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

Plan for Lecture 4

1. **Summary of Chapter 9 – Quantum particle interacting with classical electromagnetic fields**
2. **Begin reading Chapter 14 – Analysis of scattering phenomena**
   a. **Partial wave expansion of probability amplitude**
   b. **Formulation of differential cross section in terms of scattering phase shifts**

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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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Summary of results for the quantum mechanical treatment of interaction of particle of mass *m* and charge *q* with classical electromagnetic fields in terms of scalar and vector potentials *U*(r,*t*) and A(r,*t*):

Time dependent Schrödinger equation:

$$i\hbar\frac{\partial\Psi(\mathbf{r},t)}{\partial t} = H(\mathbf{r},t)\Psi(\mathbf{r},t)$$

$$H(\mathbf{r},t)=\frac{1}{2m}\left(-i\hbar\nabla - q\mathbf{A}(\mathbf{r},t)\right)^2 + V(\mathbf{r}) + qU(\mathbf{r},t)$$

Results for a different "gauge":

$$\mathbf{A}'(\mathbf{r},t)=\mathbf{A}(\mathbf{r},t)+\nabla\chi(\mathbf{r},t) \quad U'(\mathbf{r},t)=U(\mathbf{r},t)-\frac{\partial\chi(\mathbf{r},t)}{\partial t} \quad \text{where } \nabla^2\chi(\mathbf{r},t)-\frac{1}{c^2}\frac{\partial^2\chi(\mathbf{r},t)}{\partial t^2}=0$$

Schrödinger equation for gauge transformed Hamiltonian: $i\hbar\frac{\partial\Psi'(\mathbf{r},t)}{\partial t} = H'(\mathbf{r},t)\Psi'(\mathbf{r},t)$

$\Rightarrow$ It can be shown that: $\Psi'(\mathbf{r},t)=\Psi(\mathbf{r},t)e^{iq\chi(\mathbf{r},t)/\hbar}$

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Summary – continued -- Effects of the electromagnetic field on the particle current operator.

As shown in Chapter 2, we still expect that the particle charge density ρ and current density $\mathbf{j}$, to satisfy the continuity equation: $\frac{\partial \rho}{\partial t} + \nabla \cdot \mathbf{j} = 0$

Particle charge density: $\rho(\mathbf{r},t) = q|\Psi(\mathbf{r},t)|^2$

Particle current density $\mathbf{j}$:

$$\mathbf{j}(\mathbf{r},t) = \frac{qi\hbar}{2m}\left(\Psi(\mathbf{r},t)\nabla\Psi^*(\mathbf{r},t) - \Psi^*(\mathbf{r},t)\nabla\Psi(\mathbf{r},t)\right) - \frac{q^2}{m}\mathbf{A}(\mathbf{r},t)|\Psi(\mathbf{r},t)|^2$$

Note that with this form of the current density, the continuity equation is consistent with the Schrödinger Eq: $i\hbar\frac{\partial \Psi(\mathbf{r},t)}{\partial t} = H(\mathbf{r},t)\Psi(\mathbf{r},t)$

where $H(\mathbf{r},t) = \frac{1}{2m}\left(-i\hbar\nabla - q\mathbf{A}(\mathbf{r},t)\right)^2 + V(\mathbf{r}) + qU(\mathbf{r},t)$

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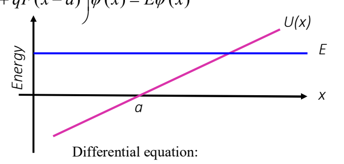
Example – A(r,*t*)=0 and *U*(r,*t*)=*F*(*x*-*a*)

Assume: $\Psi(x,t) = \psi(x)e^{-iEt/\hbar}$

$$\left(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + qF(x-a)\right)\psi(x) = E\psi(x)$$



Differential equation:

$$\left(\frac{d^2}{dx^2} - \frac{2mqF}{\hbar^2}(x-b)\right)\psi(x) = 0 \quad \text{where } b \equiv a + \frac{E}{qF}$$

$$\left(\frac{d^2}{du^2} - \alpha u\right)\psi(u) = 0 \quad \text{where } u \equiv x - b \quad \alpha \equiv \frac{2mqF}{\hbar^2}$$

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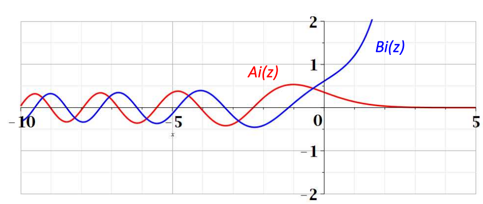
Airy functions --

$$\frac{d^2 w}{dz^2} = zw$$



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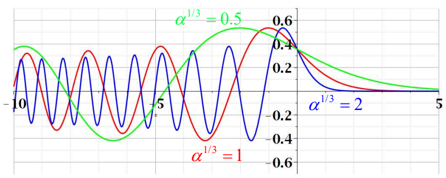
Summary of results

Differential equation:

$$\left(\frac{d^2}{dx^2} - \frac{2mqF}{\hbar^2}(x-b)\right)\psi(x) = 0 \qquad \text{where } b \equiv a + \frac{E}{qF}$$

$$\left(\frac{d^2}{du^2} - \alpha u\right)\psi(u) = 0 \qquad \text{where } u \equiv x - b \qquad \alpha \equiv \frac{2mqF}{\hbar^2}$$

$$\psi(u) = \mathcal{N} Ai(\alpha^{1/3} u)$$



Note that in this case, physical solutions exist for all energies *E*; the wavefunction oscillates for *x<a+E/qF* and decays for *x>a+E/qF* .

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Example – Particle in a magnetostatic field

Assume particle has charge q and mass m; $V(\mathbf{r}) = 0$ and $U(\mathbf{r}) = 0$

$$H = \frac{1}{2m}\left(-i\nabla - q\mathbf{A}(\mathbf{r})\right)^2$$

For a constant and uniform magnetic field $B_0\hat{\mathbf{z}}$

can choose $\mathbf{A}(\mathbf{r}) = -B_0 y\hat{\mathbf{x}}$

$$H = \frac{1}{2m}\left(-i\hbar\frac{\partial}{\partial x} + qB_0 y\right)^2 + \frac{-\hbar^2}{2m}\left(\frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}\right)$$

$$\Psi(x,y,z,t) = e^{i(p_x x + p_z z - Et)/\hbar}\psi(y)$$

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$$H = \frac{1}{2m}\left(-i\hbar\frac{\partial}{\partial x} + qB_0 y\right)^2 + \frac{-\hbar^2}{2m}\left(\frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}\right)$$

$$H\Psi = e^{i(p_x x + p_z z - Et)/\hbar}\left(-\frac{\hbar^2}{2m}\frac{d^2\psi(y)}{dy^2} + \left(\frac{1}{2}m\omega_c^2(y-y_0)^2 + \frac{p_z^2}{2m}\right)\psi(y)\right) = E\Psi$$

Differential equation for $\psi(y)$:

$$-\frac{\hbar^2}{2m}\frac{d^2\psi(y)}{dy^2} + \frac{1}{2}m\omega_c^2(y-y_0)^2\psi(y) = \left(E - \frac{p_z^2}{2m}\right)\psi(y)$$

$$\text{where } \omega_c \equiv \frac{qB_0}{m} \qquad y_0 = -\frac{p_x}{qB_0}$$

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Energy eigenvalues:

$$E_n(p_z) = \hbar\omega_c\left(n+\frac{1}{2}\right)+\frac{p_z^2}{2m} \qquad \text{where } \omega_c \equiv \frac{qB_0}{m}$$

Eigenfunctions

Hermite polynomial

$$\psi_n(y) = \mathcal{N} e^{-(y-y_0)^2/(2\alpha^2)} H_n((y-y_0)/\alpha)$$

$$\text{where } \alpha \equiv \sqrt{\frac{\hbar}{qB_0}} = \sqrt{\frac{\hbar}{m\omega_c}} \qquad y_0 = -\frac{p_x}{qB_0}$$

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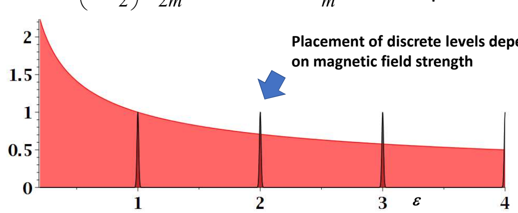
DOS plot for magnetostatic acting on charged particle

Note that this is an approximate model of an ideal metal in a magnetic field which results in oscillatory resistivity for example.

Energy eigenvalues:

$$E_n(p_z) = \hbar\omega_c\left(n+\frac{1}{2}\right)+\frac{p_z^2}{2m} \qquad \text{where } \omega_c \equiv \frac{qB_0}{m}$$

Placement of discrete levels depends on magnetic field strength



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Effects of magnetostatic fields on particles' intrinsic magnetic moment.

If a particle has an intrinsic magnetic moment $\mathbf{m}$, its interaction potential with a magnetostatic field is $-\mathbf{m}\cdot\mathbf{B}$. For an electron, $\mathbf{m} = -g\mu_B\mathbf{S}/\hbar$ where $\mathbf{S}$ the spin angular momentum operator of the electron with eigenvalues $\pm\frac{1}{2}\hbar$, $\mu_B = \frac{e\hbar}{2m_e}$, and $|g| = 2.00231930436256$. This adds an interaction to the Hamiltonian $\Delta H_{spin} = g\mu_B\mathbf{B}\cdot\mathbf{S}/\hbar$. This formalism is appropriate for all particles with intrinsic spin, each with its own gyromagnetic ratio. For example, there is also an interaction of the magnetic field with a proton, with a smaller factor by 10^{-3}.

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Interaction of magnetostatic field B with a hydrogen atom (including contribution of intrinsic electron spin, omitting contribution of intrinsic proton spin).

Isolated H atom: $H^0 = \frac{\mathbf{p}^2}{2m} + V(r)$

H atom in magnetic field **B** and vector potential $\mathbf{A} = -\frac{1}{2}\mathbf{r}\times\mathbf{B}$

$$H = \frac{(\mathbf{p}+e\mathbf{A})^2}{2m} + V(r) + g\mu_B \mathbf{S}\cdot\mathbf{B}/\hbar = H^0 + H^1 + H^2$$

Terms of linear order in **A**:

$$\frac{e}{2m}(\mathbf{p}\cdot\mathbf{A}+\mathbf{A}\cdot\mathbf{p}) = -\frac{e}{4m}\left(\mathbf{p}\cdot(\mathbf{r}\times\mathbf{B})+(\mathbf{r}\times\mathbf{B})\cdot\mathbf{p}\right) = \frac{e}{2m}(\mathbf{r}\times\mathbf{p})\cdot\mathbf{B} = \frac{e}{2m}\mathbf{L}\cdot\mathbf{B}$$

$$H^1 = \mu_B(\mathbf{L}+g\mathbf{S})\cdot\mathbf{B}/\hbar$$

$$\mu_B = \frac{e\hbar}{2m} \qquad |g| = 2.00231930436256$$

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Analysis of magnetostatic effects on atomic structure using perturbation theory, also including the effects of spin-orbit interation

$$H = \frac{(\mathbf{p}+e\mathbf{A})^2}{2m} + V(r) + G(r)\mathbf{S}\cdot\mathbf{L} + g\mu_B\mathbf{B}\cdot\mathbf{S}/\hbar$$

$$H^0 = \frac{\mathbf{p}^2}{2m} + V(r)$$

Keeping terms of linear order in **B** and spin-orbit interation :

$$\mathbf{J} = \mathbf{L} + \mathbf{S}$$

$$H^1 = G(r)\mathbf{S}\cdot\mathbf{L} + \mu_B(\mathbf{L}+g\mathbf{S})\cdot\mathbf{B}/\hbar$$

$$= \frac{G(r)}{2}\left(\mathbf{J}^2-\mathbf{L}^2-\mathbf{S}^2\right) + \mu_B\left(\mathbf{J}+(g-1)\mathbf{S}\right)\cdot\mathbf{B}/\hbar$$

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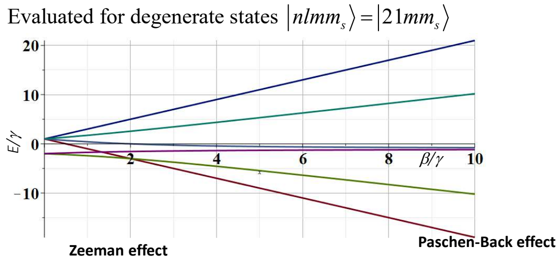
First order perturbation theory analysis for *n*=2 levels of H atom

$$H^1 = G(r)\mathbf{S}\cdot\mathbf{L} + \mu_B(\mathbf{L}+g\mathbf{S})\cdot\mathbf{B}/\hbar$$

Evaluated for degenerate states $|nlmm_s\rangle = |21mm_s\rangle$



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Aharonov-Bohm effect – an interference phenomenon concerning a particle interacting with a vector potential

Reference: End of Chap. 9 in Professor Carlson's text
Online sources -- http://mafija.fmf.uni-lj.si/seminar/files/2010_2011/seminar_aharonov.pdf

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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

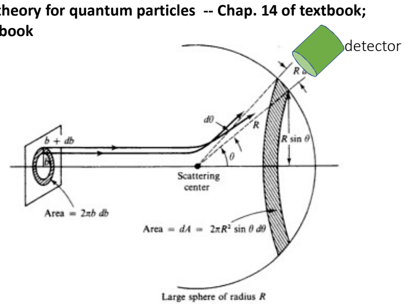

Figure 5.5 The scattering problem and relation of cross section to impact parameter.

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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:

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

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.

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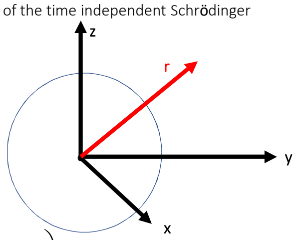
Representation of a free particle in quantum mechanics --

Continuum solutions of the time independent Schrödinger equation.



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

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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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Free particle partial waves -- continued

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

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

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

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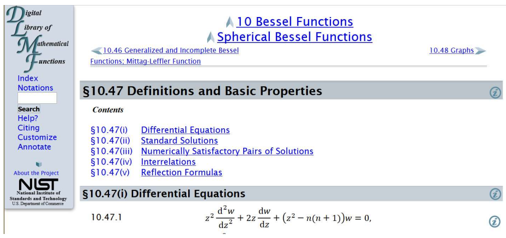
Properties of spherical Bessel functions

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
10.48 Graphs

§10.47 Definitions and Basic Properties

Contents

§10.47(i) Differential Equations
§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 $$z^2\frac{d^2w}{dz^2}+2z\frac{dw}{dz}+\left(z^2-n(n+1)\right)w=0,$$

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Spherical Bessel functions of order *n*

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

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

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

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

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

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

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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:

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

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

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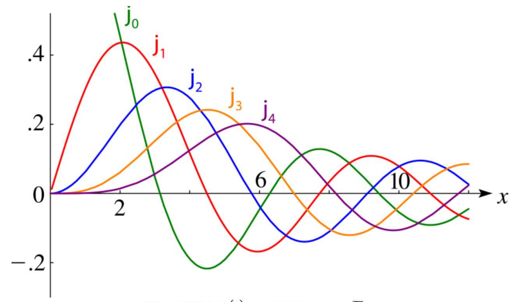

Figure 10.48.1: $j_n(x)$, $n = 0(1)4$, $0 \le x \le 12$.

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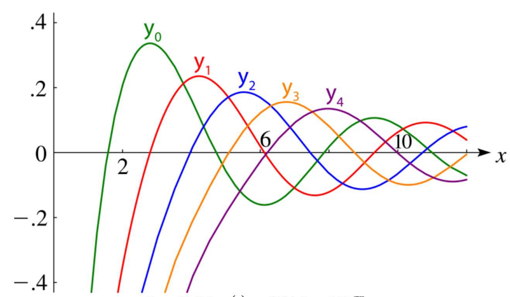

Figure 10.48.2: $y_n(x)$, $n = 0(1)4$, $0 < x \le 12$.

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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 $r = D$:

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

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

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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:

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

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

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

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What we will show next time, 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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