

- Answer all questions, using the paper provided. Begin each problem on a separate sheet. The pages will be separated for grading, so clearly label the problem number and put your name on EACH PAGE.
- One 8.5 by 11 inch cheat sheet (front and back) allowed. No other books, calculators or notes allowed.
- SHOW ALL WORK.
- Potentially useful information:

$$d^3x = r^2 dr \sin \theta d\theta d\phi; \quad 0 \leq \theta \leq \pi; \quad 0 \leq \phi \leq 2\pi$$

$$\int x e^{ax} dx = \frac{e^{ax}}{a^2} (ax - 1) \quad \int x^2 e^{ax} dx = \frac{x^2 e^{ax}}{a} - \frac{2}{a} \int x e^{ax} dx$$

$$\int x^m e^{ax} dx = e^{ax} \sum_{r=0}^m (-1)^r \frac{m! x^{m-r}}{(m-r)! a^{r+1}}$$

$$\int (\sin^2 ax) dx = \frac{x}{2} - \frac{1}{4a} \sin 2ax \quad \int (\cos^2 ax) dx = \frac{x}{2} + \frac{1}{4a} \sin 2ax$$

$$\int (\sin ax) (\cos ax) dx = \frac{1}{2a} \sin^2 ax \quad \int (\sin^2 ax) (\cos^2 ax) dx = \frac{x}{8} - \frac{1}{32a} \sin 4ax$$

$$\int (\sin ax) (\cos^m ax) dx = -\frac{\cos^{m+1} ax}{(m+1)a} \quad \int (\sin^m ax) (\cos ax) dx = \frac{\sin^{m+1} ax}{(m+1)a}$$

$$L_x = i\hbar(\sin \phi \partial/\partial \theta + \cot \theta \cos \phi \partial/\partial \phi) \quad L_y = i\hbar(-\cos \phi \partial/\partial \theta + \cot \theta \sin \phi \partial/\partial \phi)$$

$$L_z = -i\hbar \partial/\partial \phi$$

n	l	m_l	Eigenfunctions
1	0	0	$\psi_{100} = \frac{1}{\sqrt{\pi}} \left(\frac{Z}{a_0}\right)^{3/2} e^{-Zr/a_0}$
2	0	0	$\psi_{200} = \frac{1}{4\sqrt{2\pi}} \left(\frac{Z}{a_0}\right)^{3/2} \left(2 - \frac{Zr}{a_0}\right) e^{-Zr/2a_0}$
2	1	0	$\psi_{210} = \frac{1}{4\sqrt{2\pi}} \left(\frac{Z}{a_0}\right)^{3/2} \frac{Zr}{a_0} e^{-Zr/2a_0} \cos \theta$
2	1	± 1	$\psi_{21\pm 1} = \frac{1}{8\sqrt{\pi}} \left(\frac{Z}{a_0}\right)^{3/2} \frac{Zr}{a_0} e^{-Zr/2a_0} \sin \theta e^{\pm i\phi}$
3	0	0	$\psi_{300} = \frac{1}{81\sqrt{3\pi}} \left(\frac{Z}{a_0}\right)^{3/2} \left(27 - 18\frac{Zr}{a_0} + 2\frac{Z^2 r^2}{a_0^2}\right) e^{-Zr/3a_0}$
3	1	0	$\psi_{310} = \frac{\sqrt{2}}{81\sqrt{\pi}} \left(\frac{Z}{a_0}\right)^{3/2} \left(6 - \frac{Zr}{a_0}\right) \frac{Zr}{a_0} e^{-Zr/3a_0} \cos \theta$
3	1	± 1	$\psi_{31\pm 1} = \frac{1}{81\sqrt{\pi}} \left(\frac{Z}{a_0}\right)^{3/2} \left(6 - \frac{Zr}{a_0}\right) \frac{Zr}{a_0} e^{-Zr/3a_0} \sin \theta e^{\pm i\phi}$
3	2	0	$\psi_{320} = \frac{1}{81\sqrt{6\pi}} \left(\frac{Z}{a_0}\right)^{3/2} \frac{Z^2 r^2}{a_0^2} e^{-Zr/3a_0} (3 \cos^2 \theta - 1)$
3	2	± 1	$\psi_{32\pm 1} = \frac{1}{81\sqrt{\pi}} \left(\frac{Z}{a_0}\right)^{3/2} \frac{Z^2 r^2}{a_0^2} e^{-Zr/3a_0} \sin \theta \cos \theta e^{\pm i\phi}$
3	2	± 2	$\psi_{32\pm 2} = \frac{1}{162\sqrt{\pi}} \left(\frac{Z}{a_0}\right)^{3/2} \frac{Z^2 r^2}{a_0^2} e^{-Zr/3a_0} \sin^2 \theta e^{\pm 2i\phi}$

1. (25 points total) *Short answer.*

(a) (4 points) The simple harmonic oscillator has a nonzero ground state energy. Why can't the ground state have zero energy?

(b) (4 points) Consider the isotropic harmonic oscillator in 3 dimensions, which would be described by the potential $V(\vec{r}) = (C/2)(x^2 + y^2 + z^2) = (C/2)r^2$. True or false: The eigenfunctions of this potential are states of definite total angular momentum. Explain *briefly*.

(c) (4 points) What is the largest number of electrons that can occupy the ground state in a multi-electron atom? (Ignore spin-orbit interaction and assume there is no magnetic field.) Why is there a maximum?

(d) (5 points) Consider an electron in a hydrogen atom with total angular momentum quantum number $j = 5/2$. What are the possible values of the electron's orbital angular momentum quantum number l ? For each l , what are the possible values of the principle quantum number n ?

(e) (3 points) Suppose you calculated the energy splitting in hydrogen due to the fine structure, and you found it to be about 50 keV. Why would you think this answer is wrong?

(f) (5 points) What are the selection rules on j and l for electric dipole transitions in the hydrogen atom? Where does each one come from? Be specific.

2. (10 points total) If a hydrogen atom is placed in a magnetic field that is very strong compared to its internal field, its orbital and spin magnetic dipole moments precess independently about the external field, and its energy depends on the quantum numbers m_l and m_s which specify their components along the external field direction.

(a) (5 points) What are the atom's orbital and spin magnetic dipole moments, in terms of the quantum numbers m_l and m_s , and whatever else they depend on?

(b) (5 points) Evaluate the splitting of the energy levels according to the values of m_l and m_s .

3. (17 points total) Consider the hydrogen atom (ignoring the spin-orbit interaction), with eigenfunctions given on the front page of the exam.

(a) (3 points) For a given eigenfunction ψ_{nlm} , what is the energy?

(b) (9 points) Consider the r dependence.

i. Find the expectation value of r for the $n = 1, l = 0$ state by explicit calculation. Check units.

ii. Do you expect the expectation value of r for, say, the $n = 2, l = 0$ state to be bigger or smaller? Why?

(c) (5 points) Suppose we had singly ionized helium (2 protons and 2 neutrons in the nucleus, one electron) instead of hydrogen.

i. By what factor would the energy levels E_n change with respect to hydrogen?

ii. By what factor would the *fractional* energy spacing $\frac{E_{n+1} - E_n}{E_n}$ change with respect to hydrogen?

4. (28 points total) Consider a particle in one dimension.

(a) (10 points) What is tunneling? Give a simple example of a potential in one dimension that can lead to tunneling. What total energy gives rise to the tunneling state?

(b) (10 points) Consider a 1-dimensional step potential, with $V = 0$ for $x < 0$ and $V = V_0$ for $x > 0$. Let a particle with mass m be incident from $x < 0$, with total energy $E < V_0$. Do you expect the energy to be quantized? Find the wave function for all x . You may keep it in terms of one arbitrary normalization constant.

(c) (8 points) For the potential in part (b), find the reflection and transmission coefficients at the step ($x = 0$).

5. (20 points total) Many of the properties we have found for quantum mechanical systems can be described in terms of the mathematical operators that correspond to physical quantities. A very important role is played by the “commutator” of two operators. The commutator has to do with what happens when you apply two operators to a wave function in different orders, for example taking $A(B\psi)$ vs. $B(A\psi)$, where A and B are operators such as L^2 or the energy operator H . If $A(B\psi) = B(A\psi)$, the two operators are said to commute.

(a) (5 points) It turns out that if two operators do not commute, then you cannot have wavefunctions that are eigenfunctions of both operators simultaneously. Show that this is true by showing that if two operators do have simultaneous eigenfunctions, then they commute. That is, show that if

$$A\psi = a\psi \quad \text{and} \quad B\psi = b\psi$$

for the same ψ , where a and b are just numbers, then

$$A(B\psi) = B(A\psi).$$

(Hint: If this is too abstract, you may substitute specific operators for A and B . For example, you could use the hydrogen atom energy operator H and the total angular momentum operator L^2 .)

(b) (8 points) Take the hydrogen atom, without spin-orbit coupling, and show explicitly that for the eigenstate ψ_{210} , L_z and either L_x or L_y do not commute. That is, show one of

$$L_z(L_x\psi_{210}) \neq L_x(L_z\psi_{210}) \quad \text{or} \quad L_z(L_y\psi_{210}) \neq L_y(L_z\psi_{210}).$$

(c) (7 points) Now add in spin-orbit coupling.

i. What is the energy shift (generally, not for a specific eigenstate) in terms of the electron's spin and orbital angular momentum vectors?

ii. Using the results of parts (a) and (b), and assuming the result in (b) applies to all eigenstates, give an argument for why m_l is no longer a good quantum number when you introduce spin-orbit coupling. (Hint: Think of your result in (i) as an operator, and note that overall constants do not affect commutation properties.)

P237 Final Exam Solns
Spring 2005

①

1. a) If the SHO had 0 energy in its ground state, it would be exactly localized and its velocity and momentum would be exactly zero. Therefore the corresponding uncertainties would also be 0, and $\Delta x \Delta p = 0$, violating the uncertainty principle.

b) True, because potential is spherically symmetric.

c) False. Electrons are $1/2$ particles and the wave function must be anti-symmetric under particle exchange.

d) At most two electrons can occupy the ground state ($n=1, l=0, m_l=0$), because no more than one electron can be in a given quantum state. In the ground state we can have $n=1, l=0, m_l=0$, and $m_s = \pm 1/2$.

d) $j = 5/2$. Since $j = l \pm \frac{1}{2}$, $l = 2$ or $l = 3$
 $l = 2: n \geq 3 \quad (3, 4, 5, \dots)$
 $l = 3: n \geq 4 \quad (4, 5, \dots)$

e) 50 KeV is much larger than the energy of the hydrogen levels themselves; it would be enough to ionize the atom, unsplit

1. cont

(2)

f) Selection rules for electric dipole transitions:

$$\Delta l = \pm 1$$

$$\Delta j = 0, \pm 1$$

$|\Delta l|$ odd comes from parity. We must have

$$P_{fi} = \left| \int \psi_f^* (-e\vec{r}) \psi_i d^3r \right| \neq 0$$

$\psi_f + \psi_i$ have parity $(-1)^l$; $\vec{r}$ has parity -1 .

Integrand must be even $(+1)$ so must have $|\Delta l|$ odd.

$\Delta j = 0, \pm 1$ follows fr/ photon carrying away 1 unit of angular momentum. $\Delta l = \pm 1$ follows from $\Delta j = 0, \pm 1$ and Δl odd

(3)

2. a) Orbital + spin magnetic dipole moments

$$\text{orb: } \vec{\mu}_L = \frac{-g_L \mu_B}{\hbar} \vec{L}$$

$$L_z = \hbar m_L$$

$$= -\frac{e}{2m} \vec{L}$$

$$g_L = 1, \mu_B = \frac{e \hbar}{2m}$$

$$\text{spin: } \vec{\mu}_S = \frac{-g_S \mu_B}{\hbar} \vec{S}$$

$$\text{and } S_z = \hbar m_S$$

$$= -\frac{e}{m} \vec{S}$$

$$g_S = 2, \text{ same } \mu_B$$

$$b) \Delta E = -\vec{\mu} \cdot \vec{B}$$

$$\text{orb: } \Delta E = -\vec{\mu}_L \cdot \vec{B} = -\mu_{L,z} B = +\frac{e}{2m} L_z B$$

assuming z direction = direction of $\vec{B}$

$$= \frac{e}{2m} \hbar B m_L = \boxed{+g_L \mu_B m_L B}$$

$$\text{spin: } \Delta E = -\vec{\mu}_S \cdot \vec{B} = -\mu_{S,z} B$$

$$= +\frac{e}{m} \hbar B m_S = \boxed{+g_S \mu_B m_S B}$$

(4)

3. H atom

$$a) E_n = -\frac{\mu Z^2 e^4}{(4\pi\epsilon_0)^2 2\hbar^2 n^2} = -\frac{\mu e^4}{(4\pi\epsilon_0)^2 2\hbar^2 n^2} \quad \text{since } Z=1 \text{ for hydrogen}$$

$$= \frac{-13.6 \text{ eV}}{n^2}$$

b) i. Find $\bar{r}$ for $n=1, l=0$:

$$\begin{aligned} \bar{r} &= \int \psi_{100}^* r \psi_{100} d^3r \quad \psi_{100} = \frac{1}{\sqrt{\pi}} \left(\frac{1}{a_0}\right)^{3/2} e^{-r/a_0} \\ &= \frac{1}{\pi a_0^3} \int_0^\infty e^{-2r/a_0} r^3 dr \int_0^\pi \sin\theta d\theta \int_0^{2\pi} d\phi \end{aligned}$$

From integral given on front of test,

$$\int_0^\infty x^m e^{ax} dx = e^{ax} \sum_{r=0}^m (-1)^r \frac{m! x^{m-r}}{(m-r)! a^{r+1}} \Big|_0^\infty$$

where $a = -2/a_0$

Note that the right hand side vanishes at the upper limit for all r because of the $e^{-(2/a_0)x}$ term. At the lower limit, all terms vanish except $r=m$ because of the x^{m-r} term.

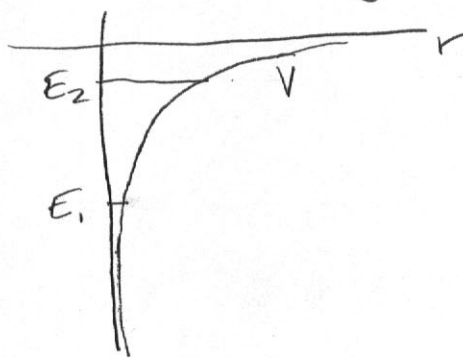
$$\therefore \int_0^\infty x^m e^{ax} dx = -e^{ax} (-1)^m \frac{m!}{a^{m+1}} = \frac{3!}{(-2/a_0)^4} = \frac{3a_0^4}{8}$$

3b) cont

(5)

$$\text{so } \bar{r} = \frac{1}{\pi a_0^3} \frac{3a_0^4}{8} \frac{1}{Z} = \boxed{\frac{3}{2} a_0 = \bar{r}}$$

ii) For $n=2$ we expect $\bar{r}$ to be bigger. Mathematically, we get an extra power of r in the integrand, which gives more weight to higher values of r . Physically, look at the energy with respect to the potential:



E_2 allows the wave fn to be large to higher values of r .

c) Helium ($Z=2$) instead of hydrogen

i. $E_n \propto Z^2$ so E_n for helium is bigger by a factor of 4 than E_n for hydrogen.

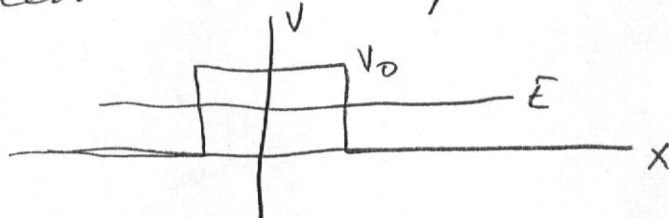
ii. The Z dependence cancels in the ratio $\frac{E_{n+1} - E_n}{E_n}$ so the fractional energy spacing does not change, i.e. the factor is 1.

[Note that the increased mass of the helium nucleus doesn't matter much here; the reduced mass is still approximately the same as the electron mass]

④ Particle in 1-D

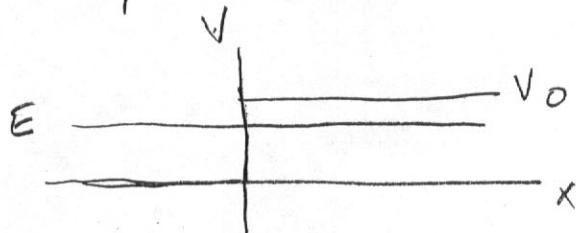
⑥

- a) Tunneling happens when a particle goes from one region to another when the region in between is classically inaccessible. E.g.:



Total energy must be $E < V_0$ for tunneling.

- b) 1-D step potential



We do not expect the energy to be quantized, because $E > V_0$ as $x \rightarrow \infty$.

Find w.f. for all x :

$$x < 0: \quad \psi(x) = A e^{i k_1 x} + B e^{-i k_1 x} \quad K_1 = \frac{\sqrt{2mE}}{\hbar}$$

$$x > 0: \quad \psi(x) = \cancel{C} e^{K_2 x} + D e^{-K_2 x} \quad K_2 = \sqrt{2m(V_0 - E)}$$

take $C = 0$, since this term is not finite.

boundary conditions:

$$\psi \text{ continuous at } x=0: \quad A + B = D$$

$$\frac{d\psi}{dx} \text{ continuous at } x=0: \quad i k_1 A - i k_1 B = -K_2 D$$

$$\Rightarrow A - B = \frac{i K_2}{k_1} D$$

Solving for A + B in terms of D:

$$2A = \left(1 + \frac{ik_2}{k_1}\right) D \Rightarrow A = \frac{1}{2} \left(1 + \frac{ik_2}{k_1}\right) D$$

$$2B = \left(1 - \frac{ik_2}{k_1}\right) D \Rightarrow B = \frac{1}{2} \left(1 - \frac{ik_2}{k_1}\right) D$$

$$\therefore \begin{cases} x < 0: & \psi(x) = \frac{D}{2} \left(1 + \frac{ik_2}{k_1}\right) e^{ik_1 x} + \frac{D}{2} \left(1 - \frac{ik_2}{k_1}\right) e^{-ik_1 x} \\ x > 0: & \psi(x) = D e^{-k_2 x} \end{cases}$$

c) Current $\vec{j} = \frac{\hbar}{2mi} \left[\Psi^* \nabla \Psi - (\nabla \Psi^*) \Psi \right]$ in 3D

In 1-D, $\vec{j} = \hat{x} \frac{\hbar}{2mi} \left[\psi^* \frac{d\psi}{dx} - (\frac{d\psi^*}{dx}) \psi \right]$ assuming energy eigenstate so time dep. cancels

$j_{inc} = \hat{x} \frac{\hbar}{2mi} \left[\psi_{inc}^* \frac{d\psi_{inc}}{dx} - \left(\frac{d\psi_{inc}^*}{dx} \right) \psi \right]$ $\psi_{inc} = A e^{ik_1 x}$

$$|A|^2 (ik_1 - (-ik_1)) = \frac{2|A|^2 ik_1}{\hbar}$$

$$= \hat{x} \frac{\hbar k_1}{m} |A|^2 = \frac{\hbar k_1}{m} \frac{|D|^2}{4} \left(1 + \frac{k_2^2}{k_1^2}\right)$$

$j_{refl} = \hat{x} \frac{\hbar}{2mi} \left[|B|^2 (-ik_1 - ik_1) \right]$ $\psi_{refl} = B e^{-ik_1 x}$

$$= \hat{x} \frac{\hbar k_1}{m} |B|^2 = -\hat{x} \frac{\hbar k_1}{m} \frac{|D|^2}{4} \left(1 + \frac{k_2^2}{k_1^2}\right)$$

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$$j_{\text{trans}} = \frac{\hbar}{2mi} \left[\psi_{\text{trans}}^* \frac{d\psi_{\text{trans}}}{dx} - \frac{d\psi_{\text{trans}}^*}{dx} \psi \right]$$
$$= \frac{\hbar}{2mi} |D|^2 \left[-k_2 e^{-2k_2 x} - (-k_2) e^{-2k_2 x} \right]$$

$= 0$

$= 0$

reflection coefficient

$$R = \frac{|j_{\text{refl}}|}{|j_{\text{inc}}|} = \frac{\frac{\hbar k_1}{m} \frac{|D|^2}{4} \left(1 + \frac{k_2^2}{k_1^2} \right)}{\frac{\hbar k_1}{m} \frac{|D|^2}{4} \left(1 + \frac{k_2^2}{k_1^2} \right)}$$

$= 1$

transmission coefficient

$$T = \frac{|j_{\text{trans}}|}{|j_{\text{inc}}|} = 0 = 1 - R$$

(9)

5. a) Show $A\psi = a\psi + B\psi = b\psi \Rightarrow A(B\psi) = B(A\psi)$

$$A(B\psi) = A(b\psi) = bA\psi = ba\psi = ab\psi$$

$$B(A\psi) = B(a\psi) = aB\psi = ab\psi$$

b) For H atom, show

$$L_z(L_x \psi_{210}) \neq L_x(L_z \psi_{210})$$

$$\psi_{210} = \underbrace{\frac{1}{4\sqrt{2}\pi} \left(\frac{r}{a_0}\right)^{3/2} \frac{r}{a_0} e^{-r/2a_0}}_{\text{let } = R} \cos\theta$$

let $= R$; L_x, L_y, L_z don't do anything to R

$$L_z(L_x \psi_{210}): L_x \psi_{210} = i\hbar \left(\sin\varphi \frac{\partial}{\partial \theta} + \cot\theta \cos\varphi \frac{\partial}{\partial \varphi} \right) R \cos\theta$$

$$= i\hbar R \sin\varphi \frac{\partial}{\partial \theta} \cos\theta$$

$$= -i\hbar R \sin\varphi \sin\theta$$

$$L_z(L_x \psi_{210}) = (-i\hbar)^2 R \frac{\partial}{\partial \varphi} [\sin\varphi \sin\theta]$$

$$= -\hbar^2 R \cos\varphi \sin\theta$$

$$L_x(L_z \psi_{210}): L_z \psi_{210} = -i\hbar \frac{\partial}{\partial \varphi} R \cos\theta = 0$$

$$\Rightarrow L_x(L_z \psi_{210}) = 0$$

$$\therefore L_z L_x \psi_{210} \neq L_x L_z \psi_{210}$$

5 b) cont

Similarly, for $L_y + L_z$:

(10)

$$\begin{aligned} L_z(L_y \psi_{210}): L_y \psi_{210} &= i\hbar(-\cos\varphi \frac{\partial}{\partial\theta} + \cot\theta \sin\varphi \frac{\partial}{\partial\varphi}) R \cos\theta \\ &= -i\hbar R \cos\varphi \frac{\partial}{\partial\theta} \cos\theta \\ &= i\hbar R \cos\varphi \sin\theta \end{aligned}$$

$$\begin{aligned} L_z(L_y \psi_{210}) &= -(i\hbar)^2 R \frac{\partial}{\partial\varphi} (\cos\varphi \sin\theta) \\ &= \hbar^2 R \sin\varphi \sin\theta \end{aligned}$$

$$L_y(L_z \psi_{210}) = L_y(0) = 0$$

$$\therefore L_z L_y \psi_{210} \neq L_y L_z \psi_{210}$$

c) Spin-orbit coupling:

$$i. \Delta E_{\text{spin-orbit}} = \frac{1}{2m^2 c^2} \frac{1}{r} \frac{dV(r)}{dr} \vec{S} \cdot \vec{L}$$

ii. We can write $\vec{S} \cdot \vec{L}$ as $S_x L_x + S_y L_y + S_z L_z$

Since L_z doesn't commute with L_y and L_x , it doesn't commute with the energy operator that includes the spin-orbit interaction. Therefore if the atom is in an eigenstate of the energy, it cannot be in an eigenstate of L_z . Since $L_z = \hbar m_l$, m_l is no longer a good quantum number.