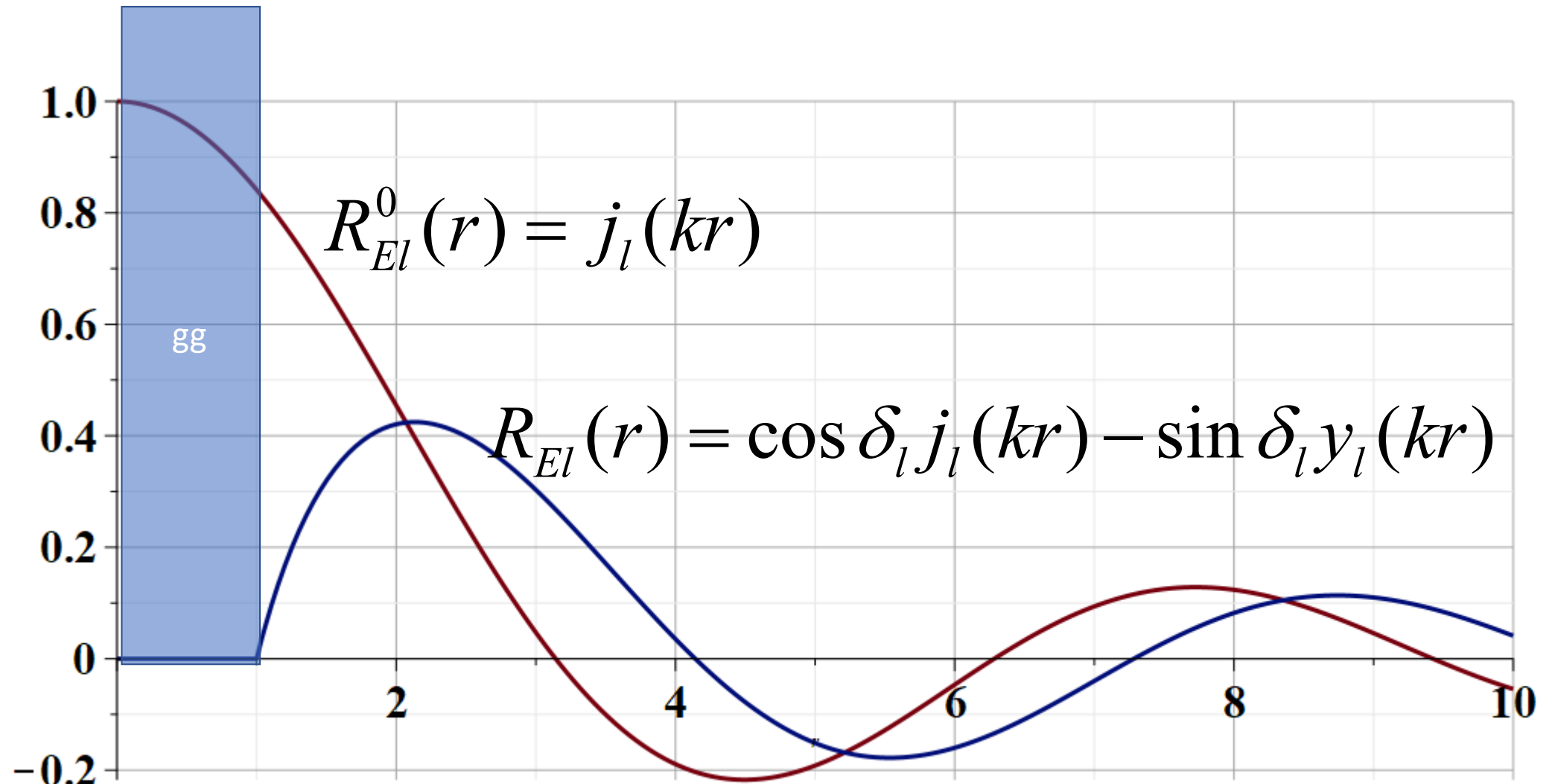
$$V(r) = \begin{cases} \infty & \text{for } r < D \\ 0 & \text{for } r \geq D \end{cases}$$

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

$$\text{In this case: } R_{El}(r) = \begin{cases} 0 & \text{for } r < D \\ \cos \delta_l j_l(kr) - \sin \delta_l y_l(kr) & \text{for } r \geq D \end{cases}$$

$$\text{where } \tan \delta_l = \frac{j_l(kD)}{y_l(kD)}$$

Illustration of phase shift for $l=0$ and infinite wall potential



➔ Phase shift is a measure of scattering strength

We can show that the scattering phase shift is a measure of the quantum mechanical scattering cross section:

Differential scattering cross section

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

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

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

➔ More details on Friday