

# **PHY 742 Quantum Mechanics II**

## **12-12:50 PM MWF Olin 103**

### **Plan for Lecture 7**

#### **Scattering theory (Chap. 14) –**

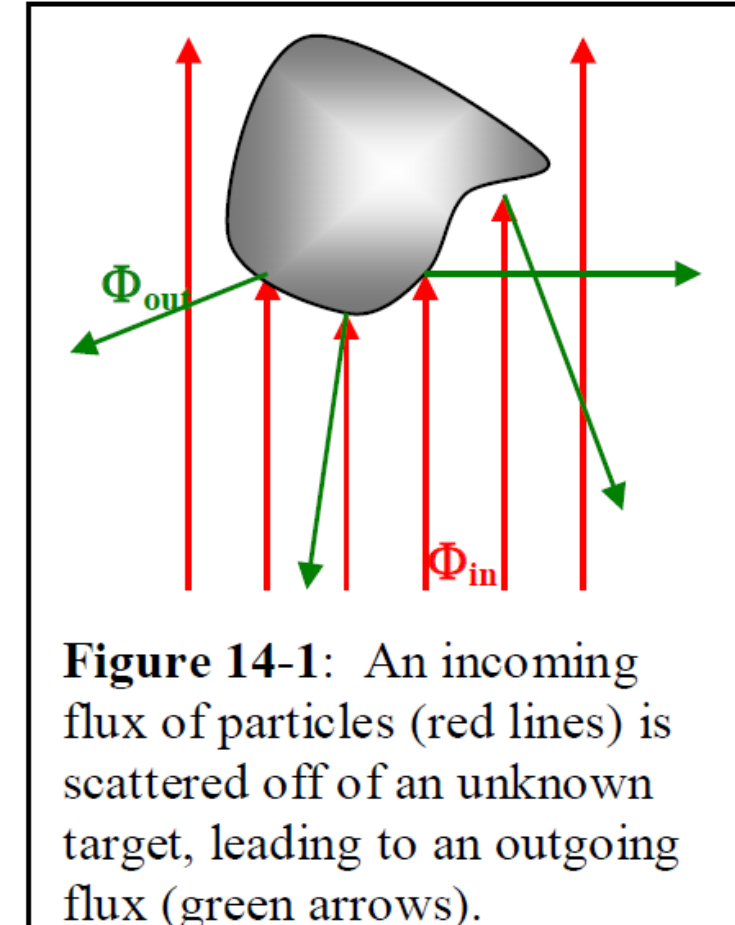
- 1. Introduction and geometry**
- 2. Scattering from spherically symmetric target**
- 3. Scattering phase shifts**

# XIV. Scattering

Let us now turn our attention to the related topic of scattering. In a scattering experiment, some sort of projectile is fired at a target, and the resulting outgoing particles are observed, as sketched in Fig. 14-1. The properties of the target, the projectiles, and their interaction are then related to the rates of incoming and scattered particles. The experimental results are normally given in terms of cross-section.

## A. Cross-Section and Differential Cross-Section

In general, many particles will be fired at a target, and only a small fraction of them will actually scatter. Generally the particles are sufficiently spread out that only one at a time strikes the target. It makes sense that the rate at which collisions occur  $\Gamma$  would be proportional to the number density  $n_{\text{in}}$  of the particles. It also might be sensible to imagine that it will be proportional to the difference in speed  $|v|$  of the projectiles compared to the target, since the faster



**Figure 14-1:** An incoming flux of particles (red lines) is scattered off of an unknown target, leading to an outgoing flux (green arrows).

# 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	<a href="#">#1</a>	01/14/2022
2	Wed: 01/12/2022	Chap. 12 C	Approximate solutions for stationary states -- Perturbation theory	<a href="#">#2</a>	01/19/2022
3	Fri: 01/14/2022	Chap. 12 D	Approximate solutions for stationary states -- Degenerate perturbation theory	<a href="#">#3</a>	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	<a href="#">#4</a>	01/24/2022
5	Fri: 01/21/2022	Chap. 13	Examples of the use of perturbation theory	<a href="#">#5</a>	01/26/2022
6	Mon: 01/24/2022	Chap. 13 & 12 B	Hyperfine perturbation and also the WKB approximation	<a href="#">#6</a>	01/28/2022
7	Wed: 01/26/2022	Chap. 14	Scattering theory		
8	Fri: 01/28/2022	Chap. 14	Scattering theory		

## Your questions –

**From Can:** On page 13, the first equation is  $R(r) = A j_l(kr) + B y_l(kr)$ , can any function be written into  $A j_l(kr) + B y_l(kr)$ ? Or just some special aspects in this problem so that we can write in this way.

**Comment:** When solving a second order differential equation, there are two independent solutions and a linear combination of the two is also a solution. In this case (outside the range of the potential  $V(x)$ ) the two independent solutions are  $j_l(kr)$  and  $y_l(kr)$ .

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 ..

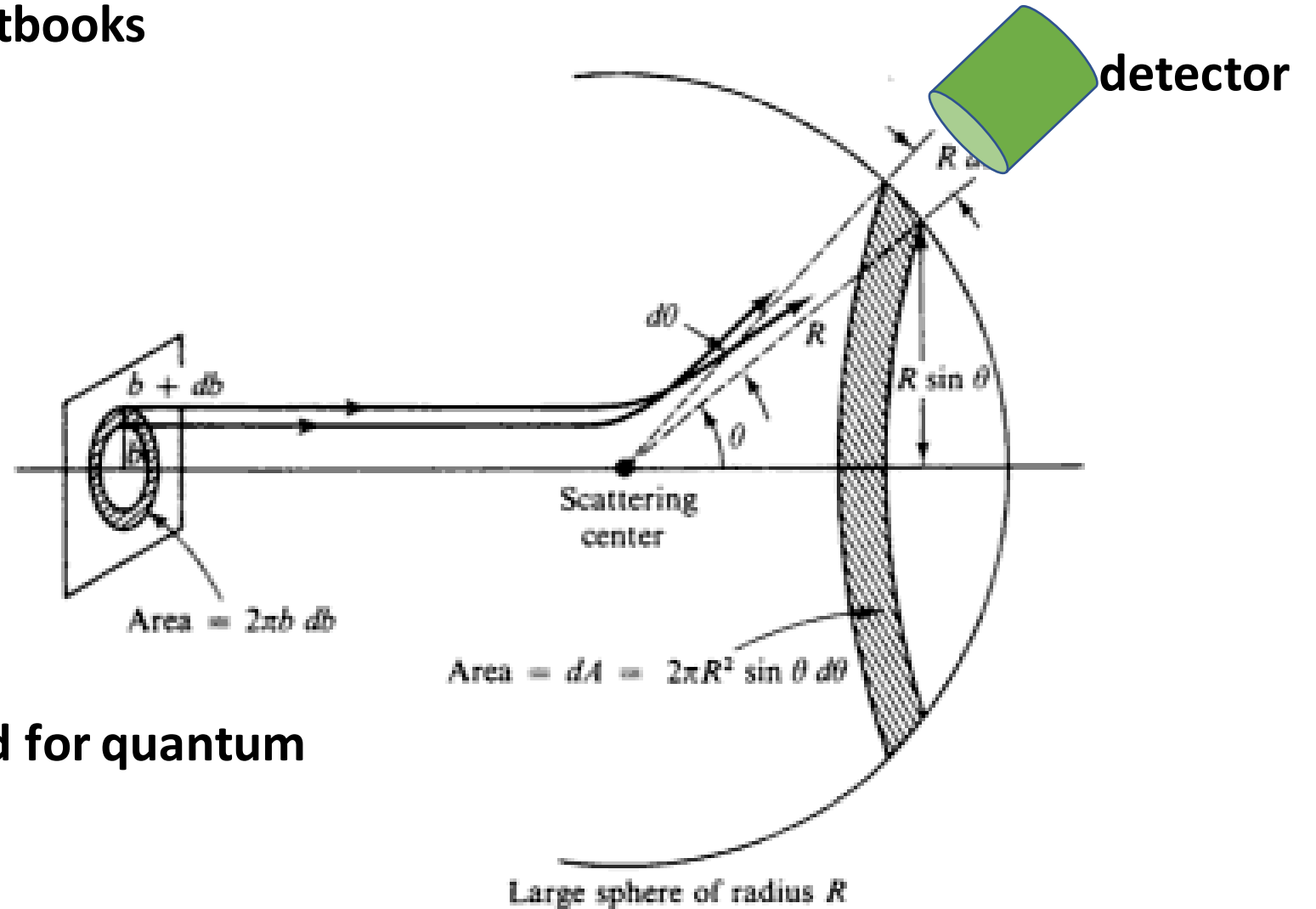


Figure 5.5 The scattering problem and relation of cross section to impact parameter.

## 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  $\theta$

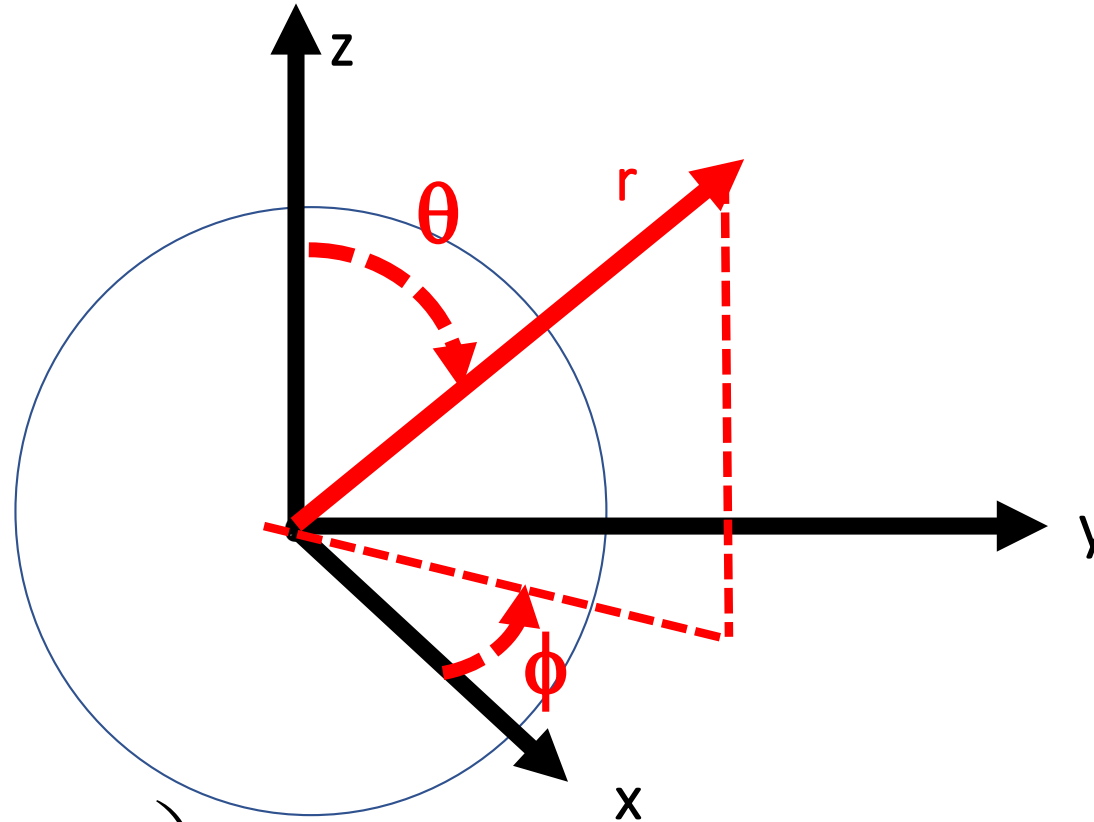
**In classical mechanics, for an isotropic target, it is possible to calculate the cross section in terms of the impact parameter  $b$ :**

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

**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. The same parameters are still relevant except for the notion of impact parameter  $b$ .**

# 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 Bessel Functions](#) [Spherical Bessel Functions](#)

[10.46 Generalized and Incomplete Bessel Functions; Mittag-Leffler Function](#)

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### §10.47 Definitions and Basic Properties



#### *Contents*

- [§10.47\(i\) Differential Equations](#)
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### §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  $n+1/2$


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


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

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

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

Note alternative notation:

$$n_n(z) \leftrightarrow y_n(z)$$

$$N_n(z) \leftrightarrow Y_n(z)$$

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

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 :

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

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

All  $j_l(x)$  are well behaved for  $x=0$

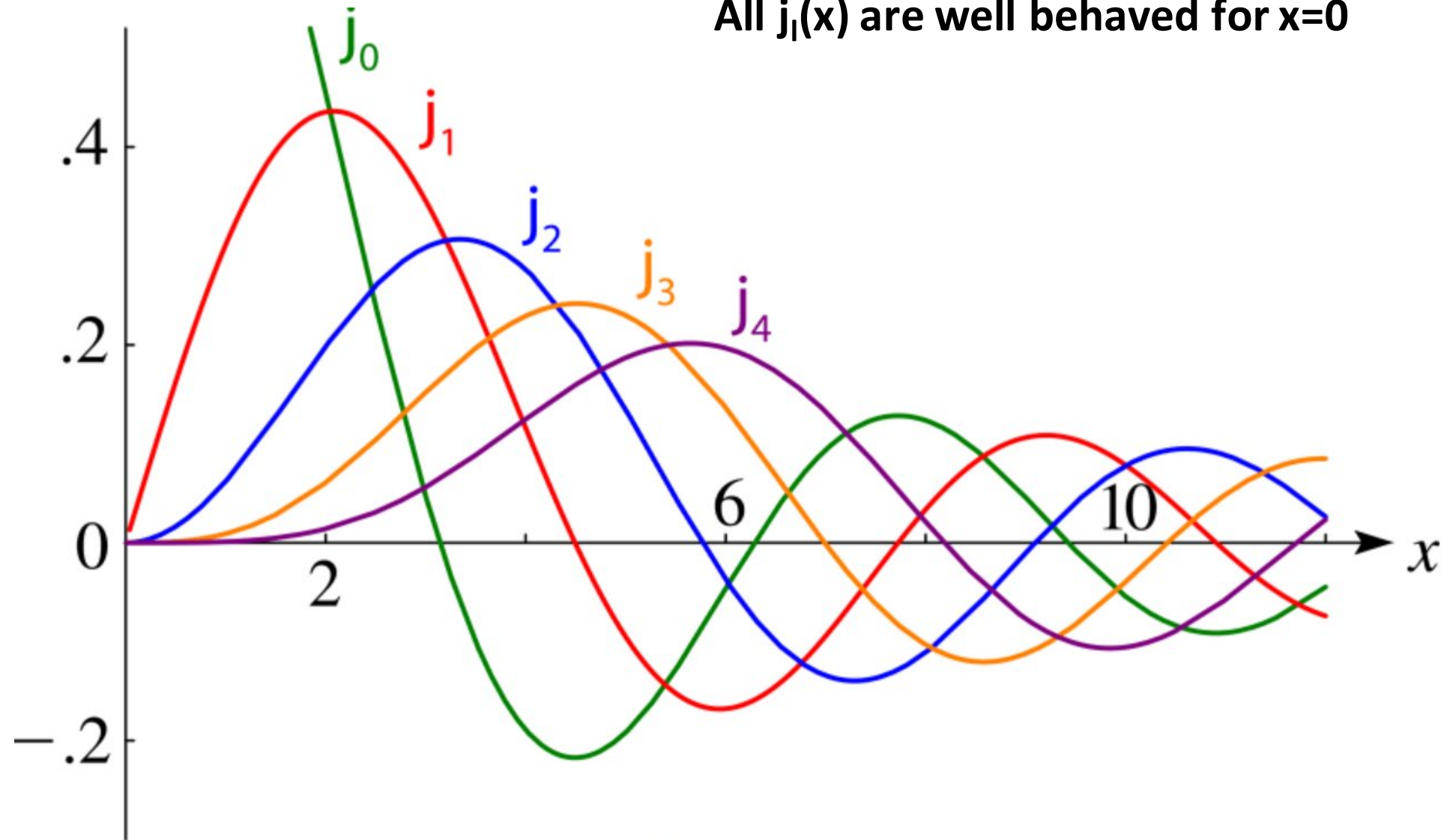


Figure 10.48.1:  $j_n(x)$ ,  $n = 0(1)4$ ,  $0 \leq x \leq 12$ .

All  $y_i(x)$  diverge for  $x=0$

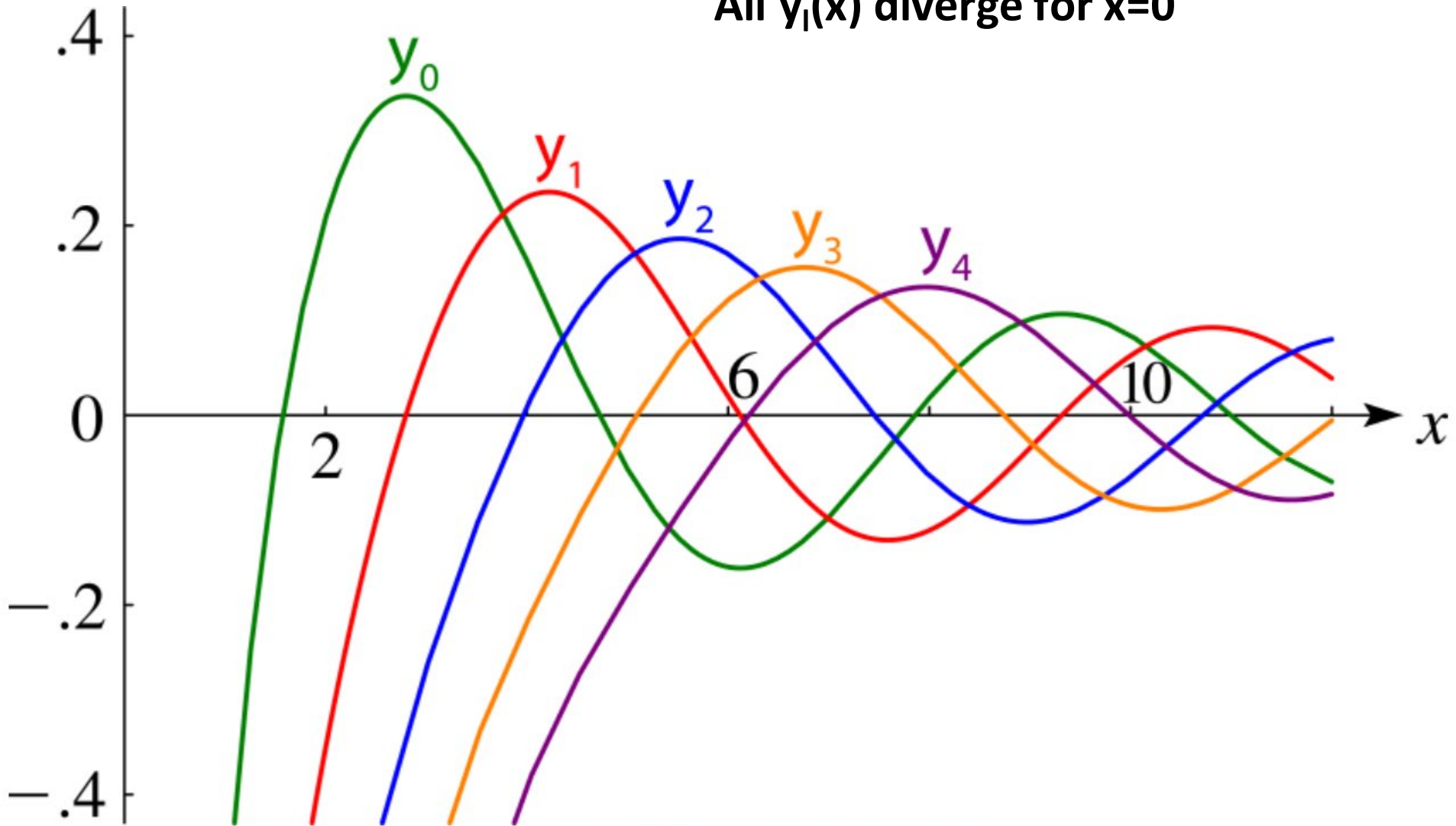


Figure 10.48.2:  $y_n(x)$ ,  $n = 0(1)4$ ,  $0 < x \leq 12$ .

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

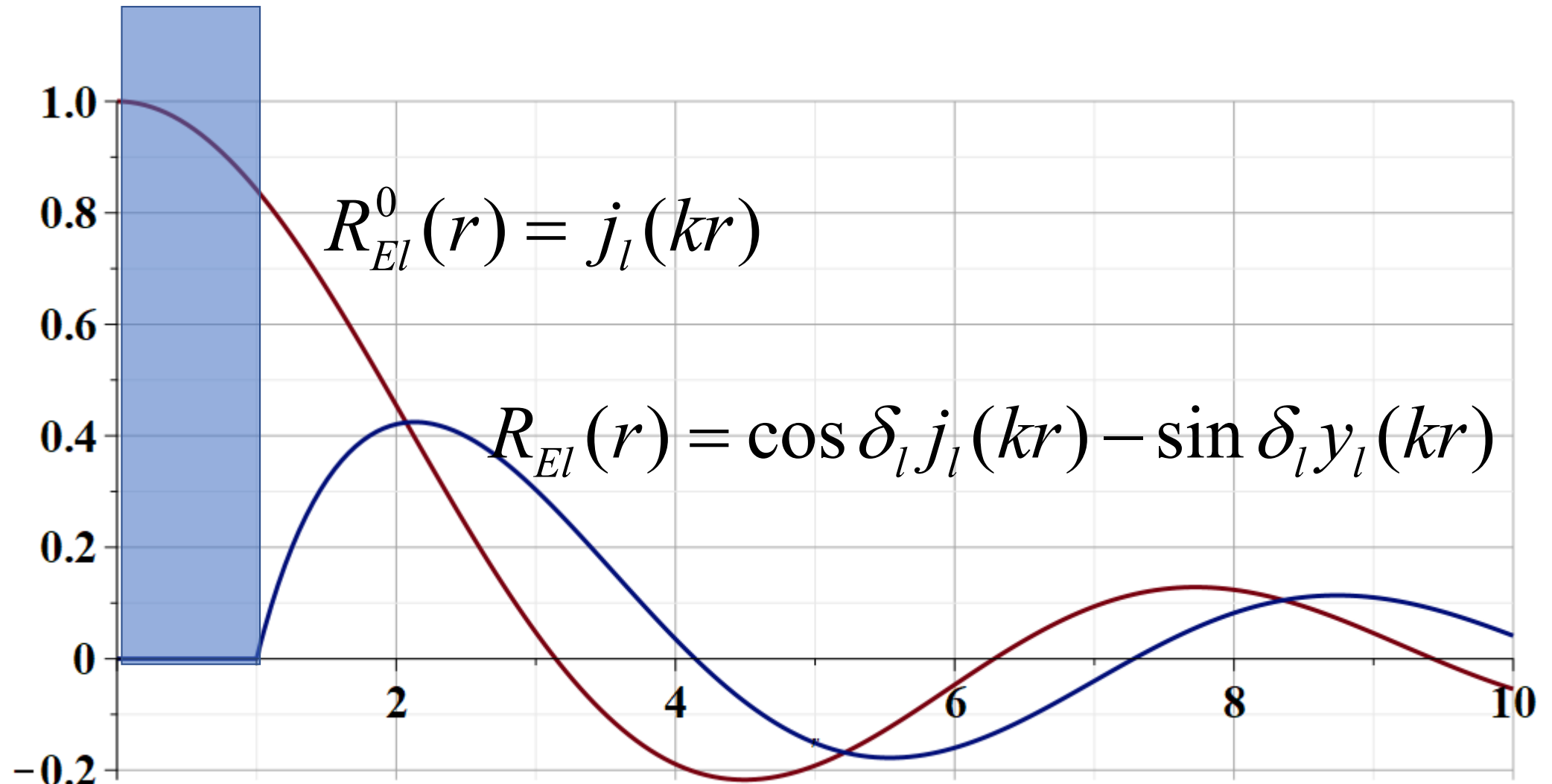
$$V(r) = \begin{cases} \infty & \text{for } r < D \\ 0 & \text{for } r \geq D \end{cases}$$

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

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

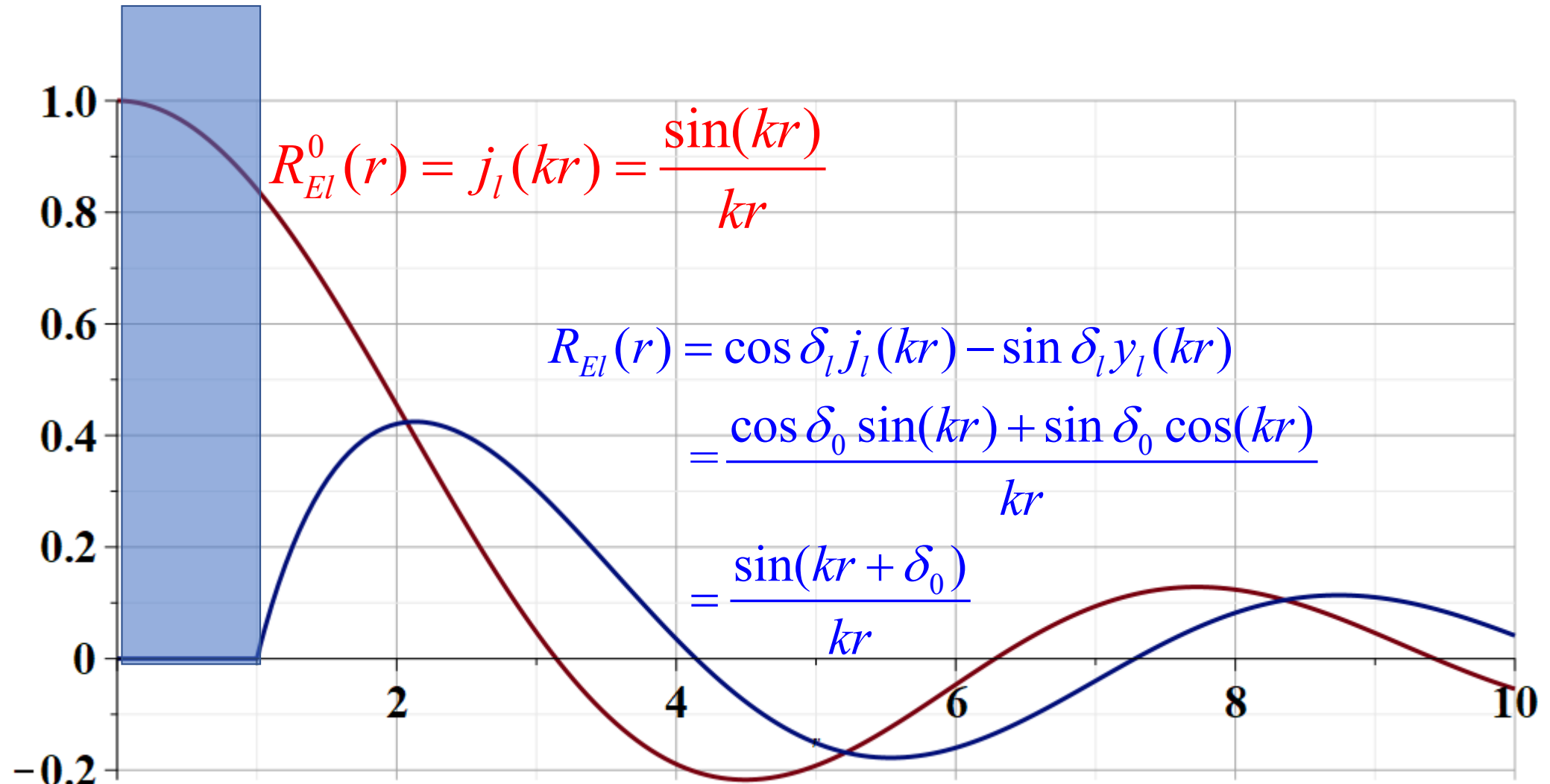
$$\text{where } \tan \delta_l = \frac{j_l(kD)}{y_l(kD)}$$

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



➔ Phase shift is a measure of scattering strength

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



For  $l > 0$ , the relationships are similar when  $kr \rightarrow \infty$

**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**