Phys 3810, Spring 2009
Exam #3

1. If we operate with L_+ on $Y_2^2(\theta,\phi)$, what do we expect to get? *Show* that we get this result.

Since L_+ is the raising operator, and there is no state "above" Y_2^2, we expect it to give zero! To show this explicitly,

$$\begin{aligned} L_+Y_2^2(\theta,\phi) &= \hbar e^{+i\phi}\left(\frac{\partial}{\partial\theta}+i\cot\theta\frac{\partial}{\partial\phi}\right)\sqrt{\frac{15}{32\pi}}\sin^2\theta\, e^{+2i\phi} \\ &= \hbar\sqrt{\frac{15}{32\pi}}e^{+i\phi}\left(2\sin\theta\cos\theta+i\cos\theta\sin\theta(2i)\right)e^{+2i\phi}=0 \end{aligned}$$

In the second step we used $\cot\theta=\frac{\cos\theta}{\sin\theta}$ to cancel a factor of $\sin\theta$; in the third step, the stuff in the paranthesis cancels.

2. What did the Stern–Gerlach experiment demonstrate?

Through exerting different forces on electrons in different spin orientations with a non-uniform magnetic field, the Stern-Gerlach expt showed that when we make a measurement of the electron's spin in a given direction, there are only two results, thus showing the quantization of spin magnetic moment (and by extension, spin angular momentum).

3. Suppose a spin-$\frac{1}{2}$ particle is in the state

$$\chi=\frac{1}{\sqrt{6}}\begin{pmatrix}2\\1-i\end{pmatrix}$$

What are the probabilities of getting $+\hbar/2$ and $-\hbar/2$ if you measure S_x? What is the expectation value of S_x for this state?

Decompose the state into eigenstates of S_x. Using the eigenvectors for S_x, this gives

$$\frac{1}{\sqrt{6}}\begin{pmatrix}2\\1-i\end{pmatrix}=\frac{a}{\sqrt{2}}\begin{pmatrix}1\\1\end{pmatrix}+\frac{b}{\sqrt{2}}\begin{pmatrix}1\\-1\end{pmatrix}$$

and solve for a and b. Get:

$$\frac{2}{\sqrt{3}}=a+b \qquad\qquad \frac{1-i}{\sqrt{3}}=a-b$$

which (adding and subtracting) gives

$$2a=\frac{3-i}{\sqrt{3}} \qquad\Longrightarrow\qquad a=\frac{3-i}{\sqrt{12}}$$

$$2b=\frac{1+i}{\sqrt{3}} \qquad\Longrightarrow\qquad b=\frac{1+i}{\sqrt{2}}$$

so we've shown

$$\chi = \frac{3-i}{\sqrt{12}}\chi_+^{(x)} + \frac{1+i}{\sqrt{12}}\chi_-^{(x)}$$

so the probability to measure $+\hbar/2$ for S_x is

$$P_{x,+} = \frac{1}{12}(3-i)(3+i) = \frac{10}{12} = \frac{5}{6}$$

and the probability to measure $-\hbar/2$ for S_x is

$$P_{x,-} = \frac{1}{12}(1+i)(1-i) = \frac{2}{12} = \frac{1}{6}$$

One can use these probabilities to get the expectation value of S_x:

$$\langle S_x\rangle = \frac{5}{6}(+\hbar/2) + \frac{1}{6}(-\hbar/2) = \frac{4}{12}\hbar = \frac{\hbar}{3}$$

One can also compute it directly:

$$\langle S_x\rangle = \chi^\dagger S_x \chi = \frac{1}{6}\begin{pmatrix} 2 & 1+i \end{pmatrix}\frac{\hbar}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}\begin{pmatrix} 2 \\ 1-i \end{pmatrix}$$

and this gives:

$$\langle S_x\rangle = \frac{\hbar}{12}\begin{pmatrix} 2 & 1+i \end{pmatrix}\begin{pmatrix} 2 \\ 1-i \end{pmatrix} = \frac{\hbar}{12}(2-2i+2+2i) = \frac{4\hbar}{12} = \frac{\hbar}{3}$$

4. Construct the S^2, S_z and S_+ matrices for a spin–2 particle.

$$S^2 = 6\hbar^2\begin{pmatrix} 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 \end{pmatrix} \qquad S_z = \hbar\begin{pmatrix} 2 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 0 & -2 \end{pmatrix}$$

The action of S_+ on the states is, for example

$$S_+|2\ -2\rangle = \hbar\sqrt{2\cdot 3-(-2)(-1)}|2\ -1\rangle = 2\hbar|2\ -1\rangle$$

Proceeding in this way, we get

$$S_+|2\ -2\rangle = 2\hbar|2\ -1\rangle \qquad S_+|2\ -1\rangle = \sqrt{6}\hbar|2\ 0\rangle \qquad S_+|2\ 0\rangle = \sqrt{6}\hbar|2\ 1\rangle$$

$$S_+|2\ 1\rangle = 2\hbar|2\ 2\rangle \qquad S_+|2\ 2\rangle = 0$$

$$S_+ = \hbar\begin{pmatrix} 0 & 2 & 0 & 0 & 0 \\ 0 & 0 & \sqrt{6} & 0 & 0 \\ 0 & 0 & 0 & \sqrt{6} & 0 \\ 0 & 0 & 0 & 0 & 2 \\ 0 & 0 & 0 & 0 & 0 \end{pmatrix}$$

5. Is the following a permissible wave function for a system of two non-interacting particles?

$$\frac{1}{\sqrt{2}}[\psi_a(\mathbf{r}_1)\psi_b(\mathbf{r}_2) + \psi_a(\mathbf{r}_2)\psi_b(\mathbf{r}_1)]\ \frac{1}{\sqrt{2}}(\uparrow\downarrow + \downarrow\uparrow)$$

If not (and of course it isn't) tell how you would fix it to make it permissible.

No, as both space and spin parts of the wave function are symmetric under exchange of the particle numbers. One of them must be antisymmetric, which can be accomplished by replacing the $+$ sign between the two terms of either one by a $-$.

6. Consider a quantum state where an angular momentum $s_1 = 2$ combines with an angular momentum $s_2 = 1$ to give a state with total angular momentum $s = 2$ and z component 1:

$$|s\ m\rangle \ = \ |2\ 1\rangle$$

Give the expansion of this state in terms of the states of *individual* angular momenta, that is, states of the form

$$|2\ m_1\rangle\,|1\ m_2\rangle$$

(A chart of C-G coefficients will be provided.)

The table tells you:

$$|2\ 1\rangle \ = \ \frac{1}{\sqrt{3}}|2\ 2\rangle\,|1\ -1\rangle + \frac{1}{\sqrt{6}}|2\ 1\rangle\,|1\ 0\rangle - \frac{1}{\sqrt{2}}|2\ 0\rangle\,|1\ 1\rangle$$

7. The CO molecule has a vibrational spectrum wherein the frequency of the emitted photon is 8.66×10^{13} Hz. (This gives the energy difference of the vibrational states. Find the force constant k for this molecule.

Hint: You need to use the reduced mass for a two–particle system;

$$m_C = 12.01\ \text{u} \qquad m_O = 16.00\ \text{u} \qquad 1\ \text{u} = 1.66 \times 10^{-27}\ \text{kg}$$

The reduced mass of the two--particle system is

$$\mu = \frac{m_1 m_2}{m_1 + m_2} = \frac{(12.01)(16.00)}{28.01\ \text{u}} = 6.86\ \text{u}\left(\frac{1.66 \times 10^{-27}\ \text{kg}}{1\ \text{u}}\right) = 1.14 \times 10^{-26}\ \text{kg}$$

The frequency ν of *vibration* of the system is the same as the frequency of the radiation from a transition between adjacent states. Use the harmonic oscillator *with the mass m replaced by the reduced mass* μ, then

$$\omega = \sqrt{\frac{k}{\mu}} \qquad \Longrightarrow \qquad k = \omega^2\mu = (2\pi\nu)^2\mu$$

Plug in numbers:

$$k = (2\pi(8.66 \times 10^{13}\ \text{Hz}))^2(1.14 \times 10^{-26}\ \text{kg}) = 3.38 \times 10^3\ \tfrac{\text{N}}{\text{m}}$$

Caution: Bad number was given in this problem; frequency of CO spectrum is in fact 6.42×10^{13} Hz.

8. Write out the complete hamiltonian for the helium atom, assuming the nucleus is stationary. Give a short description of each of the terms and explain why the Schrödinger equation for this hamiltonian is so hard to solve.

If we make the *gross* approximation of ignoring the interaction between the electrons, what are the solutions?

The hamiltonian (which acts on the two-particle wave function $\psi(\mathbf{r}_1, \mathbf{r}_2)$) is

$$H = -\frac{\hbar^2}{2m}\nabla_1^2 - \frac{\hbar^2}{2m}\nabla_2^2 - \frac{2e^2}{4\pi\epsilon_0 r_1} - \frac{2e^2}{4\pi\epsilon_0 r_1} + \frac{e^2}{4\pi\epsilon_0|\mathbf{r}_1 - \mathbf{r}_2|}$$

The first two terms here are operators for the kinetic energies of the two electrons; the third and fourth and the potential energies for the attraction of the electrons to the nucleus and the last is the repulsion energy for the two electrons.

The reason why the Schrödinger equation with this H is hard to solve is that with the e--e repulsion term we can't separate the equation into single--particle equations. The true solution is unavoidably a function of both particle coordinates and because of this difficulty, solutions must be approximate and numerical.

9. For a multi-particle system, what is meant by "exchange force"?

It is a name given to the gross effects of symmetrization or antisymmetrization (but not a *genuine* potential) on a multi-particle wave function. The effect is to bring the particles closer together (on average) for a symmetrized wave function and to keep them farther apart (on average) for an antisymmetrized wave function.

10. Summarize the simple model of (3d) electron gas given in the text (and also in your stat mech class).

The model to treat the electrons moving freely (no potential at all) except for the hard walls of the box which contains them. The electrons are added to the levels of the 3D box (2 electrons per level, one for each spin direction) in accoradance with the number of electrons in the system, which is really given by their density. The maximum electron energy is the "Fermie energy".

11. In the computer "project" for this semester, the boundary conditions imposed on the wave function $u(r)$ were

$$u(0) = 0. \qquad\qquad u'(0) = 1.$$

Give the *reasons* why we imposed these conditions. Actually, one of them was arbitrary! Why were we able to get away with this arbitrary choice?

As $R(r) = \frac{u(r)}{r}$ and we would like the radial wavefunction to be finite at the origin, we need to have $u(0) = 0$ to make this ratio finite as $r \rightarrow 0$.

As for the derivative condition, it is arbitrary. But any value will work because the function and all its derivatives are proportional to the normalization and we do not care about the normalization in this exercise. The value 1 was chosen just because the solution for $u(r)$ is something like a sine function near the origin and the slope of $\sin(x)$ is 1 at the origin, so the solution will be a function of (convenient) order 1, but still not normalized.

Numbers

$$\hbar = 1.05457 \times 10^{-34}\ \mathrm{J \cdot s} \qquad m_{\mathrm{e}} = 9.10938 \times 10^{-31}\ \mathrm{kg} \qquad m_{\mathrm{p}} = 1.67262 \times 10^{-27}\ \mathrm{kg}$$

$$e = 1.60218 \times 10^{-19}\ \mathrm{C} \qquad c = 2.99792 \times 10^{8}\ \tfrac{\mathrm{m}}{\mathrm{s}}$$

Physics

$$i\hbar\frac{\partial \Psi}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2 \Psi}{\partial x^2} + V\Psi \qquad P_{ab} = \int_a^b |\Psi(x,t)|^2\,dx \qquad p \to \frac{\hbar}{i}\frac{d}{dx}$$

$$\int_{-\infty}^{\infty} |\Psi(x,t)|^2\,dx = 1 \qquad \langle x \rangle = \int_{-\infty}^{\infty} x|\Psi(x,t)|^2\,dx \qquad \langle p \rangle = \int_{-\infty}^{\infty} \Psi^* \left(\frac{\hbar}{i}\frac{\partial}{\partial x}\right)\Psi\,dx$$

$$\sigma = \sqrt{\langle j^2 \rangle - \langle j \rangle^2} \qquad \sigma_x\sigma_p \geq \frac{\hbar}{2}$$

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + V\psi = E\psi \qquad \phi(t) = e^{-iEt/\hbar} \qquad \Psi(x,t) = \sum_{n=1}^{\infty} c_n\psi_n(x)e^{-iE_nt/\hbar} = \sum_{n=1}^{\infty}\Psi_n(x,t)$$

$$\infty \text{ Square Well:} \qquad E_n = \frac{n^2\pi^2\hbar^2}{2ma^2} \qquad \psi_n(x) = \sqrt{\frac{2}{a}}\sin\left(\frac{n\pi}{a}x\right)$$

$$\int \psi_m(x)^*\psi_n(x)\,dx = \delta_{mn} \qquad c_n = \int \psi_n(x)^* f(x)\,dx \qquad \sum_{n=1}^{\infty}|c_n|^2 = 1 \qquad \langle H \rangle = \sum_{n=1}^{\infty}|c_n|^2 E_n$$

$$\text{Harmonic Oscillator:} \qquad V(x) = \tfrac{1}{2}m\omega^2x^2 \qquad \frac{1}{2m}[p^2 + (m\omega x)^2]\psi = E\psi$$

$$a_{\pm} \equiv \frac{1}{\sqrt{2\hbar m\omega}}(\mp ip + m\omega x) \qquad [A,B] = AB - BA \qquad [x,p] = i\hbar$$

$$H(a_+\psi) = (E + \hbar\omega)(a_+\psi) \qquad H(a_-\psi) = (E - \hbar\omega)(a_+\psi) \qquad a_-\psi_0 = 0$$

$$\psi_0(x) = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} e^{-\frac{m\omega}{2\hbar}x^2} \qquad \psi_1(x) = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4}\sqrt{\frac{2m\omega}{\hbar}}\,x e^{-\frac{m\omega}{2\hbar}x^2}$$

$$\text{Free particle:} \qquad \Psi_k(x) = Ae^{i(kx - \frac{\hbar k^2}{2m})t} \qquad v_{\text{phase}} = \frac{\omega}{k} \qquad v_{\text{group}} = \frac{d\omega}{dk}$$

$$\Psi(x,t) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}\phi(k)e^{i(kx - \frac{\hbar k^2}{2m}t)}\,dk \qquad \phi(k) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}\Psi(x,0)e^{-ikx}\,dx$$

$$\text{Delta Fn Potl:} \qquad \psi(x) = \frac{\sqrt{m\alpha}}{\hbar}e^{-m\alpha|x|/\hbar^2} \qquad E = -\frac{m\alpha^2}{2\hbar^2}$$

$$f_p(x) = \frac{1}{\sqrt{2\pi\hbar}}\exp(ipx/\hbar) \qquad [\hat{A},\hat{B}] \equiv \hat{A}\hat{B} = \hat{B}\hat{A} \qquad \Phi(p,t) = \frac{1}{\sqrt{2\pi\hbar}}\int_{-\infty}^{\infty}e^{-ipx/\hbar}\Psi(x,t)\,dx$$

$$\sigma_A^2\sigma_B^2 \geq \left(\frac{1}{2i}\langle[\hat{A},\hat{B}]\rangle\right)^2 \qquad \sigma_x\sigma_p \geq \frac{\hbar}{2} \qquad \Delta E\Delta t \geq \frac{\hbar}{2}$$

$$-\frac{\hbar^2}{2m}\left[\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial\psi}{\partial r}\right)+\frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial\psi}{\partial\theta}\right)+\frac{1}{r^2\sin^2\theta}\frac{\partial^2\psi}{\partial\phi^2}\right]+V(r)\psi=E\psi$$

$$\psi(r,\theta,\phi)=R(r)\Theta(\theta)\Phi(\phi)\qquad \frac{d^2\Phi}{d\phi^2}=-m^2\Phi\qquad \sin\theta\frac{d}{d\theta}\left(\sin\theta\frac{d\Theta}{d\theta}\right)+[\ell(\ell+1)\sin^2\theta-m^2]\Theta=0$$

$$Y_0^0=\sqrt{\frac{1}{4\pi}}\qquad Y_1^0=\sqrt{\frac{3}{4\pi}}\cos\theta\qquad Y_1^{\pm1}=\mp\sqrt{\frac{3}{8\pi}}\sin\theta e^{\pm i\phi}$$

$$Y_2^0=\sqrt{\frac{5}{16\pi}}(3\cos^2\theta-1)\qquad Y_2^{\pm1}=\mp\sqrt{\frac{15}{8\pi}}\sin\theta\,\cos\theta e^{\pm i\phi}\qquad Y_2^{\pm2}=\sqrt{\frac{15}{32\pi}}\sin^2\theta\,e^{\pm 2i\phi}\text{etc.}$$

$$u(r)\equiv rR(r)\qquad -\frac{\hbar^2}{2m}\frac{d^2u}{dr^2}+\left[V+\frac{\hbar^2}{2m}\frac{l(l+1)}{r^2}\right]u=Eu$$

$$a=\frac{4\pi\epsilon_0\hbar^2}{me^2}=0.529\times10^{-10}\text{ m}\qquad E_n=-\left[\frac{m}{2\hbar^2}\left(\frac{e^2}{4\pi\epsilon_0}\right)^2\right]\frac{1}{n^2}\equiv\frac{E_1}{n^2}\qquad \text{for}\quad n=1,2,3,\ldots$$

where $E_1=-13.6$ eV.

$$R_{10}(r)=2a^{-3/2}e^{-r/a}\qquad R_{20}(r)=\frac{1}{\sqrt{2}}a^{-3/2}\left(1-\frac{1}{2}\frac{r}{a}\right)e^{-r/2a}\qquad R_{21}(r)\frac{1}{\sqrt{24}}a^{-3/2}\,\frac{r}{a}\,e^{-r/2a}$$

$$\lambda f=c\qquad E_\gamma=hf\qquad \frac{1}{\lambda}=R\left(\frac{1}{n_f^2}-\frac{1}{n_i^2}\right)\qquad \text{where}\qquad R=\frac{m}{4\pi c\hbar^3}\left(\frac{c^2}{4\pi\epsilon_0}\right)^2=1.097\times10^7\text{ m}^{-1}$$

$$\mathbf{L}=\mathbf{r}\times\mathbf{p}\qquad [L_x,L_y]=i\hbar L_z\qquad [L_y,L_z]=i\hbar L_x\qquad [L_z,L_x]=i\hbar L_y$$

$$L_z=\frac{\hbar}{i}\frac{\partial}{\partial\phi}\qquad L_\pm=\pm\hbar e^{\pm i\phi}\left(\frac{\partial}{\partial\theta}\pm i\cot\theta\frac{\partial}{\partial\phi}\right)\qquad L^2=-\hbar^2\left[\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right)+\frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\right]$$

$$L^2f_l^m=\hbar^2l(l+1)f_l^m\qquad L_zf_l^m=\hbar mf_l^m$$

$$[S_x,S_y]=i\hbar S_z\qquad [S_y,S_z]=i\hbar S_x\qquad [S_z,S_x]=i\hbar S_y$$

$$S^2|s\;m\rangle=\hbar^2s(s{+}1)|s\;m\rangle\qquad S_z|s\;m\rangle=\hbar m|s\;m\rangle\qquad S_\pm|s\;m\rangle=\hbar\sqrt{s(s+1)-m(m\pm1)}\,|s\;m{\pm}1\rangle$$

$$\chi=\begin{pmatrix}a\\b\end{pmatrix}=a\chi_++b\chi_-\quad\text{where}\quad \chi_+=\begin{pmatrix}1\\0\end{pmatrix}\quad\text{and}\quad \chi_-=\begin{pmatrix}0\\1\end{pmatrix}$$

$$\mathsf{S}^2=\frac{3}{4}\hbar^2\begin{pmatrix}1&0\\0&1\end{pmatrix}\qquad \mathsf{S}_z=\frac{\hbar}{2}\begin{pmatrix}1&0\\0&-1\end{pmatrix}$$

$$\mathsf{S}_x = \frac{\hbar}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \qquad \mathsf{S}_y = \frac{\hbar}{2}\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \qquad \mathsf{S}_z = \frac{\hbar}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \qquad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \qquad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

$$\chi_+^{(x)} = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 1 \end{pmatrix} \qquad \chi_-^{(x)} = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ -1 \end{pmatrix} \qquad \chi_+^{(y)} = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ i \end{pmatrix} \qquad \chi_-^{(y)} = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ -i \end{pmatrix}$$

$$\mathbf{B} = B_0\mathbf{k} \qquad H = -\gamma B_0 \mathsf{S}_z \qquad E_+ = -(\gamma B_0 \hbar)/2 \qquad E_- = +(\gamma B_0 \hbar)/2$$

$$\chi(t) = a\chi_+ e^{-iE_+t/\hbar} + b\chi_- e^{-iE_-t/\hbar} = \begin{pmatrix} ae^{-iE_+t/\hbar} \\ be^{-iE_-t/\hbar} \end{pmatrix}$$

$$-\frac{\hbar^2}{2M}\nabla_R^2\psi - \frac{\hbar^2}{2\mu}\nabla_r^2\psi + V(\mathbf{r})\psi = E\psi \qquad \psi(\mathbf{r}_1, \mathbf{r}_2) = \pm\psi(\mathbf{r}_2, \mathbf{r}_1)$$