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

Plan for Lecture 6

1. **Continue reading Chapter 14 – Analysis of scattering phenomena**
   a. **Summary of phase shift analysis and examples**
   b. **Approximate treatments of scattering – Born approximation**

1

PHY 742 Quantum Mechanics II>

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

Instructor: Natalie Holzwarth | **Phone:**758-5510 | **Office:**300 OPL | **e-mail:**natalie@wfu.edu

Course schedule for Spring 2020

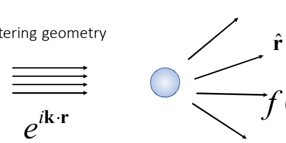
(Preliminary schedule -- subject to frequent adjustment.)

	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	Chap. 14	Scattering theory	#5	01/31/2020
6	Mon: 01/27/2020	Chap. 14	Scattering theory	#6	02/03/2020
7	Wed: 01/29/2020				
8	Fri: 01/31/2020				

2

Representation of scattering in terms of probability amplitude

Scattering geometry



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

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

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

3

Summary of analysis for spherical target in terms of scattering phase shifts:

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

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

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

4

Summary of analysis for spherical target in terms of scattering phase shifts -- continued:

How to determine phase shifts $\delta_l(E)$ for interaction potential $V(r)$:

Partial wave differential equation:

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

Spherical Bessel function

Spherical Neumann function

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

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

$$\tan\delta_l(E) = \frac{L_l(E) j_l(kD) - kj_l'(kD)}{L_l(E) y_l(kD) - ky_l'(kD)} \quad \text{where} \quad \frac{d\ln\left(R_{El}(r)\right)}{dr} = \left.\frac{\frac{dR_{El}(r)}{dr}}{R_{El}(r)}\right|_{r=D} \equiv L_l(E)$$

5

Slight simplification in functions --

Define slightly more convenient radial function: $R_{El}(r) \equiv \frac{P_{El}(r)}{r}$

Partial wave differential equation for $P_{El}(r)$:

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

Similarly, we can define the scaled spherical Bessel and Neumann functions:

$jj_l(x) = xj_l(x)$ and $yy_l(x) = xy_l(x)$

Continuity conditions at $r=D$: $P_{El}(D) = \mathcal{N}\left(\cos\delta_l jj_l(kD) - \sin\delta_l yy_l(kD)\right)$

$$\frac{dP_{El}(D)}{dr} = \mathcal{N}\left(\cos\delta_l \frac{djj_l(kD)}{dr} - \sin\delta_l \frac{dyy_l(kD)}{dr}\right)$$

$$\tan\delta_l(E) = \frac{LL_l(E) jj_l(kD) - kjj_l'(kD)}{LL_l(E) yy_l(kD) - kyy_l'(kD)} \quad \text{where} \quad \left.\frac{d\ln\left(P_{El}(r)\right)}{dr}\right|_{r=D} \equiv LL_l(E)$$

6

Slight simplification in functions – continued (Note: This notation is not standard.)

Scaled Bessel and Neumann functions:

$$jj_0(x) = \sin(x) \qquad yy_0(x) = -\cos(x)$$

$$jj_1(x) = \frac{\sin(x)}{x} - \cos(x) \qquad yy_1(x) = -\frac{\cos(x)}{x} - \sin(x)$$

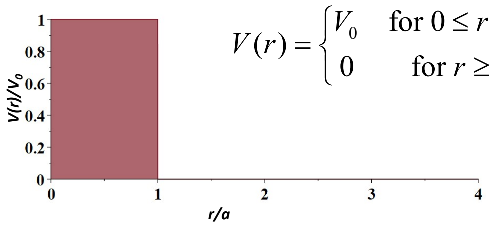
Similarly, we have scaled modified Bessel and Neumann functions

$$ii_0(x) = \sinh(x) \qquad kk_0(x) = \frac{\pi}{2}e^{-x}$$

$$ii_1(x) = -\frac{\sinh(x)}{x} + \cosh(x) \qquad kk_1(x) = \frac{\pi}{2}e^{-x}\left(\frac{1}{x}+1\right)$$

7

Example --



$$V(r) = \begin{cases} V_0 & \text{for } 0 \le r \le a \\ 0 & \text{for } r \ge a \end{cases}$$

For the case that $E < V_0$, define $\kappa = \sqrt{\frac{2m(V_0 - E)}{\hbar^2}}$ and $k = \sqrt{\frac{2mE}{\hbar^2}}$

8

Example -- continued

Partial wave differential equation for $P_{El}(r)$:

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

Focusing on the solution for $l = 0$: For $r \le a$:

$$\left(\frac{d^2}{dr^2} - \kappa^2\right)P_{E0}(r) = 0 \qquad \text{Physical solution: } P_{E0}(r) = \sinh(\kappa r)$$

where $\kappa = \sqrt{\frac{2m(V_0 - E)}{\hbar^2}}$ and $k = \sqrt{\frac{2mE}{\hbar^2}}$

$$LL_0(E) = \kappa\frac{\cosh \kappa a}{\sinh \kappa a} \equiv \frac{1}{\lambda_0} \qquad \tan\delta_0(E) = \frac{\sin(ka)/\lambda_0 - k\cos(ka)}{-\cos(ka)/\lambda_0 + k\sin(ka)}$$

9

Example -- continued

$$\tan\delta_0(E) = \frac{\sin(ka)/\lambda_0 - k\cos(ka)}{-\cos(ka)/\lambda_0 + k\sin(ka)} \qquad \lambda_0 = \frac{\sinh\kappa a}{\kappa\cosh\kappa a}$$

For $ka \ll 1$, $\tan\delta_0(E) \approx \delta_0(E) \approx k\frac{1-a/\lambda_0}{1/\lambda_0} = -k(a-\lambda_0)$

Note that for infinite potential well, $\lambda_0 \to 0$ as derived previously.

More generally, for $ka \ll 1$ $\quad \sigma \approx 4\pi(a-\lambda_0)^2$

Even more generally, this approach can be used to determine the exact cross section for this model from scattering amplitude:

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

1/27/2020 PHY 742 -- Lecture 6 10

10

Approximate treatment of scattering – Born approximation

In this treatment, we use the notions of perturbation theory

$$H = H^0 + H^1$$

$$H^0 = -\frac{\hbar^2}{2m}\nabla^2$$

$$H^1 = V(r)$$

In this case, the relevant eigenstates of H^0 are plane waves.

$$H^0\left|\Psi_E^0\right\rangle = E\left|\Psi_E^0\right\rangle \qquad \left|\Psi_E^0\right\rangle = e^{i\mathbf{k}\cdot\mathbf{r}} \quad \text{where } k = \sqrt{\frac{2mE}{\hbar^2}}$$

11/15/2017 PHY 741 Fall 2017 -- Lecture 31 11

11

Equation for first order wavefunction:

$$\left(H^0(\mathbf{r}) - E\right)\left|\Psi^1\right\rangle = -V(r)\left|\Psi^0\right\rangle$$

Note that for

$$\left(-\frac{\hbar^2}{2m}\nabla^2 - E\right)G(\mathbf{r},\mathbf{r}',E) = -\delta\left(\mathbf{r}-\mathbf{r}'\right)$$

$$G(\mathbf{r},\mathbf{r}',E) = -\frac{2m}{\hbar^2}\frac{e^{ik|\mathbf{r}-\mathbf{r}'|}}{4\pi|\mathbf{r}-\mathbf{r}'|}$$

$$\left|\Psi^1\right\rangle = -\int d^3r' G(\mathbf{r},\mathbf{r}',E)V(r')\Psi^0(\mathbf{r}')$$

$$\left|\Psi\right\rangle \approx e^{i\mathbf{k}\cdot\mathbf{r}} - \frac{2m}{4\pi\hbar^2}\int d^3r' \frac{e^{ik|\mathbf{r}-\mathbf{r}'|}}{|\mathbf{r}-\mathbf{r}'|}V(r')e^{i\mathbf{k}\cdot\mathbf{r}'}$$

11/15/2017 PHY 741 Fall 2017 -- Lecture 31 12

12

$$|\Psi\rangle \approx e^{i\mathbf{k}\cdot\mathbf{r}} - \frac{2m}{4\pi\hbar^2}\int d^3r' \frac{e^{ik|\mathbf{r}-\mathbf{r}'|}}{|\mathbf{r}-\mathbf{r}'|} V(r')e^{i\mathbf{k}\cdot\mathbf{r}'}$$

For $r \gg r'$, $|\mathbf{r}-\mathbf{r}'| \approx r - \mathbf{r}'\cdot\hat{\mathbf{r}}$

$$|\Psi\rangle \approx e^{i\mathbf{k}\cdot\mathbf{r}} - \frac{2m}{4\pi\hbar^2}\frac{e^{ikr}}{r}\int d^3r' e^{-ik\hat{\mathbf{r}}\cdot\mathbf{r}'} V(r')e^{i\mathbf{k}\cdot\mathbf{r}'}$$

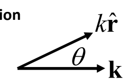
$$\approx e^{i\mathbf{k}\cdot\mathbf{r}} - \frac{2m}{4\pi\hbar^2}\frac{e^{ikr}}{r}\int d^3r' e^{i(\mathbf{k}-k\hat{\mathbf{r}})\cdot\mathbf{r}'} V(r')$$

Scattering amplitude in the Born approximation:

$$f(\hat{\mathbf{k}},\hat{\mathbf{r}}) = -\frac{2m}{4\pi\hbar^2}\int d^3r' e^{i(\mathbf{k}-k\hat{\mathbf{r}})\cdot\mathbf{r}'} V(r')$$

13

Example – screened Coulomb interaction



$$V(r) = -\frac{Ze^2}{r}e^{-\gamma r}$$

$$f(\hat{\mathbf{k}},\hat{\mathbf{r}}) = -\frac{2m}{4\pi\hbar^2}\int d^3r' e^{i(\mathbf{k}-k\hat{\mathbf{r}})\cdot\mathbf{r}'} V(r')$$

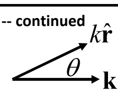
$$= \frac{2m}{\hbar^2}\frac{Ze^2}{K}\int_0^\infty dr'\ e^{-\gamma r'}\sin(Kr')$$

$$= \frac{2m}{\hbar^2}\frac{Ze^2}{\left(K^2+\gamma^2\right)}$$

where $K = |\mathbf{k} - k\hat{\mathbf{r}}| = 2k\sin(\theta/2)$

14

Example – screened Coulomb interaction -- continued



$K = |\mathbf{k} - k\hat{\mathbf{r}}| = 2k\sin(\theta/2)$

$$V(r) = -\frac{Ze^2}{r}e^{-\gamma r}$$

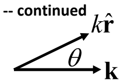
$$f(\hat{\mathbf{k}},\hat{\mathbf{r}}) = \frac{2m}{\hbar^2}\frac{Ze^2}{\left(K^2+\gamma^2\right)}$$

Differential cross section:

$$\frac{d\sigma}{d\Omega} = \left|f(\hat{\mathbf{k}},\hat{\mathbf{r}})\right|^2 = \left(\frac{2mZe^2}{\hbar^2}\right)^2 \left|\frac{1}{\left(K^2+\gamma^2\right)}\right|^2$$

15

Example – screened Coulomb interaction -- continued



$$V(r) = -\frac{Ze^2}{r}e^{-\gamma r}$$

$$K = |\mathbf{k} - k\hat{\mathbf{r}}| = 2k\sin(\theta/2)$$

Differential cross section:

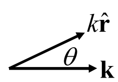
$$\frac{d\sigma}{d\Omega} = \left|f(\hat{\mathbf{k}},\hat{\mathbf{r}})\right|^2 = \left(\frac{2mZe^2}{\hbar^2}\right)^2 \left|\frac{1}{\left(K^2+\gamma^2\right)}\right|^2$$

Note that for $\gamma \to 0$:

$$\frac{d\sigma}{d\Omega} = \left|f(\hat{\mathbf{k}},\hat{\mathbf{r}})\right|^2 = \left(\frac{2mZe^2}{\hbar^2}\right)^2 \frac{1}{K^4} = \left(\frac{Ze^2}{4E}\right)^2 \frac{1}{\sin^4\left(\frac{\theta}{2}\right)}$$

16

Example – spherical well



$$V(r) = \begin{cases} V_0 & \text{for } r < a \\ 0 & \text{for } r > a \end{cases}$$

$$f(\hat{\mathbf{k}},\hat{\mathbf{r}}) = -\frac{2m}{4\pi\hbar^2}\int d^3r' e^{i(\mathbf{k}-k\hat{\mathbf{r}})\cdot\mathbf{r}'}V(r')$$

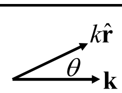
$$= -\frac{2m}{4\pi\hbar^2}\frac{4\pi V_0}{K}\int_0^a dr'\; r'\sin(Kr')$$

$$= -\frac{2m}{\hbar^2}\frac{V_0}{K^3}\left(\sin(Ka) - Ka\cos(Ka)\right)$$

where $K = |\mathbf{k} - k\hat{\mathbf{r}}| = 2k\sin(\theta/2)$

17

Example – spherical well – continued



$$V(r) = \begin{cases} V_0 & \text{for } r < a \\ 0 & \text{for } r > a \end{cases}$$

$$K = |\mathbf{k} - k\hat{\mathbf{r}}| = 2k\sin(\theta/2)$$

$$f(\hat{\mathbf{k}},\hat{\mathbf{r}}) = -\frac{2m}{\hbar^2}\frac{V_0}{K^3}\left(\sin(Ka) - Ka\cos(Ka)\right)$$

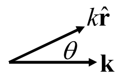
Differential cross section:

$$\frac{d\sigma}{d\Omega} = \left|f(\hat{\mathbf{k}},\hat{\mathbf{r}})\right|^2 = \left(\frac{2mV_0}{\hbar^2}\right)^2 \frac{1}{K^6}\left|\sin(Ka) - Ka\cos(Ka)\right|^2$$

Total cross section: $\sigma = \int \frac{d\sigma}{d\Omega}d\Omega = \frac{2\pi}{k^2}\int_0^{2k}\frac{d\sigma}{d\Omega}KdK$

18

Example – spherical well – continued
(Ref. Landau and Lifshitz)



$$V(r)=\begin{cases} V_0 & \text{for } r<a \\ 0 & \text{for } r>a \end{cases}$$

$$K=|\mathbf{k}-k\hat{\mathbf{r}}|=2k\sin(\theta/2)$$

$$f(\hat{\mathbf{k}},\hat{\mathbf{r}})=-\frac{2m}{\hbar^2}\frac{V_0}{K^3}\left(\sin(Ka)-Ka\cos(Ka)\right)$$

Total cross section: $\sigma=\int\frac{d\sigma}{d\Omega}d\Omega=\frac{2\pi}{k^2}\int_0^{2k}\frac{d\sigma}{d\Omega}KdK$

When the dust clears: $\sigma=\frac{2\pi}{4k^2}\left(\frac{2mV_0a^2}{\hbar^2}\right)^2\left(1-\frac{1}{(2ka)^2}+\frac{\sin(4ka)}{(2ka)^3}-\frac{\sin^2(2ka)}{(2ka)^4}\right)$

For $ka\ll 1$ $\quad\sigma\approx\frac{4\pi a^2}{9}\left(\frac{2mV_0a^2}{\hbar^2}\right)^2$ $\qquad ka\gg 1$ $\quad\sigma\approx\frac{\pi}{2k^2}\left(\frac{2mV_0a^2}{\hbar^2}\right)^2$

(Not generally consistent with phase shift analysis.)

11/15/2017 PHY 741 Fall 2017 -- Lecture 31 19

19

Beyond the Born approximation

Equation for full wavefunction:

$$\left(H^0(\mathbf{r})-E\right)|\Psi\rangle=-V(r)|\Psi\rangle$$

$$\left(-\frac{\hbar^2}{2m}\nabla^2-E\right)G(\mathbf{r},\mathbf{r}',E)=-\delta(\mathbf{r}-\mathbf{r}') \qquad G(\mathbf{r},\mathbf{r}',E)=-\frac{2m}{\hbar^2}\frac{e^{ik|\mathbf{r}-\mathbf{r}'|}}{4\pi|\mathbf{r}-\mathbf{r}'|}$$

$$|\Psi\rangle=\int d^3r'G(\mathbf{r},\mathbf{r}',E)V(r')\Psi(\mathbf{r}')$$

$$|\Psi\rangle\approx|\Psi^0\rangle+\int d^3r'G(\mathbf{r},\mathbf{r}',E)V(r')\Psi^0(\mathbf{r}')$$
$$+\int d^3r''G(\mathbf{r},\mathbf{r}'',E)V(r'')\Psi^0(\mathbf{r}'')\int d^3r'G(\mathbf{r}'',\mathbf{r}',E)V(r')\Psi^0(\mathbf{r}')$$
$$+\ldots$$

11/15/2017 PHY 741 Fall 2017 -- Lecture 31 20

20