PHY 742 Quantum Mechanics II
1-1:50 AM MWF Olin 103

Plan for Lecture 5

1. **Continue reading Chapter 14 – Analysis of scattering phenomena**
   a. **Notion of scattering phase shifts**
   b. **Relationship of scattering phase shifts and differential and total scattering cross sections**
   c. **Examples**

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PHY 742 Quantum Mechanics II>

MWF 1-1:50 PM	OPL 103	http://www.wfu.edu/~natalie/s20phy742/

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Course schedule for Spring 2020

(Preliminary schedule -- subject to frequent adjustment.)

	Lecture date	Reading	Topic	HW	Due date
1	Mon: 01/13/2020	Chap. 9	Quantum mechanics of electromagnetic forces	#1	01/22/2020
2	Wed: 01/15/2020	Chap. 9	Quantum mechanics of particle in electrostatic field	#2	01/24/2020
3	Fri: 01/17/2020	Chap. 9	Quantum mechanics of particle in magnetostatic field	#3	01/27/2020
	Mon: 01/20/2020	No class	Martin Luther King Holiday		
4	Wed: 01/22/2020	Chap. 14	Scattering theory	#4	01/29/2020
5	Fri: 01/24/2020				
6	Mon: 01/27/2020				
7	Wed: 01/29/2020				

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Introduction to scattering theory for quantum particles -- Chap. 14 of textbook; also see Merzbacher's textbook

Geometry of ideal scattering measurement

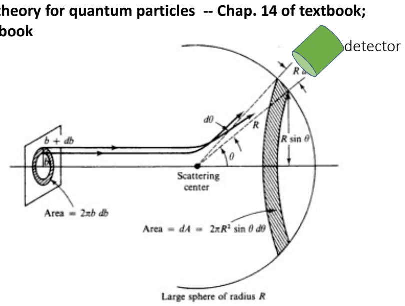

Figure 5.5 The scattering problem and relation of cross section to impact parameter.

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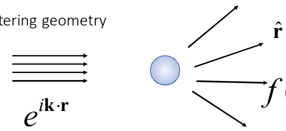
Representation of scattering in terms of probability amplitude

Scattering geometry



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

Incident plane wave with wavevector $\mathbf{k}$ and energy $E=\frac{\hbar^2k^2}{2m}$

Scattered spherical wave with scattering amplitude $f(\hat{\mathbf{k}},\hat{\mathbf{r}})$

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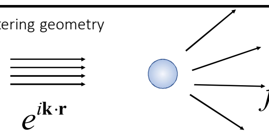
Scattering geometry



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

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

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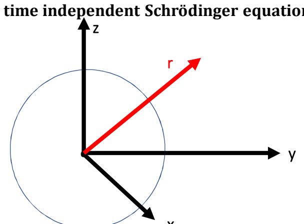
Representation of a free particle in quantum mechanics --

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 $0\le r\le D$

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

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

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

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

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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:

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

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

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

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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

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

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

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

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Some details:

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

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

Legendre polynomials $P_l(\cos\theta)$: $P_0(\cos\theta) = 1$

$P_1(\cos\theta) = \cos\theta$

$P_2(\cos\theta) = \frac{1}{2}(3\cos^2\theta - 1)$

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

$j_1(kr) = \frac{1}{3}kr - \frac{1}{30}(kr)^3 \ldots$

Legendre polynomials vs spherical harmonics --

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

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More details:

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

$$\Psi^0_E(\mathbf{r}) = e^{i\mathbf{k}\cdot\mathbf{r}} = 4\pi \sum_{lm} i^l j_l(kr) Y_{lm}{}^*(\hat{\mathbf{k}}) Y_{lm}(\hat{\mathbf{r}}) \quad \Rightarrow R^0_{El}(r) = 4\pi i^l j_l(kr) Y_{lm}{}^*(\hat{\mathbf{k}})$$

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

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

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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:

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

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More details:

For $r \to \infty$

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

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

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

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

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

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

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More details:

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

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

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

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

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

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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.

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

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

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

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

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

Different from classical case!

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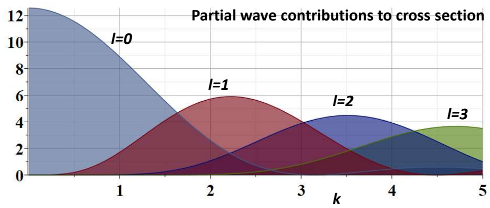
Example – scattering from an impenetrable spherical hard wall of radius *a*

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



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