PHY 741 Quantum Mechanics
12-12:50 AM MWF Olin 103

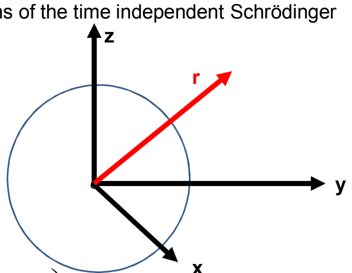
Plan for Lecture 30:

Chap. 19 in Shankar: Scattering theory

1. **Partial wave solutions of the Schrödinger equation**
2. **Scattering phase shifts**
3. **Scattering cross section**

23	Wed, 10/25/2017	Chap. 15	Multi-electron atoms	#14	10/30/2017
24	Fri, 10/27/2017		Effects of nuclear motion		
25	Mon, 10/30/2017	Chap. 17	Time-independent perturbation theory	#15	11/3/2017
26	Wed, 11/01/2017	Chap. 17	Time-independent perturbation theory		
27	Fri, 11/03/2017		Effects of a static magnetic field		
28	Mon, 11/06/2017	Chap. 18	Time-dependent perturbation theory	#16	11/10/2017
29	Wed, 11/08/2017	Chap. 18	Time-dependent perturbation theory		
30	Fri, 11/10/2017	Chap. 19	Scattering theory	#17	11/15/2017
31	Mon, 11/13/2017				
32	Wed, 11/15/2017				
33	Fri, 11/17/2017				
34	Mon, 11/20/2017				
	Wed, 11/22/2017		*Thanksgiving Holiday -- No class*		
	Fri, 11/24/2017		*Thanksgiving Holiday -- No class*		
35	Mon, 11/27/2017				
36	Wed, 11/29/2017				
37	Fri, 12/01/2017				
38	Mon, 12/04/2017		Review	Prepare presentations	

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

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

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

Free partical partial waves -- continued

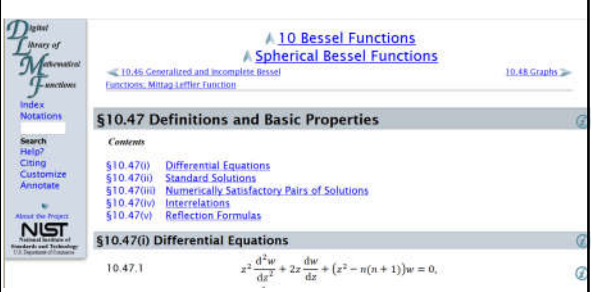
$$\left(\frac{d^2}{dr^2} + \frac{2}{r}\frac{d}{dr} - \frac{l(l+1)}{r^2} + \frac{2mE}{\hbar^2} \right) R^0_{El}(r) = 0 \qquad \text{for } E > 0$$

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

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

Properties of spherical Bessel functions

http://dlmf.nist.gov/10.47



Spherical Bessel functions of order *n*

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

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

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

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

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

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

Forms of spherical Bessel and Hankel functions:

$$j_0(x) = \frac{\sin(x)}{x} \qquad h_0(x) = \frac{e^{ix}}{ix}$$

$$j_1(x) = \frac{\sin(x)}{x^2} - \frac{\cos(x)}{x} \qquad h_1(x) = -\left(1+\frac{i}{x}\right)\frac{e^{ix}}{x}$$

$$j_2(x) = \left(\frac{3}{x^3} - \frac{1}{x}\right)\sin(x) - \frac{3\cos(x)}{x^2} \qquad h_2(x) = i\left(1+\frac{3i}{x} - \frac{3}{x^2}\right)\frac{e^{ix}}{x}$$

Assymptotic behavior :

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

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

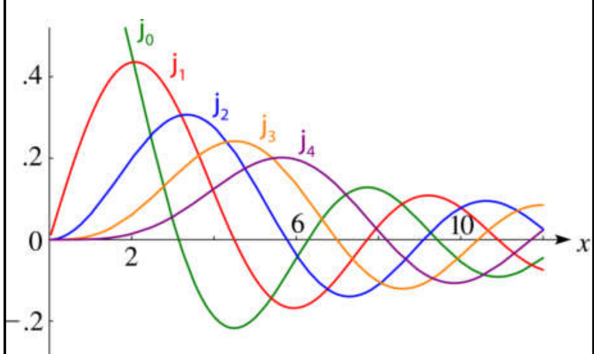


Figure 10.48.1: $j_n(x)$, $n = 0(1)4$, $0 \le x \le 12$.

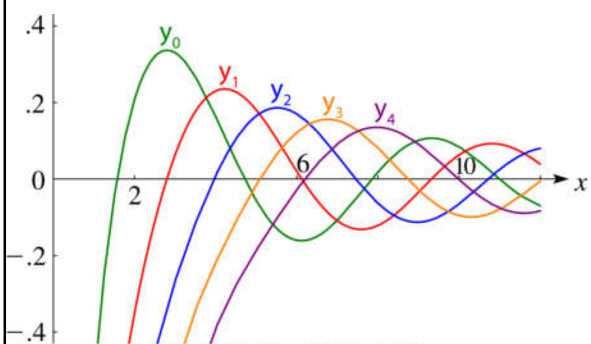


Figure 10.48.2: $y_n(x)$, $n = 0(1)4$, $0 < x \leq 12$.

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

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

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 $r = D$:

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

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

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:

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

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

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

Determination of the phase shifts:

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

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

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

In this case, $R_{El}(r) = \begin{cases} 0 & \text{for } r < D \\ \mathcal{N}\left(y_l(kD) j_l(kr) - j_l(kD) y(kr) \right) & \text{for } r > D \end{cases}$

$L_l(E) = \infty \qquad \Rightarrow \tan\,\delta_l(E) = \dfrac{j_l(kD)}{y_l(kD)}$

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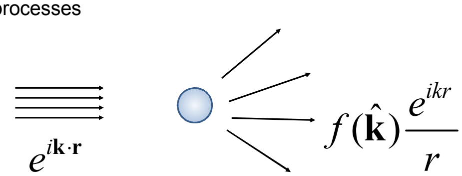
$L_l(E) = \infty \qquad \Rightarrow \tan\,\delta_l(E) = \dfrac{j_l(kD)}{y_l(kD)}$

For $l = 0$: $\quad j_0(kr) = \dfrac{\sin(kr)}{kr} \qquad y_0(kr) = -\dfrac{\cos(kr)}{kr}$

$\Rightarrow \delta_0(E) = kD$

$R_{E0}(r) = \mathcal{N}\dfrac{\sin(k(r-D))}{kr}$

More general relationship of phase shifts to scattering processes



It can be shown that:

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

General wavefunction for describing wavefunction in spherical potential:

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

Outside range of potential:

$$\Psi_E(\mathbf{r}) = \sum_{lm}\Big(A_l j_l(kr) + B_l\big(\cos(\delta_l(E))\, j_l(kr) - \sin(\delta_l(E))\, y_l(kr)\big)\Big) Y_{lm}(\hat{\mathbf{r}})$$

Far from potential:

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

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

$$\Psi_E(\mathbf{r}) \approx \sum_{lm}\left(A_l \frac{\sin(kr - l\frac{\pi}{2})}{kr} + B_l \frac{\sin(kr - l\frac{\pi}{2} + \delta_l(E))}{kr}\right) Y_{lm}(\hat{\mathbf{r}})$$

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

Choose $\quad A_l = 2\pi i^l Y^*_{lm}(\hat{\mathbf{k}}) \qquad B_l = A_l e^{i\delta_l(E)}$

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

Differential scattering cross section

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

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

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

Example -- hard sphere scattering

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

Evaluation in the limit that $E \approx 0$

$$j_l(kD) \approx \frac{(kD)^l}{(2l+1)!!} \qquad y_l(kD) \approx -\frac{(2l-1)!!}{(kD)^{l+1}}$$

$$\tan\,\delta_l(E) \approx -\frac{(kD)^{2l+1}}{\big((2l+1)!!\big)\big((2l-1)!!\big)} \approx -kD\delta_{0l}$$

Hard sphere (radius *D*) scattering -- continued

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

In the low energy limit:

$$\frac{d\sigma}{d\Omega} \approx \left(\frac{4\pi}{k}\right)^2 (kD)^2 \left(\frac{1}{4\pi}\right)^2 = D^2$$

Total cross section for this case:

$$\sigma = \int d\Omega \frac{d\sigma}{d\Omega} = 4\pi D^2$$

Recall that in classical treatment

$$\left.\frac{d\sigma}{d\Omega}\right|_{\text{classical}} = \frac{D^2}{4} \qquad \sigma_{\text{classical}} = \pi D^2$$