PHY 308 Midterm 2, Spring 2017
Stony Brook University
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7 problems and 100 points total. The following information may or may not be useful

Planck's constant: $\hbar = 1.055 \times 10^{-34}$ J-s $= 6.582 \times 10^{-16}$ eV-s
Speed of light: $c = 3 \times 10^8$ m/s
Mass of the electron: $m_e = 9.1 \times 10^{-31}$ kg
The electron volt: 1 eV $= 1.6 \times 10^{-19}$ J
The fine structure constant $\alpha = 1/137$

Table 4.2: The first few spherical harmonics, $Y_l^m(\theta, \phi)$.

$$Y_0^0 = \left(\frac{1}{4\pi}\right)^{1/2}$$

$$Y_2^{\pm 2} = \left(\frac{15}{32\pi}\right)^{1/2} \sin^2\theta e^{\pm 2i\phi}$$

$$Y_1^0 = \left(\frac{3}{4\pi}\right)^{1/2} \cos\theta$$

$$Y_3^0 = \left(\frac{7}{16\pi}\right)^{1/2} (5\cos^3\theta - 3\cos\theta)$$

$$Y_1^{\pm 1} = \mp\left(\frac{3}{8\pi}\right)^{1/2} \sin\theta e^{\pm i\phi}$$

$$Y_3^{\pm 1} = \mp\left(\frac{21}{64\pi}\right)^{1/2} \sin\theta(5\cos^2\theta - 1)e^{\pm i\phi}$$

$$Y_2^0 = \left(\frac{5}{16\pi}\right)^{1/2} (3\cos^2\theta - 1)$$

$$Y_3^{\pm 2} = \left(\frac{105}{32\pi}\right)^{1/2} \sin^2\theta \cos\theta e^{\pm 2i\phi}$$

$$Y_2^{\pm 1} = \mp\left(\frac{15}{8\pi}\right)^{1/2} \sin\theta \cos\theta e^{\pm i\phi}$$

$$Y_3^{\pm 3} = \mp\left(\frac{35}{64\pi}\right)^{1/2} \sin^3\theta e^{\pm 3i\phi}$$

TABLE 4.7: The first few radial wave functions for hydrogen, $R_{nl}(r)$.

$$R_{10} = 2a^{-3/2}\exp(-r/a)$$

$$R_{20} = \frac{1}{\sqrt{2}}a^{-3/2}\left(1 - \frac{1}{2}\frac{r}{a}\right)\exp(-r/2a)$$

$$R_{21} = \frac{1}{\sqrt{24}}a^{-3/2}\frac{r}{a}\exp(-r/2a)$$

$$R_{30} = \frac{2}{\sqrt{27}}a^{-3/2}\left(1 - \frac{2}{3}\frac{r}{a} + \frac{2}{27}\left(\frac{r}{a}\right)^2\right)\exp(-r/3a)$$

$$R_{31} = \frac{8}{27\sqrt{6}}a^{-3/2}\left(1 - \frac{1}{6}\frac{r}{a}\right)\left(\frac{r}{a}\right)\exp(-r/3a)$$

$$R_{32} = \frac{4}{81\sqrt{30}}a^{-3/2}\left(\frac{r}{a}\right)^2\exp(-r/3a)$$

$$R_{40} = \frac{1}{4}a^{-3/2}\left(1 - \frac{3}{4}\frac{r}{a} + \frac{1}{8}\left(\frac{r}{a}\right)^2 - \frac{1}{192}\left(\frac{r}{a}\right)^3\right)\exp(-r/4a)$$

$$R_{41} = \frac{\sqrt{5}}{16\sqrt{3}}a^{-3/2}\left(1 - \frac{1}{4}\frac{r}{a} + \frac{1}{80}\left(\frac{r}{a}\right)^2\right)\frac{r}{a}\exp(-r/4a)$$

$$R_{42} = \frac{1}{64\sqrt{5}}a^{-3/2}\left(1 - \frac{1}{12}\frac{r}{a}\right)\left(\frac{r}{a}\right)^2\exp(-r/4a)$$

$$R_{43} = \frac{1}{768\sqrt{35}}a^{-3/2}\left(\frac{r}{a}\right)^3\exp(-r/4a)$$

1 True/False (12 points)

Circle **T** if the statement is always true. Otherwise circle **F** for false. 2 points each

T (**F**)   The wavefunction describing a many-body quantum system that is a mixture of Fermions and Bosons must be antisymmetric under exchange of any two particles.

(**T**) **F**   Observables in quantum mechanics are represented by Hermitian Operators.

T (**F**)   All operators used in quantum mechanics are Hermitian.

T (**F**)   The wave function describing the positions of two identical deuterons (the nucleus of a deuterium atom), each with 1 proton and 1 neutron, must be symmetric with exchange of the two deuteron's position coordinates since the deuteron is a (composite) boson. → *can have antisymmetric spin w.f.*

T (**F**)   The variational principle states that for any quantum system, the expectation value of the Hamiltonian evaluated using any normalized trial wave function will always be larger than the energy of the system's ground state.   *≥*

(**T**) **F**   In the variational method, if one uses a normalized trial function ϕ orthogonal to the ground state wave function of a quantum system, then $\langle\phi|\hat{H}|\phi\rangle$ always gives an upper bound for the energy of the first excited state.

2 Multiple Choice (16 points)

Circle **one** answer for each question. 4 points each.

Which property applies to identical particles that are labeled "Fermions":
a) they possess integer spin angular momentum
b) their angular momentum cannot be added.
c) they always have $\langle \hat{S}^2 \rangle = 0$
(d) they obey the Pauli principle.

In atomic units, the mass of the proton is (circle the closest answer):
a) 1
b) 13.6
c) 1.673×10^{-27}
(d) 1836

Which of the following is *not* a valid set of quantum numbers for the orbitals of the hydrogen atom $\psi_{nlm}(r, \theta, \phi) = R_{nl}(r)Y_\ell^m(\theta, \phi)$:
a) $n = 1, \ell = 0, m = 0$
b) $n = 27, \ell = 0, m = 0$
c) $n = 2, \ell = 1, m = -1$
(d) $n = 2, \ell = 2, m = -1$
e) none of the above.

If the spin angular momenta of two spin-3/2 particles are added, the possible s values for the *total* spin angular momentum (such that $\hat{S}_{tot}^2 |\psi\rangle = s(s+1)\hbar^2 |\psi\rangle$) are
a) $s =$ -3, -2, -1, 0, 1, 2, or 3
(b) $s = 3, 2, 1$, or 0
c) $s = 3$ or 0
d) $s =$ -3, -5/2, -2, -3/2, -1, -1/2, 0, 1/2, 1, 3/2, 2, 5/2, or 3
e) $s = 3/2$ or 1/2
f) Not enough information to answer the question because it depends on if the particles are identical or not.

3 Matrix Element Potpouri (18 points)

For each of the expressions below, indicate if the answer is 0, 1, or something else. If it is "something else", just write "something else" - you don't need to calculate it. 2 points each.

For the stationary state wave functions of the hydrogen atom in spherical coordinates $\psi_{n\ell m}(r,\theta,\phi) = R_{n\ell}(r)Y_\ell^m(\theta,\phi)$, with $\int d^3\vec{r}$ representing the volume integral over all three dimensional space.

a) $\int_0^\infty dr\, r^2 |R_{n\ell}(r)|^2 =$ **1**

b) $\int_0^\infty dr\, r^2 |\psi_{n\ell m}|^2 =$ something else

c) $\langle 2s|\hat{r}^2|1s\rangle = \int d^3\vec{r}\, \psi_{200}^* \, r^2 \, \psi_{100} =$ something else

d) $\langle 2p_z|\hat{r}^2|1s\rangle = \int d^3\vec{r}\, \psi_{210}^* \, r^2 \, \psi_{100} =$ **0**

e) $\langle 2p_z|\hat{z}|1s\rangle = \int d^3\vec{r}\, \psi_{210}^* \, r\cos\theta \, \psi_{100} =$ something else

For the spherical harmonics in spherical coordinates $Y_\ell^m(\theta,\phi)$, with $\int_{4\pi} d\Omega$ representing the integral over all 4π solid angle:

f) $\int_{4\pi} d\Omega\, (Y_1^0)^* Y_0^0 =$ **0**

g) $\int_{4\pi} d\Omega\, (Y_1^0)^* \cos\theta\, Y_0^0 =$ something else

h) $\int_{4\pi} d\Omega\, (Y_2^0)^* \cos\theta\, Y_0^0 =$ **0**

i) $\int_{4\pi} d\Omega\, (Y_0^0)^* \sin\phi\, Y_0^0 =$ **0**

4 Addition of Angular Momenta (9 points)

For each expression below, give the Clebsch-Gordan coefficients $\langle j_1 j_2; m_1 m_2 | j_1 j_2; jm \rangle$ regarding the angular momentum addition of two spin-1/2 particles ($j_1 = 1/2, j_2 = 1/2$). 3 points each.

a) $\langle \frac{1}{2}\frac{1}{2}; \frac{+1}{2}\frac{+1}{2} | \frac{1}{2}\frac{1}{2}; 10 \rangle =$ **0**

b) $\langle \frac{1}{2}\frac{1}{2}; \frac{+1}{2}\frac{+1}{2} | \frac{1}{2}\frac{1}{2}; 11 \rangle =$ **1**

c) $\langle \frac{1}{2}\frac{1}{2}; \frac{+1}{2}\frac{-1}{2} | \frac{1}{2}\frac{1}{2}; 10 \rangle =$ $\dfrac{1}{\sqrt{2}}$

5 The Pauli Exclusion Principle (13 points)

Consider two non-interacting spin-$\frac{1}{2}$ particles confined to a 1D box of length 1 ($V(x) = 0$ for $0 < x < 1$ and ∞ otherwise), with the two particles in the excited configuration represented by the following Slater determinant:

$$\Psi_e = \frac{1}{\sqrt{2}} \begin{vmatrix} \phi_{1\alpha}(x_1) & \phi_{2\alpha}(x_1) \\ \phi_{1\alpha}(x_2) & \phi_{2\alpha}(x_2) \end{vmatrix} \tag{5.1}$$

and the "α" designates spin "up", viz. $\phi_{1\alpha}(x) = \phi_1(x) |{\uparrow}\rangle$. Take $\phi_1 = \sqrt{2}\sin(\pi x)$ and $\phi_2 = \sqrt{2}\sin(2\pi x)$.

a) Verify that Ψ_e satisfies the time independent Schrödinger equation. To save writing, if you desire you can use the fact that ϕ_1 and ϕ_2 are eigenstates of the 1 particle Hamiltonian without re-deriving this.

b) Make a sketch illustrating the 2-dimensional $|\Psi_e(x_1, x_2)|^2$. You can draw a contour plot, a 3D surface plot, or use shading to represent magnitude, as long as you make yourself clear. What happens when $x_1 = x_2$? Interpret your results in the context of the Pauli exclusion principle.
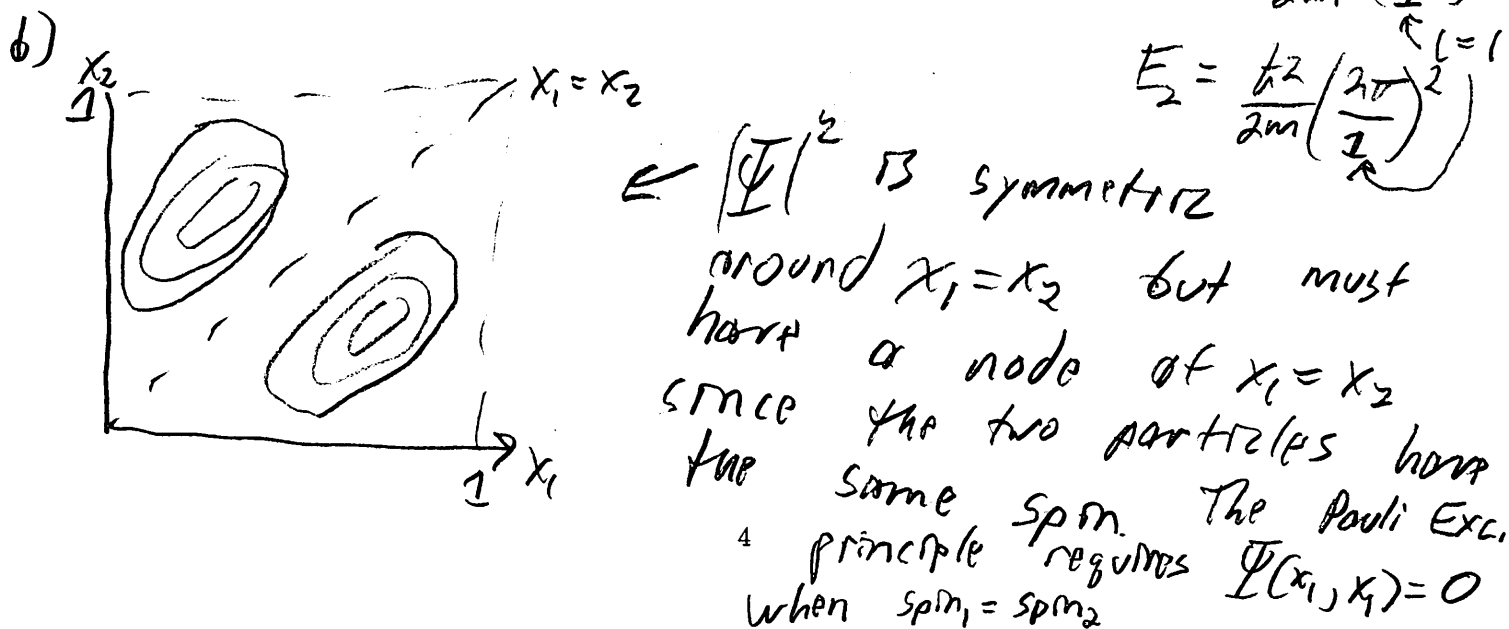
a) $\hat{H} = \dfrac{-\hbar^2}{2m}\dfrac{\partial^2}{\partial x_1^2} - \dfrac{\hbar^2}{2m}\dfrac{\partial^2}{\partial x_2^2}$ between $x=0$ and $x=1$

$= \hat{H}_1 + \hat{H}_2$

$\Psi_e = \dfrac{1}{\sqrt{2}}\Big(\phi_1(x_1)\phi_2(x_2) - \phi_2(x_1)\phi_1(x_2) \Big)\alpha(1)\alpha(2)$

$\hat{H}_1 \Psi_e = \dfrac{1}{\sqrt{2}}\Big(E_1 \phi_1(x_1)\phi_2(x_2) - E_2 \phi_2(x_1)\phi_1(x_2) \Big)\alpha(1)\alpha(2)$

$\hat{H}_2 \Psi_e = \dfrac{1}{\sqrt{2}}\Big(E_2 \phi_1(x_1)\phi_2(x_2) - E_1 \phi_2(x_1)\phi_1(x_2) \Big)\alpha(1)\alpha(2)$

$\Rightarrow \hat{H}\Psi_e = (\hat{H}_1 + \hat{H}_2)\Psi_e = (E_1 + E_2)\Psi_e$ w/ $E_1 = \dfrac{\hbar^2}{2m}\left(\dfrac{\pi}{1}\right)^2$ $\leftarrow l=1$

$E_2 = \dfrac{\hbar^2}{2m}\left(\dfrac{2\pi}{1}\right)^2$ $l=1$

b)

$\leftarrow |\Psi|^2$ is symmetric around $x_1 = x_2$ but must have a node at $x_1 = x_2$ since the two particles have same spin. The Pauli Exc. principle requires $\Psi(x_1, x_1) = 0$ when $\text{spin}_1 = \text{spin}_2$

6 Half-Hydrogen Atom (12 points)

Consider an electron bound to a point impurity at the surface of an insulator. Taking the model potential for this problem in spherical coordinates (r, θ, ϕ) to be.

$$V(r,\theta,\phi) = \begin{cases} \infty, & \theta \geq \pi/2 \\ -\frac{1}{4\pi\epsilon_0}\frac{e^2}{r} & \theta < \pi/2 \end{cases}$$

What is the normalized ground state wave function and ground state energy, both written in atomic units $(m_e = \hbar = e = 1/4\pi\epsilon_0 = 1)$?
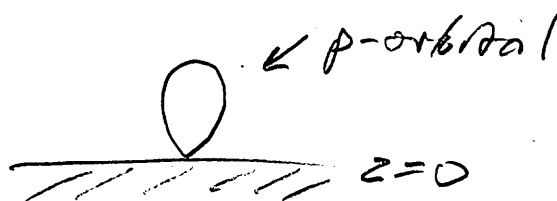
The Hamiltonian for $z > 0$ $\left(\theta < \pi/2\right)$ is the same as the Hydrogen atom, so the solns are the same, but not all soln's are able to meet the b.c.'s. The lowest energy soln that meets the b.c. $\psi \to 0$ at $\theta = \pi/2$ is ψ_{210}. We need to multiply by $\sqrt{2}$ since now we are only integrating over half of all space and we still need

$$\int d^3\vec{r} \, |\psi|^2 = 1$$

$z > 0$

So

$$\psi_{ground} = \underbrace{\sqrt{2} \underbrace{\frac{1}{\sqrt{24}} r e^{-r/2}}_{R_{21}} \underbrace{\left(\frac{3}{4\pi}\right)^{1/2} \cos\theta}_{Y_1^0}}_{\text{normalization}}$$

← p-orbital

$z = 0$

For the hydrogen atom, the electron with spin $s = 1/2$ "orbits" the proton, and it is thus convenient to describe this system with states labeled by the angular momentum quantum numbers $|\ell s; m_\ell m_s\rangle$:

$$\hat{L}^2 |\ell s; m_\ell m_s\rangle = \hbar^2 \ell(\ell+1) \tag{7.1}$$

$$\hat{L}_z |\ell s; m_\ell m_s\rangle = \hbar m_\ell \tag{7.2}$$

$$\hat{S}^2 |\ell s; m_\ell m_s\rangle = \hbar^2 \frac{1}{2}\left(\frac{1}{2}+1\right) \tag{7.3}$$

$$\hat{S}_z |\ell s; m_\ell m_s\rangle = \hbar m_s \tag{7.4}$$

Consider, now an additional term in the Hamiltonian the couples the spin and orbital angular momentum together:

$$\hat{H}_{so} = \beta \hat{\vec{S}} \cdot \hat{\vec{L}} = \beta \left(\hat{S}_x \hat{L}_x + \hat{S}_y \hat{L}_y + \hat{S}_z \hat{L}_z \right) \tag{7.5}$$

where we'll take β as a positive constant (really it would be an operator of the spatial coordinates). This is called spin-orbit coupling. Note that since this term involves all of the components $\hat{L}_i$ and $\hat{S}_i$, the states $|\ell s; m_\ell m_s\rangle$ are *not* eigenstates of this term. The operators $\hat{L}_z$ and $\hat{S}_z$ do not commute with $\hat{H}_{so}$.

In this case, it is convenient to introduce a total angular momentum $\hat{\vec{J}} = \hat{\vec{S}} + \hat{\vec{L}}$, which has its own eigenstates $|\ell s; jm\rangle$, viz.

$$\hat{J}^2 |ls; jm\rangle = \left(\hat{S}^2 + \hat{L}^2 + 2\hat{\vec{S}} \cdot \hat{\vec{L}} \right) |\ell s; jm\rangle = \hbar^2 j(j+1) |\ell s; jm\rangle \tag{7.6}$$

$$\hat{J}_z |ls; jm\rangle = \left(\hat{S}_z + \hat{L}_z \right) |\ell s; jm\rangle = \hbar m |\ell s; jm\rangle \tag{7.7}$$

a) Show that the operator $\hat{J}_z = \hat{L}_z + \hat{S}_z$ commutes with $\hat{H}_{so}$

b) Show that the opperators $\hat{S}^2$ and $\hat{L}^2$ also commute with $\hat{H}_{so}$

c) Rewrite $\hat{H}_{so}$ in terms of $\hat{J}^2$, $\hat{L}^2$, and $\hat{S}^2$, what are the energy eigenvalues you get when you act this part of the Hamiltonian on the states $|ls; jm\rangle$?

d) For an $\ell = 1$ state (p-orbital), j can have only two possible values: $j = \frac{1}{2}$ and $j = \frac{3}{2}$. What are the $\ell = 1$ energy eigenstates? What are their degeneracies?

e) Draw an energy level diagram for the Hydrogen 2p energy level without the spin-orbit coupling and with the spin orbit coupling, what is the energy splitting between the states due to H_{so} in terms of β?

a) $\beta \left[\hat{S}_x \hat{L}_x + \hat{S}_y \hat{L}_y + \hat{S}_z \hat{L}_z, \hat{L}_z + \hat{S}_z \right]$

$= \beta \left(\hat{S}_x [\hat{L}_x, \hat{L}_z] + \hat{S}_y [\hat{L}_y, \hat{L}_z] + [\hat{S}_x, \hat{S}_z] \hat{L}_x + [\hat{S}_y, \hat{S}_z] \hat{L}_y \right)$

$= \beta \left(\hat{S}_x (-i\hbar \hat{L}_y) + \hat{S}_y (+i\hbar \hat{L}_x) + (-i\hbar \hat{S}_y) \hat{L}_x + (+i\hbar \hat{S}_x) \hat{L}_y \right)$

$= 0$

b) $[\hat{H}_{so}, \hat{S}^2] = \beta \left([\hat{S}_x, \hat{S}^2]^0 \hat{L}_x + [\hat{S}_y, \hat{S}^2]^0 \hat{L}_y + [\hat{S}_z, \hat{S}^2]^0 \hat{L}_z \right)$

$\hat{S}^2$ commutes w/ all it's components.

similarly $[\hat{H}_{so}, \hat{L}^2] = \beta \left(\hat{S}_x [\hat{L}_x, \hat{L}^2]^0 + \hat{S}_y [\hat{L}_y, \hat{L}^2] + \hat{S}_z [\hat{L}_z, \hat{L}^2]^0 \right)$

c) $\hat{H}_{so} = \beta \vec{S} \cdot \vec{L} = \frac{\beta}{2} \left(\hat{J}^2 - \hat{S}^2 - \hat{L}^2 \right)$

so $\hat{H}_{so} | \ell s; j m \rangle = \frac{\beta \hbar^2}{2} \left(j(j+1) - s(s+1) - \ell(\ell+1) \right)$

d) For $\ell = 1$, $s = \frac{1}{2}$ j can be $\frac{3}{2}$ or $\frac{1}{2}$

$\hat{H}_{so} | 1 \frac{1}{2}; \frac{3}{2} m \rangle = \frac{\beta \hbar^2}{2} \left(\frac{3}{2} \left(\frac{3}{2} + 1 \right) - \frac{1}{2} \left(\frac{1}{2} + 1 \right) - 1 (1+1) \right)$

$= \frac{\beta \hbar^2}{2} \left(\frac{15}{4} - \frac{3}{4} - 2 \right) = \frac{+ \beta \hbar^2}{2}$

$\hat{H}_{so} | 1 \frac{1}{2}; \frac{1}{2} m \rangle = \frac{\beta \hbar^2}{2} \left(\frac{1}{2} \left(\frac{1}{2} + 1 \right) - \frac{1}{2} \left(\frac{1}{2} + 1 \right) - 2 \right)$

$= - \beta \hbar^2$

e) 2×3-fold degenerat

$2p$ $j = \frac{3}{2}$ 4-fold deg.

$\uparrow \beta \hbar^2/2$

$\uparrow \beta \hbar^2$

$j = \frac{1}{2}$

splitting $= \frac{3}{2} \beta \hbar^2$