PHY 742 Quantum Mechanics II
12-12:50 PM MWF Olin 103

Notes for Lecture 34

Review

- Overview
- Examples

27	Fri: 04/08/2022		Multi electron atoms	#21	04/11/2022
28	Mon: 04/11/2022		Multi electron atoms	#22	04/18/2022
29	Wed: 04/13/2022		Multi electron atoms		
	Fri: 04/15/2022	*No class*	Holiday		
30	Mon: 04/18/2022		Hubbard model with multiple electrons	#23	04/22/2022
31	Wed: 04/20/2022		Hubbard model with multiple electrons		
32	Fri: 04/22/2022		BCS model of superconductivity		
33	Mon: 04/25/2022		BCS model of superconductivity		
34	Wed: 04/27/2022		Review		
35	Fri: 04/29/2022		Review		

Main topics, covering Chapters 12-18 + of Professor E. Carlson's textbook

- **Approximation methods for Quantum Mechanical problems; time-dependent and time independent**
- **Quantum mechanical scattering theory**
- **Dirac equation**
- **Quantization of the electromagnetic field**
- **Treatment of multiparticle systems**
- **Special cases**

Example solution --

HW #7 for PHY 742

PHY 742 -- Assignment #7

January 28, 2022

Continue reading Chapter 14 in **Carlson's** textbook.

1. Consider the function e^{ix} , where x is a positive quantity.
   a. Write the function as an expansion in terms of spherical bessel functions.
   b. Using Maple or Mathematica or other software, plot the real and imaginary parts of the function as a function for x in the range of 0 and 5, both for the function itself and a finite number of expansion terms.
   c. Comment on the accuracy of the expansion.

From Lecture #8 --

From Lecture 8 --

Some details: Note that this is also covered in Jackson in Sec. 10.3

It can be shown that: $e^{i\mathbf{k}\cdot\mathbf{r}} = \sum_l i^l (2l+1) j_l(kr) P_l(\hat{\mathbf{k}}\cdot\hat{\mathbf{r}}) = 4\pi \sum_{lm} i^l j_l(kr) Y_{lm}^*(\hat{\mathbf{k}}) Y_{lm}(\hat{\mathbf{r}})$

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

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

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

Note that by design:

$P_l(1) = 1$

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 --

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

This means for our problem --

exp(ix)=sum_l (i^l * (2l+1) * j_l(x))

Real(exp(ix))=j_0(x)-5*j_2(x)+9*j_4(x)-13*j_6(x)......

Imag(exp(ix))=3*j_1(x)-7*j_3(x)+11*j_5(x)-15*j_7(x)......

$$> \; jj := (l, x) \rightarrow \left(\frac{\mathrm{Pi}}{2\,x}\right)^{\frac{1}{2}} \cdot \mathrm{BesselJ}\left(l + \frac{1}{2}, x\right);$$

$$jj := (l, x) \mapsto \frac{\sqrt{2} \cdot \sqrt{\frac{\pi}{x}} \cdot \mathrm{BesselJ}\left(l + \frac{1}{2}, x\right)}{2}$$

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> plot( {cos(x), jj(0, x) - 5·jj(2, x) + 9·jj(4, x) - 13· jj(6, x) }, x = 0.001 ..10, thickness = 3, gridlines, font = [ariel,
    bold, 24])
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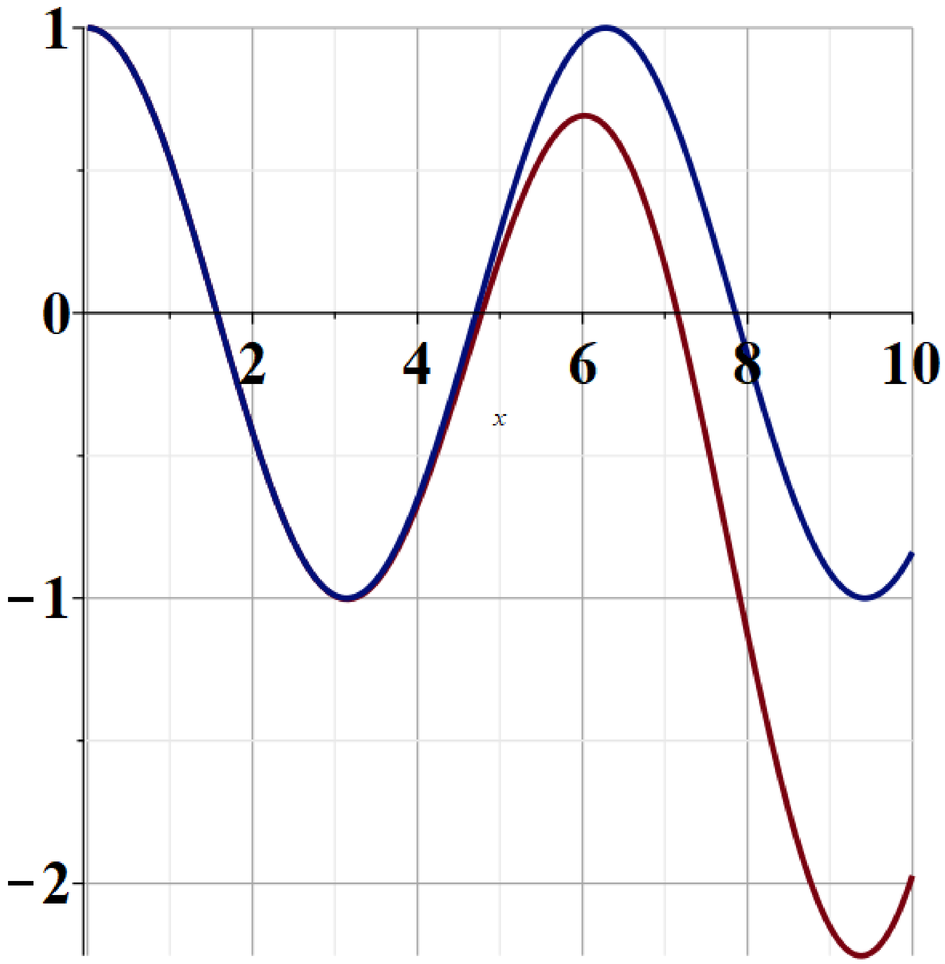
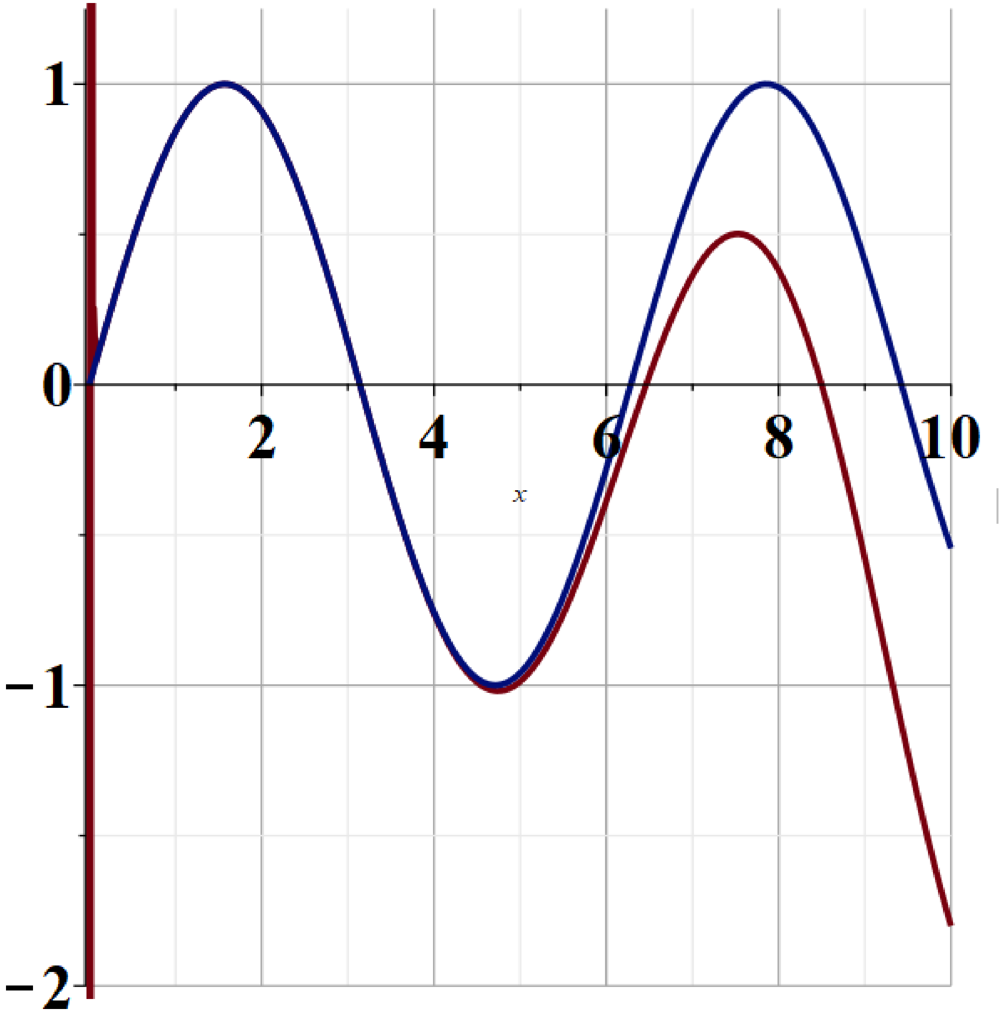


$$> plot(\{\sin(x), 3 \cdot jj(1, x) - 7 \cdot jj(3, x) + 11 \cdot jj(5, x) - 15 \cdot jj(7, x)\}, x = 0.001..10, thickness = 3, gridlines, font = [ariel, bold, 24])$$



Do you think this expansion is useful?

Is it helpful to encourage you to plot these functions to see how the expansion works/fails?

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

Another example – from Lecture 30 on the 2-site Hubbard model

Two-site Hubbard model

$$H = -t\left(c^{\dagger}_{1\uparrow}c_{2\uparrow} + c^{\dagger}_{2\uparrow}c_{1\uparrow} + c^{\dagger}_{1\downarrow}c_{2\downarrow} + c^{\dagger}_{2\downarrow}c_{1\downarrow}\right) + U\left(n_{1\uparrow}n_{1\downarrow} + n_{2\uparrow}n_{2\downarrow}\right)$$

Matrix elements of Hamiltonian for all 2 particle states with spin 0:

$$H = \begin{array}{c} \\ A \\ B \\ C \end{array}\!\!\begin{array}{c} \begin{array}{ccc} A & B & C \end{array} \\ \begin{pmatrix} U & 0 & -\sqrt{2}t \\ 0 & U & -\sqrt{2}t \\ -\sqrt{2}t & -\sqrt{2}t & 0 \end{pmatrix} \end{array}$$

$$|A\rangle \equiv c^{\dagger}_{1\uparrow}c^{\dagger}_{1\downarrow}|0\rangle$$

$$|B\rangle \equiv c^{\dagger}_{2\uparrow}c^{\dagger}_{2\downarrow}|0\rangle$$

$$|C\rangle \equiv \frac{1}{\sqrt{2}}\left(c^{\dagger}_{1\uparrow}c^{\dagger}_{2\downarrow} + c^{\dagger}_{2\uparrow}c^{\dagger}_{1\downarrow}\right)|0\rangle$$

Note that this is corrected from the original slides

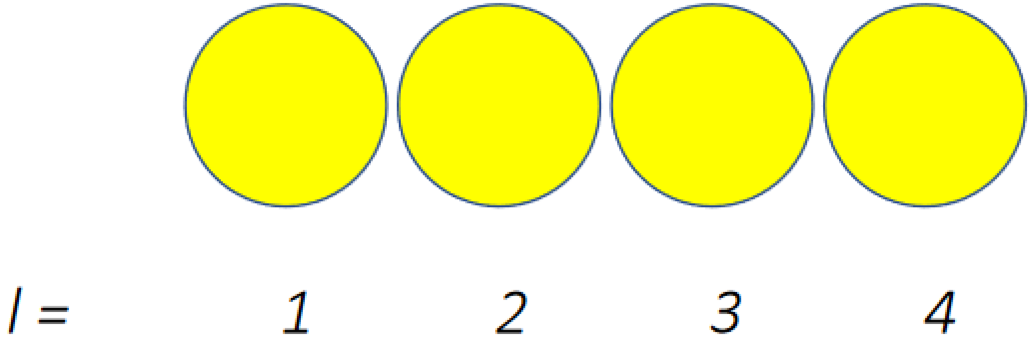
We claim that these states correspond to a total spin S=0; how can we analyze this?

Total spin S=0:

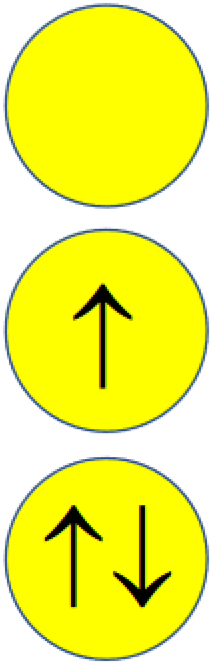
$$|A\rangle \equiv c^\dagger_{1\uparrow} c^\dagger_{1\downarrow} |0\rangle$$

$$|B\rangle \equiv c^\dagger_{2\uparrow} c^\dagger_{2\downarrow} |0\rangle$$

$$|C\rangle \equiv \frac{1}{\sqrt{2}}\left(c^\dagger_{1\uparrow} c^\dagger_{2\downarrow} + c^\dagger_{2\uparrow} c^\dagger_{1\downarrow} \right)|0\rangle$$



Possible configurations of a single site



$|0\rangle$

$c^\dagger_{\uparrow}|0\rangle$

$c^\dagger_{\uparrow} c^\dagger_{\downarrow}|0\rangle$

Possible total spin S=1 states:

$$|D\rangle = c^\dagger_{1\uparrow} c^\dagger_{2\uparrow} |0\rangle$$

$$|E\rangle = \frac{1}{\sqrt{2}}\left(c^\dagger_{1\uparrow} c^\dagger_{2\downarrow} - c^\dagger_{2\uparrow} c^\dagger_{1\downarrow} \right)|0\rangle$$

$$|F\rangle = c^\dagger_{1\downarrow} c^\dagger_{2\downarrow} |0\rangle$$

How can we calculate the total spin for our states?

Basic properties of indistinguishable Fermi particles

$$\Psi(1,2) = -\Psi(2,1)$$

Typically, we can write $\Psi(1,2) = \psi_{space}(\mathbf{r}_1,\mathbf{r}_2)\psi_{spin}(\sigma_1,\sigma_2)$

$\Rightarrow$ If $\psi_{space}(\mathbf{r}_1,\mathbf{r}_2) = \psi_{space}(\mathbf{r}_2,\mathbf{r}_1)$ then $\psi_{spin}(\sigma_1,\sigma_2) = -\psi_{spin}(\sigma_2,\sigma_1)$ $\left(S=0\right)$

$\Rightarrow$ If $\psi_{space}(\mathbf{r}_1,\mathbf{r}_2) = -\psi_{space}(\mathbf{r}_2,\mathbf{r}_1)$ then $\psi_{spin}(\sigma_1,\sigma_2) = \psi_{spin}(\sigma_2,\sigma_1)$ $\left(S=1\right)$

How can we analyze this in second quantization?

How do you calculate total spin in second quantization?

$$S_z = \frac{1}{2}\left(\sigma_1 + \sigma_2\right)$$

Possible total spin S=1 states:

$$\left|D\right\rangle = c_{1\uparrow}^{\dagger} c_{2\uparrow}^{\dagger} \left|0\right\rangle$$

➔**<S$_z$>=1**

$$\left|E\right\rangle = \frac{1}{\sqrt{2}}\left(c_{1\uparrow}^{\dagger} c_{2\downarrow}^{\dagger} - c_{2\uparrow}^{\dagger} c_{1\downarrow}^{\dagger}\right)\left|0\right\rangle$$

➔**<S$_z$>=0**

$$\left|F\right\rangle = c_{1\downarrow}^{\dagger} c_{2\downarrow}^{\dagger} \left|0\right\rangle$$

➔**<S$_z$>=-1**

Need to show that $\left\langle E\right|\left(S_x^2 + S_y^2 + S_z^2\right)\left|E\right\rangle = 2$

Remember, we are dealing with two spin ½ particles. For now, label these s_a and s_b

The quantum mechanical two particle spin operator

$$\mathbf{S}_{op}^2 = (s_{a\ op} + s_{b\ op})^2 = s_{a\ op}^2 + s_{b\ op}^2 + \left(2 s_{az\ op} s_{bz\ op} + s_{a+\ op} s_{b-\ op} + s_{a-\ op} s_{b+\ op}\right)$$

where $s_{a+\ op}\left|\uparrow\right\rangle = 0$ and $s_{a-\ op}\left|\uparrow\right\rangle = \frac{1}{2}\left|\downarrow\right\rangle$ etc.

Note that: $\left(s_{a+\ op} s_{b-\ op} + s_{a-\ op} s_{b+\ op}\right)\left|E\right\rangle = \frac{2}{4}\frac{1}{\sqrt{2}}\left(c_{1\downarrow}^\dagger c_{2\uparrow}^\dagger - c_{2\downarrow}^\dagger c_{1\uparrow}^\dagger\right)\left|0\right\rangle = \left|E\right\rangle$

$$\left|D\right\rangle = c_{1\uparrow}^\dagger c_{2\uparrow}^\dagger \left|0\right\rangle \qquad \left\langle D\right| S_{op}^2 \left|D\right\rangle = \frac{3}{4} + \frac{3}{4} + \frac{2}{4} = 2$$

$$\left|E\right\rangle = \frac{1}{\sqrt{2}}\left(c_{1\uparrow}^\dagger c_{2\downarrow}^\dagger - c_{2\uparrow}^\dagger c_{1\downarrow}^\dagger\right)\left|0\right\rangle \qquad \left\langle E\right| S_{op}^2 \left|E\right\rangle = \frac{3}{4} + \frac{3}{4} + \frac{2}{4} = 2$$

$$\left|F\right\rangle = c_{1\downarrow}^\dagger c_{2\downarrow}^\dagger \left|0\right\rangle \qquad \left\langle F\right| S_{op}^2 \left|F\right\rangle = \frac{3}{4} + \frac{3}{4} + \frac{2}{4} = 2$$