Assignments for Mid-Spring_2023 of Atomic and Molecular Physics

1. Show that the conditions of the quantum numbers of one-electron atom shown in the following two boxes are equivalent.

$\lvert m_l \rvert = 0, 1, 2, 3, \ldots$ $l = \lvert m_l \rvert, \lvert m_l \rvert + 1, \lvert m_l \rvert + 2, \lvert m_l \rvert + 3, \ldots$ $n = l + 1, l + 2, l + 3, \ldots$	$n = 1, 2, 3, \ldots$ $l = 0, 1, 2, \ldots, n - 1$ $m_l = -l, -l + 1, \ldots, 0, \ldots, +l - 1, l$

2.

Work out all of the **canonical commutation relations** for components of the operators **r** and **p**: $[x, y]$, $[x, p_y]$, $[x, p_x]$, $[p_y, p_z]$, and so on.

3.

Use separation of variables in *cartesian* coordinates to solve the infinite *cubical* well (or "particle in a box"):

$$V(x, y, z) = \begin{cases} 0, & \text{if } x, y, z \text{ are all between 0 and } a; \\ \infty, & \text{otherwise.} \end{cases}$$

(a) Find the stationary states, and the corresponding energies.

(b) Call the distinct energies $E_1, E_2, E_3, \ldots$, in order of increasing energy. Find E_1, E_2, E_3, E_4, E_5, and E_6. Determine their degeneracies (that is, the number of different states that share the same energy). *Comment:* In *one* dimension degenerate bound states do not occur (see Problem 2.45), but in three dimensions they are very common.

(c) What is the degeneracy of E_{14}, and why is this case interesting?

4.

Consider the **infinite spherical well**, $V(r) = \begin{cases} 0, & \text{if } r \le a; \\ \infty, & \text{if } r > a. \end{cases}$

Find the wave functions and the allowed energies.

5. Verify that the eigenfunction ,

$$\psi_{21\pm1} = \frac{1}{8\sqrt{\pi}} \left(\frac{Z}{a_0}\right)^{3/2} \frac{Zr}{a_0} e^{-Zr/2a_0} \sin\theta \, e^{\pm i\varphi}$$

and the associated eigenvalue E2, satisfy the time-independent Schroedinger equation

$$-\frac{\hbar^2}{2\mu}\nabla^2\psi(r,\theta,\varphi) + V(r)\psi(r,\theta,\varphi) = E\psi(r,\theta,\varphi)$$

for the one-electron atom with Z = 1

6. (a) Calculate the location at which the radial probability density is a maximum for the ground state of the hydrogen atom. (b) Next calculate the expectation value for the radial coordinate in this state. (c) Then interpret these results in terms of the results of measurements of the location of the electron in the atom.

$$\psi_{100} = \frac{1}{\sqrt{\pi}}\left(\frac{Z}{a_0}\right)^{3/2} e^{-Zr/a_0}$$

7. In its ground state, the size of the hydrogen atom can be taken to be the radius of the n = 1 shell for Z = 1, which is essentially $a_0 = 4\pi\epsilon_0\hbar^2/\mu e^2 \simeq 0.5$ Å.

Show that this fundamental atomic dimension can be obtained directly from consideration of the uncertainty principle.

8. Evaluate the average of the probability density functions for the following set of degenerate states corresponding to the energy E2

$$\psi_{200} = \frac{1}{4\sqrt{2\pi}}\left(\frac{Z}{a_0}\right)^{3/2}\left(2 - \frac{Zr}{a_0}\right)e^{-Zr/2a_0} \quad ; \qquad \psi_{210} = \frac{1}{4\sqrt{2\pi}}\left(\frac{Z}{a_0}\right)^{3/2}\frac{Zr}{a_0}e^{-Zr/2a_0}\cos\theta$$

$$\psi_{21\pm1} = \frac{1}{8\sqrt{\pi}}\left(\frac{Z}{a_0}\right)^{3/2}\frac{Zr}{a_0}e^{-Zr/2a_0}\sin\theta\, e^{\pm i\varphi}$$

9.

Work out the radial wave functions R_{30}, R_{31}, and R_{32}, using the recursion formula

$$c_{j+1} = \frac{2(j+l+1-n)}{(j+1)(j+2l+2)}c_j. \qquad R_{nl}(r) = \frac{1}{r}\rho^{l+1}e^{-\rho}v(\rho)$$

10.

(a) Find $\langle r\rangle$ and $\langle r^2\rangle$ for an electron in the ground state of hydrogen. Express your answers in terms of the Bohr radius.

(b) Find $\langle x\rangle$ and $\langle x^2\rangle$ for an electron in the ground state of hydrogen. *Hint:* This requires no new integration—note that $r^2 = x^2 + y^2 + z^2$, and exploit the symmetry of the ground state.

(c) Find $\langle x^2\rangle$ in the state $n = 2$, $l = 1$, $m = 1$. *Warning:* This state is *not* symmetrical in x, y, z. Use $x = r\sin\theta\cos\phi$.

11.

A hydrogen atom starts out in the following linear combination of the stationary states $n = 2$, $l = 1$, $m = 1$ and $n = 2$, $l = 1$, $m = -1$:

$$\Psi(\mathbf{r}, 0) = \frac{1}{\sqrt{2}}(\psi_{211} + \psi_{21-1})$$

(a) Construct $\Psi(\mathbf{r}, t)$. Simplify it as much as you can.

(b) Find the expectation value of the potential energy, $\langle V \rangle$. (Does it depend on t?) Give both the formula and the actual number, in electron volts.

12.

A **hydrogenic atom** consists of a single electron orbiting a nucleus with Z protons ($Z = 1$ would be hydrogen itself, $Z = 2$ is ionized helium, $Z = 3$ is doubly ionized lithium, Determine the Bohr energies $E_n(Z)$, the binding energy $E_1(Z)$, the Bohr radius $a(Z)$, and the Rydberg constant $R(Z)$ for a hydrogenic atom.
(Express your answers as appropriate multiples of the hydrogen values.)
Where in the electromagnetic spectrum would the Lyman series fall, for $Z = 2$ and $Z = 3$?

13.

(a) Starting with the canonical commutation relations for position and momentum $[r_i, p_j] = -[p_i, r_j] = i\hbar\delta_{ij}$, $[r_i, r_j] = [p_i, p_j] = 0$, work out the following commutators:
$[L_z, x] = i\hbar y$, $[L_z, y] = -i\hbar x$, $[L_z, z] = 0$,
$[L_z, p_x] = i\hbar p_y$, $[L_z, p_y] = -i\hbar p_x$, $[L_z, p_z] = 0$.

(b) Use these results to obtain $[L_z, L_x] = i\hbar L_y$ directly from Equation 4.96.

(c) Evaluate the commutators $[L_z, r^2]$ and $[L_z, p^2]$ (where, of course, $r^2 = x^2 + y^2 + z^2$ and $p^2 = p_x^2 + p_y^2 + p_z^2$).

(d) Show that the Hamiltonian $H = (p^2/2m) + V$ commutes with all three components of $\mathbf{L}$, provided that V depends only on r. (Thus H, L^2, and L_z are mutually compatible observables.)

14.

(a) Prove that for a particle in a potential $V(\mathbf{r})$ the rate of change of the expectation value of the orbital angular momentum $\mathbf{L}$ is equal to the expectation value of the torque: $\frac{d}{dt}\langle \mathbf{L} \rangle = \langle \mathbf{N} \rangle$ where $\mathbf{N} = \mathbf{r} \times (-\nabla V)$

(b) Show that $d\langle \mathbf{L} \rangle / dt = 0$ for any spherically symmetric potential. (This is one form of the quantum statement of **conservation of angular momentum**.)

15.

Suppose a spin-1/2 particle is in the state $\chi = \frac{1}{\sqrt{6}} \begin{pmatrix} 1+i \\ 2 \end{pmatrix}$

What are the probabilities of getting $+\hbar/2$ and $-\hbar/2$, if you measure S_z and S_x?

16.

An electron is in the spin state $\chi = A \begin{pmatrix} 3i \\ 4 \end{pmatrix}$

(a) Determine the normalization constant A.

(b) Find the expectation values of S_x, S_y, and S_z.

(c) Find the "uncertainties" σ_{S_x}, σ_{S_y}, and σ_{S_z}. (*Note:* These sigmas are standard deviations, not Pauli matrices!)

(d) Confirm that your results are consistent with all three uncertainty principles

17.

For the most general normalized spinor χ $\chi = \begin{pmatrix} a \\ b \end{pmatrix} = a\chi_+ + b\chi_-$, compute $\langle S_x \rangle$, $\langle S_y \rangle$, $\langle S_z \rangle$, $\langle S_x^2 \rangle$, $\langle S_y^2 \rangle$, and $\langle S_z^2 \rangle$. Check that $\langle S_x^2 \rangle + \langle S_y^2 \rangle + \langle S_z^2 \rangle = \langle S^2 \rangle$

18.

(a) Find the eigenvalues and eigenspinors of $\mathbf{S}_y$.

(b) If you measured S_y on a particle in the general state χ (Equation 4.139), what values might you get, and what is the probability of each? Check that the probabilities add up to 1. *Note:* a and b need not be real!

(c) If you measured S_y^2, what values might you get, and with what probabilities?

19.

Larmor precession: Imagine a particle of spin 1/2 at rest in a uniform magnetic field,

$$\mathbf{B} = B_0 \hat{k}.$$

Write down the interaction Hamiltonian. Determine the eigenvalues and stationary state. What is the general state? Determine the expectation value of the spin angular momentum and show that it undergoes precession around the Z axis with Larmor frequency. Determine the expression for Larmor frequency.

20. Vector treatment of Stern-Gerlach experiment. In an inhomogeneous magnetic field, there is not only a torque, but a Force acts on a stream of magnetic dipole: $\mathbf{F} = \nabla(\boldsymbol{\mu} \cdot \mathbf{B})$

$$\mathbf{B}(x, y, z) = -\alpha x \hat{\imath} + (B_0 + \alpha z)\hat{k}, \quad \mathbf{F} = \gamma\alpha(-S_x \hat{\imath} + S_z \hat{k})$$

But because of the Larmor precession about B_0, S_x oscillates rapidly, and *averages* to zero; the *net* force is in the z direction: $F_z = \gamma\alpha S_z$

In the frame of the moving magnetic dipoles, the Hamiltonian has the form

$$H(t) = \begin{cases} 0, & \text{for } t < 0, \\ -\gamma(B_0 + \alpha z)S_z, & \text{for } 0 \le t \le T, \\ 0, & \text{for } t > T. \end{cases}$$

Where T is the time taken by the dipole to cross the region of the magnetic field and B_0 is the Uniform part of the field.

Determine the general spin state after passing through the Stern-Gerlach set-up. Determine the momentum experienced by the dipoles in the z direction.

(a) If you measured the component of spin angular momentum along the x direction, at time t, what is the probability that you would get $+\hbar/2$?

(b) Same question, but for the y-component.

(c) Same, for the z component.

21.

An electron is at rest in an oscillating magnetic field $\mathbf{B} = B_0 \cos(\omega t)\hat{k}$, where B_0 and ω are constants.

(a) Construct the Hamiltonian matrix for this system.

(b) The electron starts out (at $t = 0$) in the spin-up state with respect to the x-axis (that is: $\chi(0) = \chi_+^{(x)}$). Determine $\chi(t)$ at any subsequent time. *Beware:* This is a time-*dependent* Hamiltonian, so you cannot get $\chi(t)$ in the usual way from stationary states. Fortunately, in this case you can solve the time-dependent Schrödinger equation (Equation 4.162) directly.

(c) Find the probability of getting $-\hbar/2$, if you measure S_x. *Answer:*

$$\sin^2\left(\frac{\gamma B_0}{2\omega}\sin(\omega t)\right).$$

(d) What is the minimum field (B_0) required to force a complete flip in S_x?

22. Hydrogen, deuterium, and singly ionized helium are all examples of one-electron atoms. The deuterium nucleus has the same charge as the hydrogen nucleus, and almost exactly twice the mass. The helium nucleus has twice the charge of the hydrogen nucleus, and almost exactly four times the mass. Make an accurate prediction of the ratios of the ground state energies of these atoms. (Hint: Remember the variation in the reduced mass.)

23. (a) Evaluate, in electron volts, the energies of the three levels of the hydrogen atom in the states for n = 1, 2, 3. (b) Then calculate the frequencies in hertz, and the wavelengths in angstroms, of all the photons that can be emitted by the atom in transitions between these levels. (c) In what range of the electromagnetic spectrum are these photons?

24. (a) Calculate the location at which the radial probability density is a maximum for the n = 2, 1 = 1 state of the hydrogen atom. (b) Then calculate the expectation value of the radial coordinate in this state. (c) Explain the physical significance of the difference in the answers to (a) and (b).

25. (a) Calculate the expectation value V for the potential energy in the ground state of the hydrogen atom. (b) Show that in the ground state E = V/2, where E is the total energy. (c) Use the relation E = K + V to calculate the expectation value K of the kinetic energy in the ground state, and show that K = — V/2. These relations are obtained for any state of motion of any quantum mechanical (or classical) system with a potential in the form V(r) ~— 1/r. They are sometimes called the virial theorem.

26. (a) Calculate the expectation value V of the potential energy in the n = 2, 1 = 1 state of the hydrogen atom. (b) Do the same for the n = 2, 1 = 0 state. (c) Discuss the results of (a) and (b), in connection with the virial theorem of earlier Problem, and explain how they bear on the origin of the 1 degeneracy.

27. Consider the probability of finding the electron in the hydrogen atom somewhere inside a cone of semiangle 23.5° of the +z axis ("arctic polar region"). (a) If the electron were equally likely to be found anywhere in space, what would be the probability of finding the electron in the arctic polar region? (b) Suppose the atom is in the state n = 2, *l* = 1, m_l= 0; recalculate the probability of finding the electron in the arctic polar region.

28. Consider the hydrogen atom eigenfunction Ψ_{432}. What are (a) the total energy in eV; (b) the expectation value of the radial coordinate in A; (c) the total angular momentum; (d) the z component of the angular momentum; (e) the uncertainty in the angular momentum; (f) the uncertainty in the z component of the angular momentum?

29.

(a) Evaluate $L_{x_{op}}\psi_{21-1}$ for the hydrogen atom. (b) Why does the result indicate that ψ_{21-1} is not an eigenfunction of $L_{x_{op}}$?

30.

Prove that $L^2_{op}\psi_{nlm_l} = l(l+1)\hbar^2\psi_{nlm_l}$

31.

We know that $\psi = e^{ikx}$ is an eigenfunction of the total energy operator e_{op} for the one-dimensional problem of the zero potential. (a) Show that it is also an eigenfunction of the linear momentum operator p_{op}, and determine the associated momentum eigenvalue. (b) Repeat for $\psi = e^{-ikx}$. (c) Interpret what the results of (a) and (b) mean concerning measurements of the linear momentum. (d) We also know that $\psi = \cos kx$ and $\psi = \sin kx$ are eigenfunctions of the zero potential e_{op}. Are they eigenfunctions of p_{op}? (e) Interpret the results of (d).

32.

Assume that a magnetic dipole, whose moment has magnitude μ_l, is aligned parallel to an external magnetic field, whose strength has magnitude B. Take $\mu_l = 1$ Bohr magneton (typical of the magnetic dipole moment of an atom), and $B = 1$ tesla (typical of the field produced by a fairly powerful electromagnet). Calculate the energy required to turn the magnetic dipole so that it is aligned antiparallel to the field.

33. A beam of hydrogen atoms, emitted from an oven running at a temperature T = 400°K, is sent through a Stern-Gerlach magnet of length X =1 m. The atoms experience a magnetic field with a gradient of 10 tesla/m. Calculate the transverse deflection of a typical atom in each component of the beam, due to the force exerted on its spin magnetic dipole moment, at the point where the beam leaves the magnet.

34. stimate the magnitude of the orientational potential energy AE for the n = 2, l = 1 state of the hydrogen atom, to check whether it is of the same order of magnitude as the observed fine-structure splitting of the corresponding energy level. (There is no spin-orbit energy in the n = 1 state, since for n = 1 the only possible value for lis l = 0, which means L = 0.)

35. Estimate the magnitude of the magnetic field B acting on the spin magnetic dipole moment of the electron in the earlier problem.

36. Enumerate the possible values of the quantum numbers j and m_i, for states in which 1 = 2 and, of course, s = 1/2.

37.

The field of an electromagnet is given by $B = 0.02 + 0.0115z^2$, with B in tesla and z = distance in cm from the north pole of the magnet. A magnetic dipole whose moment has magnitude 1.34×10^{-23} amp-m^2 is located 8.00 cm from the north pole, the dipole moment vector at 40° to the local magnetic field direction. What are (a) the torque on the dipole, (b) the force on the dipole, and (c) the energy released if the magnetic dipole is turned parallel to the field?

38. A beam of hydrogen atoms in their ground state is sent through a Stern-Gerlach magnet, which splits it into two components according to the two spin orientations. One component is stopped by a diaphragm at the end of the magnet, and the other continues into a second Stern-Gerlach magnet which is coaxial with the beam leaving the first magnet,

but is rotated relative to the first magnet about their approximately common axes through an angle a. There is a second diaphragm fixed on the end of the second magnet which also allows only one component to pass. Describe qualitatively how the intensity of the beam passing the second diaphragm depends on a.

39. Determine the field gradient of a 50 cm long Stern-Gerlach magnet that would produce a 1 mm separation at the end of the magnet between the two components of a beam of silver atoms emitted with typical kinetic energy from a 960°C oven. The magnetic dipole moment of silver is due to a single *1* = 0 electron, just as for hydrogen.

40. If a hydrogen atom is placed in a magnetic field which 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) Evaluate the splitting of the energy levels according to the values of m_l and m_s. (b) Draw the pattern of split levels originating from the $n = 2$ level, enumerating the quantum numbers of each component of the pattern. (c) Calculate the strength of the external magnetic field that would produce an energy difference between the most widely separated $n = 2$ levels which equals the difference between the energies of the n = 1 and n = 2 levels in the absence of the field.

41.

Prove that the only possible values of the quantum number j from the series $j = l + 1/2$, $l - 1/2$, $l - 3/2$, . . . , that satisfy the inequality $\sqrt{j(j+1)} \geq \left|\sqrt{l(l+1)} - \sqrt{s(s+1)}\right|$ with $s = 1/2$, are $j = l + 1/2$, $l - 1/2$, if $l \neq 0$, or $j = 1/2$, if $l = 0$.

42.

(a) Enumerate the possible values of j and m_j, for the states in which $l = 1$, and, of course, $s = 1/2$. (b) Draw the corresponding "vector model" figures. (c) Draw a figure illustrating the angular momentum vectors for a typical state. (d) Show also the spin and orbital magnetic dipole moment vectors, and their sum the total magnetic dipole moment vector. (e) Is the total magnetic dipole moment vector antiparallel to the total angular momentum vector?

43.

Consider the states in which $l = 4$ and $s = 1/2$. For the state with the largest possible j and largest possible m_j, calculate (a) the angle between $\mathbf{L}$ and $\mathbf{S}$, (b) the angle between $\boldsymbol{\mu}_l$ and $\boldsymbol{\mu}_s$, and (c) the angle between $\mathbf{J}$ and the $+z$ axis.

44. Enumerate the possible values of j and m_j for states in which / = 3 and $s = 1/2$.