

# University Quantum Mechanics II · Midterm Examination

The first eight units of Quantum Mechanics II on one paper: the spherical harmonics and the hydrogen radial functions derived rather than quoted, spin and charge in magnetic fields, composite systems and density operators, rotations and the addition of angular momentum, time-independent perturbation theory, identical particles, and the fine structure of hydrogen. Every degenerate perturbation is diagonalised in the basis its symmetry picks out, and the results the course quotes rather than derives, such as the Thomas factor and the Darwin term, are given in the stems.

| SUGGESTED TIME    | TOTAL MARKS | QUESTIONS | MULTIPLE CHOICE |
|-------------------|-------------|-----------|-----------------|
| <b>90 minutes</b> | <b>74</b>   | <b>14</b> | <b>8</b>        |

SECTION **UQMII · Midterm · University Quantum Mechanics II — Midterm examination**

IN THE FORMAT OF A university midterm: conceptual multiple choice, structured problems, a data-analysis question and an extended derivation

DEMAND **Recall 2 · Routine 5 · Demanding 6 · Discriminating 1**

*Pitched at what a strong course grade requires rather than at what a homework set rehearses. Routine substitutions carry few marks; most sit on problems that have to be set up before they can be solved, on derivations from a named law, and on checking a result against its limits. Every paper still opens with entry points, so you can tell which marks you should be securing first.*

COURSE UNITS UQMII-01 · UQMII-02 · UQMII-03 · UQMII-04 · UQMII-05 · UQMII-06 · UQMII-07 · UQMII-08

## INSTRUCTIONS

- Answer all questions in the spaces provided.
- Show your working. Method marks are awarded even where the final answer is wrong.
- Give your answers to a sensible number of significant figures, with a unit.
- The mark scheme for this paper follows the last question.

*Written by GioPhysics from its own University Physics course maps. These are practice examinations in a university style: they are not the examinations of any university, contain no past-paper questions, and carry no academic credit. For a course you are taking, your instructor's syllabus and past papers remain the authority.*

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# University Quantum Mechanics II · Midterm Examination

Answer all questions. 74 marks in 90 minutes.

**1** MULTIPLE CHOICE · ROUTINE · UQMII-01.01 · UQMII-01.02 [1]  
CORE COURSE

Separating the angular equation for  $m = 0$  and writing  $x = \cos \theta$  gives Legendre's equation,  $(1 - x^2)y'' - 2xy' + \lambda y = 0$ . Substituting  $y = \sum a_k x^k$  gives the recursion  $a_{k+2} = [k(k+1) - \lambda]a_k / [(k+1)(k+2)]$ , so the even and the odd coefficients form two independent series. Take  $\lambda = 6$ . Which statement is correct?

- A** Both series terminate, the even one as  $1 - 3x^2$  and the odd one as  $x - (2/3)x^3$ , so  $\lambda = 6$  has two independent polynomial solutions.
- B** Neither series terminates, but both converge for  $|x| < 1$ , so  $\lambda = 6$  is as acceptable as any other value;  $\lambda$  is quantised only by the boundary condition on the  $\phi$  equation.
- C** The even series terminates as  $1 - 3x^2$ ; the odd series does not, and because its coefficients fall off only as  $1/k$  it diverges logarithmically at  $x = \pm 1$ , so its coefficient must be set to zero.
- D** The even series terminates as  $1 - 3x^2$ ; the odd series does not, but its coefficients alternate in sign, so it converges at  $x = \pm 1$  and any combination of the two solutions is acceptable.

Answer

**2** MULTIPLE CHOICE · RECALL · UQMII-02.08 [1]  
CORE COURSE

For hydrogen, with  $a_0$  the Bohr radius, compare the 3s state ( $n = 3, l = 0$ ) with a 3d state ( $n = 3, l = 2$ ). Which expectation value is the same for the two states?

- A**  $\langle 1/r \rangle$ , equal to  $1/(9a_0)$  in both, because the virial theorem fixes  $\langle V \rangle = 2E_3$
- B**  $\langle r \rangle$ , equal to  $9a_0$  in both, the radius of the third Bohr orbit
- C**  $\langle 1/r^2 \rangle$ , because the centrifugal term averages to the same value in every state of a given  $n$
- D**  $\langle r^2 \rangle$ , because the mean-square radius is fixed by the energy through  $\langle T \rangle = -E_3$

Answer

3

CORE  
COURSE

MULTIPLE CHOICE · DEMANDING · UQMII-03.06 · UQMII-03.07

[1]

A particle of charge  $q$  and mass  $m$  moves in the potentials  $\phi$  and  $A$  with Hamiltonian  $\hat{H} = (\hat{p} - qA)^2/(2m) + q\phi$ , where  $\hat{p} = -i\hbar\nabla$ . Under the gauge transformation  $A \rightarrow A + \nabla\Lambda$ ,  $\phi \rightarrow \phi - \partial\Lambda/\partial t$ , with  $\Lambda(r, t)$  any real function, the Schrödinger equation keeps its form provided  $\psi \rightarrow e^{i(q\Lambda/\hbar)}\psi$ . Which expectation value is the same in every gauge, whatever  $\Lambda$  is?

- A  $\langle \hat{p} \rangle$ , because  $\hat{p} = -i\hbar\nabla$  is the same operator in every gauge
- B  $\langle \hat{H} \rangle$ , because the Hamiltonian generates the same physical time evolution in every gauge
- C The phase of  $\psi$  at a fixed point  $r_0$ , because multiplying  $\psi$  by  $e^{i(q\Lambda/\hbar)}$  leaves  $|\psi|^2$  unchanged
- D  $\langle \hat{p} - qA \rangle$ , which equals  $m$  times the rate of change of  $\langle r \rangle$

Answer

4

CORE  
COURSE

MULTIPLE CHOICE · ROUTINE · UQMII-04.03 · UQMII-04.04 · UQMII-04.05

[1]

A source emits spin- $\frac{1}{2}$  particles, each prepared either in  $|+z\rangle$  or in  $|+x\rangle = (|+z\rangle + |-z\rangle)/\sqrt{2}$ , with probability  $\frac{1}{2}$  each, and the record of which state was prepared is discarded. What is the purity  $\text{Tr}(\rho^2)$  of the ensemble?

- A 0.50
- B 0.75
- C 0.85
- D 1.00

Answer

5

CORE  
COURSE

MULTIPLE CHOICE · ROUTINE · UQMII-05.06 · UQMII-05.07

[1]

An electron in a 2p orbital of hydrogen is in the coupled state with  $l = 1$ ,  $s = \frac{1}{2}$ ,  $j = \frac{3}{2}$  and  $m_j = \frac{3}{2}$ . The stretched state is  $|j = 3/2, m_j = 3/2\rangle = |m_l = 1\rangle|\uparrow\rangle$ , and  $J_- = L_- + S_-$ , with  $L_-|l, m\rangle = \hbar\sqrt{l(l+1) - m(m-1)}|l, m-1\rangle$  and  $S_-|\uparrow\rangle = \hbar|\downarrow\rangle$ . What is the probability that a measurement of  $S_z$  on the  $j = \frac{3}{2}$  state gives  $+\hbar/2$ ?

- A  $1/2$
- B  $2/3$
- C  $1/3$
- D 1

Answer

6

CORE  
COURSE

MULTIPLE CHOICE · DEMANDING · UQMII-06.05 · UQMII-06.06 · UQMII-06.07

[1]

A particle of mass  $m$  moves in the isotropic two-dimensional oscillator  $H_0 = (p_x^2 + p_y^2)/(2m) + \frac{1}{2}m\omega^2(x^2 + y^2)$ . Its second excited level, at  $3\hbar\omega$ , is spanned by  $|2, 0\rangle$ ,  $|1, 1\rangle$  and  $|0, 2\rangle$ , the labels counting quanta along  $x$  and along  $y$ . Here  $x = \sqrt{\hbar/(2m\omega)}(a_x + a_x^\dagger)$ , with  $y$  written likewise,  $a^\dagger|n\rangle = \sqrt{n+1}|n+1\rangle$  and  $a|n\rangle = \sqrt{n}|n-1\rangle$ . A weak perturbation  $H' = \varepsilon xy$  is added. What are the first-order shifts of this level, and which good state is left unshifted?

- A All three shifts are zero: every diagonal element  $\langle n_x, n_y | H' | n_x, n_y \rangle$  vanishes, so the level stays threefold degenerate at first order.
- B  $+\varepsilon\hbar/(m\omega)$ , 0 and  $-\varepsilon\hbar/(m\omega)$ , with  $|1, 1\rangle$  left unshifted
- C  $+\varepsilon\hbar/(\sqrt{2} m\omega)$ , 0 and  $-\varepsilon\hbar/(\sqrt{2} m\omega)$ , with  $(|2, 0\rangle - |0, 2\rangle)/\sqrt{2}$  left unshifted
- D  $+\varepsilon\hbar/(m\omega)$ , 0 and  $-\varepsilon\hbar/(m\omega)$ , with  $(|2, 0\rangle - |0, 2\rangle)/\sqrt{2}$  left unshifted

Answer

7

CORE  
COURSE

MULTIPLE CHOICE · RECALL · UQMII-07.09

[1]

The ground configuration of oxygen is  $1s^2 2s^2 2p^4$ . The  $2p^4$  shell has the same terms as  $2p^2$ , namely  $^1S$ ,  $^1D$  and  $^3P$ . According to Hund's rules, which level is the ground level of oxygen?

- A  $^3P_2$
- B  $^3P_0$
- C  $^1D_2$
- D  $^1S_0$

Answer

8

CORE  
COURSE

MULTIPLE CHOICE · ROUTINE · UQMII-08.01 · UQMII-08.08

[1]

Three small splittings are measured in the  $n = 2$  level of hydrogen: the fine-structure splitting  $2P_{3/2} - 2P_{1/2}$ , the Lamb shift  $2S_{1/2} - 2P_{1/2}$ , and the hyperfine splitting of  $2S_{1/2}$ . Using  $mc^2 = 511$  keV,  $\alpha = 1/137$ ,  $m_e/m_p = 1/1836$ , and the powers of  $\alpha$  and of  $m_e/m_p$  that set the size of each effect, which ordering, largest first, is correct?

- A fine structure, then hyperfine splitting, then Lamb shift
- B fine structure, then Lamb shift, then hyperfine splitting
- C hyperfine splitting, then fine structure, then Lamb shift
- D Lamb shift, then fine structure, then hyperfine splitting

Answer

On the unit sphere the angular-momentum operators act as  $L_z = -i\hbar \partial/\partial\phi$  and  $L_{\pm} = \pm\hbar e^{\pm i\phi}(\partial/\partial\theta \pm i \cot\theta \partial/\partial\phi)$ , and  $L_{\pm}Y_l^m = \hbar\sqrt{l(l+1) - m(m \pm 1)} Y_l^{m \pm 1}$ . The Condon-Shortley convention is used throughout, in which  $Y_1^1 = -\sqrt{3/(8\pi)} \sin\theta e^{i\phi}$ .

(a) DERIVE

[2]

Write  $Y_2^2 = g(\theta)e^{2i\phi}$ . Starting from the condition  $L_+Y_2^2 = 0$ , derive  $g(\theta)$  up to a constant factor.

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(b) SHOW THAT

[2]

Show that normalising  $Y_2^2$  over the sphere, with  $C$  real and positive, gives  $C = (1/4)\sqrt{15/(2\pi)}$ .

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(c) DETERMINE

[2]

Determine  $Y_2^1$  by applying  $L_-$  to  $Y_2^2$ , keeping the sign that the operator produces.

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(d) STATE

[1]

State the parity of  $Y_2^1$  and the number of values of  $\theta$  strictly between 0 and  $\pi$  at which it vanishes.

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(e) EXPLAIN

[2]

In general the recursion for  $\cos\theta Y_l^m$  gives a combination of  $Y_{l+1}^m$  and  $Y_{l-1}^m$ . Explain why  $\cos\theta Y_1^1$  is a multiple of  $Y_2^1$  alone, find the multiple, and say what this implies for a z-polarised electric-dipole transition from an  $l = 1, m = 1$  state.

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In a crystal of cuprous oxide, an electron in the conduction band and a hole in the valence band bind into a hydrogen-like exciton. Model it as two particles of charges  $-e$  and  $+e$  with effective masses  $0.99m_e$  (electron) and  $0.58m_e$  (hole), interacting through the Coulomb potential screened by the relative permittivity  $\epsilon_r = 7.5$ ,  $V(r) = -e^2/(4\pi\epsilon_0\epsilon_r r)$ . Once the centre-of-mass motion is separated, the relative motion is that of one particle of reduced mass  $\mu$ , whose radial function  $u(r) = rR(r)$  obeys  $-(\hbar^2/2\mu)u'' + [V(r) + \hbar^2 l(l+1)/(2\mu r^2)]u = Eu$ . For a bound state write  $\kappa = \sqrt{-2\mu E}/\hbar$ ,  $\rho = \kappa r$ ,  $a^* = 4\pi\epsilon_0\epsilon_r \hbar^2/(\mu e^2)$  and  $\rho_0 = 2/(\kappa a^*)$ . Substituting  $u = \rho^{l+1}e^{-\rho}v(\rho)$  gives  $\rho v'' + 2(l+1-\rho)v' + [\rho_0 - 2(l+1)]v = 0$ . For hydrogen with an infinitely heavy nucleus,  $\hbar^2/(2m_e a_0^2) = 13.606$  eV and  $a_0 = 0.05292$  nm.

- (a) **DERIVE** [2]  
Substituting  $v(\rho) = \sum_j c_j \rho^j$ , derive the recursion relation between  $c_{j+1}$  and  $c_j$ .

- (b) **EXPLAIN** [2]  
The series solves the differential equation for any value of  $E$ . Explain why a physical solution must nevertheless have a terminating series, and why this condition fixes the energy.

- (c) **SHOW THAT** [2]  
Show that the bound-state energies are  $E_n = -(\mu/m_e)(13.606 \text{ eV})/(\epsilon_r n^2)$ , with  $n = N + l + 1$ , where  $N$  is the degree of the terminated polynomial, and that  $l \leq n - 1$ .

- (d) **CALCULATE** [3]  
Calculate  $\mu$  as a multiple of  $m_e$ , the exciton Rydberg energy  $R^* = -E_1$  in meV, and the effective Bohr radius  $a^*$  in nm.

- (e) **DETERMINE** [2]  
For these states Kramers' relation reads  $((s+1)/n^2)\langle r^s \rangle - (2s+1)a^*\langle r^{s-1} \rangle + (s/4)[(2l+1)^2 - s^2]a^{*2}\langle r^{s-2} \rangle = 0$ . Absorption lines of the exciton P series ( $l = 1$ ) have been resolved up to  $n = 25$ . Determine  $\langle r \rangle$  for the  $n = 25$ ,  $l = 1$  exciton.

The neutron is a spin- $\frac{1}{2}$  particle whose magnetic moment is  $\mu = \gamma S$ , with  $\gamma = -1.832 \times 10^8 \text{ rad s}^{-1} \text{ T}^{-1}$ , so the moment points opposite to the spin. In a magnetic field  $B$  its spin Hamiltonian is  $H = -\mu \cdot B = -\gamma B \cdot S$ , and the spin operators obey  $[S_x, S_y] = i\hbar S_z$  and its cyclic permutations. In every part the neutrons travel at 2200 m/s, and their motion through the apparatus is treated classically, so that a neutron spends a time  $L/v$  in a region of length  $L$ .

(a) DERIVE

[2]

For a uniform static field  $B = B\hat{z}$ , derive from the Heisenberg equation of motion the equations of motion of  $S_x$ ,  $S_y$  and  $S_z$ , written as one vector equation, and hence the angular frequency  $\omega_L$  at which  $\langle S \rangle$  precesses about  $B$  and the sense of the precession.

(b) CALCULATE

[2]

In one arm of a neutron interferometer the neutrons cross a region 2.0 cm long in which a uniform field  $B$  is applied perpendicular to their path. Calculate the time each neutron spends in the field, and the field  $B_{2\pi}$  for which its spin precesses through exactly one turn.

(c) PREDICT

[2]

The two arms are recombined, and the count rate at one output port is recorded as  $B$  is raised from zero; at  $B = 0$  this port is at an interference maximum. In the field the spin state is acted on by the rotation operator  $\exp(-i\phi\hat{n}\cdot\sigma/2)$ , where  $\phi$  is the precession angle and  $\hat{n}$  the field direction. Predict the count rate at  $B = B_{2\pi}$ , and the smallest nonzero field at which the port returns to its  $B = 0$  count rate.

(d) DESCRIBE

[2]

A resonance spin flipper is a region with a static field  $B_0$  along  $z$  and a field of magnitude  $B_1 \ll B_0$  rotating in the  $xy$ -plane at angular frequency  $\omega$ , in the same sense as the precession. Describe how transforming to the frame that rotates with  $B_1$  reduces the problem to precession about a static effective field, giving that field's components and the flip probability that follows.

(e) CALCULATE

[2]

The flipper is 5.0 cm long and  $B_0 = 10.0 \text{ mT}$ . Calculate the frequency  $\omega/2\pi$  at which  $B_1$  must rotate, and the smallest value of  $B_1$  that turns a neutron spin polarised along  $+z$  into one polarised along  $-z$ .

Two atoms of mass  $m$  are held in a narrow one-dimensional box trap, modelled as an infinite square well on  $0 < x < L$ . The single-particle states are  $\psi_n(x) = \sqrt{2/L} \sin(n\pi x/L)$ , with energies  $E_n = n^2 E_1$ , where  $E_1 = \pi^2 \hbar^2 / (2mL^2)$ . The atoms interact weakly through a short-range repulsion  $H' = g\delta(x_1 - x_2)$ , with  $g > 0$ , which is treated as a perturbation of  $H_0 = H_1 + H_2$ .  $P_{12}$  exchanges every label of the two atoms, coordinates and internal states alike. You may use  $\int_0^L \psi_1(x)^4 dx = 3/(2L)$ .

(a) EXPLAIN

[2]

$P_{12}$  commutes with  $H_0 + H'$ . Explain why this alone does not require the two-atom state to be symmetric or antisymmetric under exchange, and state what does.

(b) SHOW THAT

[2]

Show that  $\int_0^L \psi_1(x)^2 \psi_2(x)^2 dx = 1/L$ .

(c) DETERMINE

[3]

For two distinguishable atoms the unperturbed level  $5E_1$  is twofold degenerate, spanned by  $|12\rangle = \psi_1(x_1)\psi_2(x_2)$  and  $|21\rangle = \psi_2(x_1)\psi_1(x_2)$ . Determine the matrix of  $H'$  in this subspace, its first-order energy shifts and the corresponding good states.

(d) CALCULATE

[2]

Take  $g = 0.10E_1L$ . Calculate, to first order in  $g$  and in units of  $E_1$ , the ground-state energy of two identical spinless bosons, and of two identical fermions in the same internal state.

(e) COMPARE

[2]

Two spin- $1/2$  fermions, for example atoms in two internal states labelled  $\uparrow$  and  $\downarrow$ , occupy  $\psi_1$  and  $\psi_2$  in the same trap,  $H'$  does not act on spin, and  $g = 0.10E_1L$  as in (d). Compare the first-order energies of the states with total spin  $S = 0$  and  $S = 1$ , and account for the difference.

A source emits pairs of spin- $\frac{1}{2}$  particles intended to be in the singlet state. Alice measures the spin component of one particle along a direction at angle  $a$  in the  $xz$ -plane and Bob that of the other along angle  $b$ , each recording  $+1$  or  $-1$ . For each setting the correlation  $E$  is the mean of the product of the two results; for the ideal singlet  $E(a, b) = -\cos(a - b)$ . Every local hidden-variable model obeys  $|S| \leq 2$ , where  $S = E(a, b) - E(a, b') + E(a', b) + E(a', b')$ . The run used  $a = 0^\circ$ ,  $a' = 90^\circ$ ,  $b = 45^\circ$  and  $b' = 135^\circ$ , and the table gives the number of detected pairs with each combination of results, Alice's sign first. Treat each detected pair as an independent trial.

**Coincidence counts at the four analyser settings**

| Settings                        | N <sub>++</sub> (counts) | N <sub>+-</sub> (counts) | N <sub>-+</sub> (counts) | N <sub>--</sub> (counts) |
|---------------------------------|--------------------------|--------------------------|--------------------------|--------------------------|
| $a = 0^\circ, b = 45^\circ$     | 43                       | 215                      | 205                      | 50                       |
| $a = 0^\circ, b' = 135^\circ$   | 192                      | 48                       | 46                       | 196                      |
| $a' = 90^\circ, b = 45^\circ$   | 52                       | 214                      | 196                      | 58                       |
| $a' = 90^\circ, b' = 135^\circ$ | 48                       | 196                      | 189                      | 49                       |

- (a) **CALCULATE** [2]  
Calculate  $E$  for each of the four settings.

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- (b) **DETERMINE** [2]  
Determine  $S$ , and the fraction of the ideal-singlet value that it reaches.

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- (c) **ESTIMATE** [2]  
Estimate the standard uncertainty in  $S$  from counting statistics, stating the assumptions you make.

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- (d) **EVALUATE** [2]  
Evaluate whether these data rule out every local hidden-variable model, and say what else a conclusive test must secure.

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- (e) **JUSTIFY** [2]  
Quantum mechanics predicts that Alice's results alone cannot reveal which setting Bob chose. Justify this from the singlet's reduced density operator, and test it against the data for Alice's setting  $a$ .

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A hydrogen-like ion has one electron of mass  $m$  bound to a point nucleus of charge  $Ze$ , treated as infinitely heavy, so that  $V(r) = -Ze^2/(4\pi\epsilon_0 r)$  and the unperturbed energies  $E_n = -(Z\alpha)^2 mc^2/(2n^2)$  are degenerate in  $l$ ,  $m_l$  and  $m_s$ . With  $a = a_0/Z$ , so that  $\hbar^2/(ma) = Ze^2/(4\pi\epsilon_0)$  and  $E_n = -Ze^2/(8\pi\epsilon_0 a n^2)$ , the unperturbed states give  $\langle 1/r \rangle = 1/(n^2 a)$ ,  $\langle 1/r^2 \rangle = 1/[n^3(l + \frac{1}{2})a^2]$ ,  $\langle 1/r^3 \rangle = 1/[n^3 l(l + \frac{1}{2})(l + 1)a^3]$  for  $l \geq 1$ , and  $|\psi_{n00}(0)|^2 = 1/(\pi n^3 a^3)$ . The fine-structure Hamiltonian is  $H_{\text{rel}} + H_{\text{SO}} + H_{\text{D}}$ , with  $H_{\text{rel}} = -p^4/(8m^3 c^2)$ ;  $H_{\text{SO}} = [1/(2m^2 c^2)](1/r)(dV/dr) \mathbf{L} \cdot \mathbf{S}$ , which already contains the Thomas factor of  $\frac{1}{2}$ , quoted from relativistic kinematics; and the Darwin term  $H_{\text{D}} = [\pi \hbar^2/(2m^2 c^2)][Ze^2/(4\pi\epsilon_0)]\delta^3(r)$ , quoted from the Dirac equation. Take  $mc^2 = 0.5110$  MeV,  $\alpha = 1/137.04$  and  $\hbar = 4.136 \times 10^{-15}$  eV s.

(a) JUSTIFY [2]

Each level  $n$  is degenerate, yet each fine-structure term can be evaluated with the non-degenerate formula  $E^{(1)} = \langle H' \rangle$  in the coupled basis  $|n, l, j, m_j\rangle$ . Justify this, naming the operators each term commutes with.

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(b) SHOW THAT [3]

Starting from  $p^2/(2m) = H_0 - V$ , show that the relativistic shift is  $E_{\text{rel}} = -[E_n^2/(2mc^2)][4n/(l + \frac{1}{2}) - 3]$ .

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(c) DERIVE [3]

Derive the first-order spin-orbit shift  $E_{\text{SO}}$  of a state with  $l \geq 1$ , expressed in terms of  $E_n$ ,  $mc^2$ ,  $n$ ,  $l$  and  $j$ .

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(d) SHOW THAT [3]

Show that, once the Darwin term is included for  $l = 0$ , the three terms sum to  $E_{\text{fs}} = [E_n^2/(2mc^2)][3 - 4n/(j + \frac{1}{2})]$  for every state, so that the energy depends on  $n$  and  $j$  only.

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(e) SKETCH [2]

For  $\text{He}^+$  ( $Z = 2$ ), sketch the fine structure of the  $n = 2$  level: draw the unperturbed level and the fine-structure levels labelled  $2S_{1/2}$ ,  $2P_{1/2}$  and  $2P_{3/2}$ , marking each shift in  $\mu\text{eV}$  and the  $2P_{3/2}$ - $2P_{1/2}$  splitting in GHz.

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(f) EVALUATE [2]

The measured  $2S_{1/2}$ - $2P_{1/2}$  Lamb shifts are 1.058 GHz in hydrogen and 14.04 GHz in  $\text{He}^+$ . Welton's argument gives, for an  $nS$  level,  $\Delta E \propto \alpha(Z\alpha)^4 mc^2 \ln[1/(Z\alpha)]/n^3$ , with a prefactor, and an argument of the logarithm, that it fixes only roughly. Evaluate how well this scaling accounts for the ratio of the two shifts.

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# University Quantum Mechanics II · Midterm Examination

## — mark scheme

One line per mark, as an examiner would award them. A note under a part is the error that part is set to catch.

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|----------------------------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|------------|
| <b>1</b><br>CORE<br>COURSE | MULTIPLE CHOICE · ROUTINE · UQMII-01.01 · UQMII-01.02                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                   | <b>[1]</b> |
|                            | <p>Separating the angular equation for <math>m = 0</math> and writing <math>x = \cos \theta</math> gives Legendre's equation, <math>(1 - x^2)y'' - 2xy' + \lambda y = 0</math>. Substituting <math>y = \sum a_k x^k</math> gives the recursion <math>a_{k+2} = [k(k+1) - \lambda]a_k / [(k+1)(k+2)]</math>, so the even and the odd coefficients form two independent series. Take <math>\lambda = 6</math>. Which statement is correct?</p>                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                            |            |
|                            | <p><b>KEY C The even series terminates as <math>1 - 3x^2</math>; the odd series does not, and because its coefficients fall off only as <math>1/k</math> it diverges logarithmically at <math>x = \pm 1</math>, so its coefficient must be set to zero.</b></p>                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                         |            |
|                            | <p><i>A stops the odd recursion one step too early. <math>a_3 = (2 - 6)a_1/6 = -(2/3)a_1</math> is nonzero, and so is the next coefficient, <math>a_5 = (12 - 6)a_3/20</math>; the factor <math>k(k+1) - 6</math> vanishes only at <math>k = 2</math>, an even index, so only the even series is cut off. B is right that both series converge inside the interval, but the poles <math>\theta = 0</math> and <math>\theta = \pi</math>, where <math>x = \pm 1</math>, are part of the sphere and an angular function must be finite there. It is regularity at the poles that quantises <math>\lambda</math>; the <math>\phi</math> equation quantises <math>m</math>. D invents a rescue: after <math>a_3 = -(2/3)a_1</math> the odd coefficients are <math>-0.200a_1</math>, <math>-0.114a_1</math> and <math>-0.079a_1</math>, all of one sign, falling like <math>1/k</math> as the coefficients of <math>\frac{1}{2}\ln[(1+x)/(1-x)]</math> do, so the series grows without bound at the poles. C is correct: at large <math>k</math> the ratio <math>a_{k+2}/a_k \approx 1 - 2/k</math>, the terminated even series is <math>P_2 \propto 3x^2 - 1</math>, and <math>\lambda = 6 = l(l+1)</math> with <math>l = 2</math>.</i></p>                                                                                                 | U2         |
| <b>2</b><br>CORE<br>COURSE | MULTIPLE CHOICE · RECALL · UQMII-02.08                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                  | <b>[1]</b> |
|                            | <p>For hydrogen, with <math>a_0</math> the Bohr radius, compare the 3s state (<math>n = 3, l = 0</math>) with a 3d state (<math>n = 3, l = 2</math>). Which expectation value is the same for the two states?</p>                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                       |            |
|                            | <p><b>KEY A <math>\langle 1/r \rangle</math>, equal to <math>1/(9a_0)</math> in both, because the virial theorem fixes <math>\langle V \rangle = 2E_n</math></b></p>                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                    |            |
|                            | <p><i>B carries the Bohr model over: <math>n^2 a_0</math> is neither state's mean radius. Kramers' relation gives <math>\langle r \rangle = (a_0/2)[3n^2 - l(l+1)]</math>, which is <math>13.5a_0</math> for 3s and <math>10.5a_0</math> for 3d; the 3d electron, with no radial node, stays closer to a circular-orbit radius. C is the reverse of the truth: <math>\langle 1/r^2 \rangle = 1/[n^3(l + \frac{1}{2})a_0^2]</math> is <math>0.0741/a_0^2</math> for 3s and <math>0.0148/a_0^2</math> for 3d, five times smaller, and that dependence on <math>l</math> is exactly why the relativistic correction separates levels of different <math>l</math>. D starts from a true statement, <math>\langle T \rangle = -E_n</math> for every state of the level, and draws a false conclusion: <math>T</math> fixes an average of <math>p^2</math>, not of <math>r^2</math>, and <math>\langle r^2 \rangle = (n^2 a_0^2/2)[5n^2 + 1 - 3l(l+1)]</math> is <math>207a_0^2</math> for 3s and <math>126a_0^2</math> for 3d. A is correct: for the Coulomb potential the virial theorem gives <math>\langle V \rangle = 2E_n</math>, which depends on <math>n</math> alone, so <math>\langle 1/r \rangle = 1/(n^2 a_0)</math> for every <math>l</math>.</i></p>                                                                            | U1         |
| <b>3</b><br>CORE<br>COURSE | MULTIPLE CHOICE · DEMANDING · UQMII-03.06 · UQMII-03.07                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                 | <b>[1]</b> |
|                            | <p>A particle of charge <math>q</math> and mass <math>m</math> moves in the potentials <math>\phi</math> and <math>A</math> with Hamiltonian <math>\hat{H} = (\hat{p} - qA)^2/(2m) + q\phi</math>, where <math>\hat{p} = -i\hbar\nabla</math>. Under the gauge transformation <math>A \rightarrow A + \nabla\Lambda</math>, <math>\phi \rightarrow \phi - \partial\Lambda/\partial t</math>, with <math>\Lambda(r, t)</math> any real function, the Schrödinger equation keeps its form provided <math>\psi \rightarrow e^{i(q\Lambda/\hbar)}\psi</math>. Which expectation value is the same in every gauge, whatever <math>\Lambda</math> is?</p>                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                     |            |
|                            | <p><b>KEY D <math>\langle \hat{p} - qA \rangle</math>, which equals <math>m</math> times the rate of change of <math>\langle r \rangle</math></b></p>                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                   |            |
|                            | <p><i>A confuses the operator with its expectation value. The operator <math>-i\hbar\nabla</math> is indeed the same, but the state is not: <math>e^{i(q\Lambda/\hbar)}\hat{p}e^{i(q\Lambda/\hbar)} = \hat{p} + q\nabla\Lambda</math>, so <math>\langle \hat{p} \rangle</math> moves by <math>q\langle \nabla\Lambda \rangle</math>, and canonical momentum is not an observable once a vector potential is present. B fails whenever <math>\Lambda</math> depends on time: the new Hamiltonian contains <math>q\phi - q\partial\Lambda/\partial t</math>, so <math>\langle \hat{H} \rangle</math> shifts by <math>-q\langle \partial\Lambda/\partial t \rangle</math> although every measurable prediction is unchanged; it survives only for a time-independent <math>\Lambda</math>. C reads a statement about <math> \psi ^2</math> as a statement about <math>\psi</math>: the modulus is unchanged, but the phase at <math>r_0</math> moves by <math>q\Lambda(r_0, t)/\hbar</math>, which is why the phase of <math>\psi</math> at one point carries no physical meaning. D is correct: <math>e^{i(q\Lambda/\hbar)}(\hat{p} - qA - q\nabla\Lambda)e^{i(q\Lambda/\hbar)} = \hat{p} - qA</math>, so the mechanical momentum, which the Heisenberg equation identifies as <math>m \, d\hat{r}/dt</math>, is gauge-invariant.</i></p> | U1         |

4

CORE  
COURSE

MULTIPLE CHOICE · ROUTINE · UQMII-04.03 · UQMII-04.04 · UQMII-04.05

[1]

A source emits spin- $\frac{1}{2}$  particles, each prepared either in  $|+z\rangle$  or in  $|+x\rangle = (|+z\rangle + |-z\rangle)/\sqrt{2}$ , with probability  $\frac{1}{2}$  each, and the record of which state was prepared is discarded. What is the purity  $\text{Tr}(\rho^2)$  of the ensemble?

KEY **B 0.75**

*A treats any equal mixture of two different states as maximally mixed. That holds only when the two states are orthogonal, so that their Bloch vectors cancel; here  $|( +z | +x )|^2 = \frac{1}{2}$ , and the Bloch vector is  $r = \frac{1}{2}(0, 0, 1) + \frac{1}{2}(1, 0, 0) = (\frac{1}{2}, 0, \frac{1}{2})$ . C is the larger eigenvalue of  $\rho$ ,  $(1 + |r|)/2 = (1 + 0.707)/2 = 0.854$ : the largest probability  $\langle \psi | \rho | \psi \rangle$  with which any one pure state, here spin up along the bisector of the z- and x-axes, is found in the ensemble, not its purity. D is what the superposition  $(|+z\rangle + |+x\rangle)/\sqrt{2 + \sqrt{2}}$  would give: a pure state pointing along that bisector. Mixing, unlike superposing, puts the Bloch vector inside the ball, here at length 0.707. B is correct:  $\text{Tr}(\rho^2) = (1 + |r|^2)/2 = (1 + \frac{1}{2})/2 = 0.75$ , which equals the sum of the squared eigenvalues,  $0.854^2 + 0.146^2$ .*

U3

5

CORE  
COURSE

MULTIPLE CHOICE · ROUTINE · UQMII-05.06 · UQMII-05.07

[1]

An electron in a 2p orbital of hydrogen is in the coupled state with  $l = 1$ ,  $s = \frac{1}{2}$ ,  $j = \frac{3}{2}$  and  $m_j = \frac{1}{2}$ . The stretched state is  $|j = 3/2, m_j = 3/2\rangle = |m_l = 1\rangle |\uparrow\rangle$ , and  $J_- = L_- + S_-$ , with  $L_- |l, m\rangle = \hbar \sqrt{l(l+1) - m(m-1)} |l, m-1\rangle$  and  $S_- |\uparrow\rangle = \hbar |\downarrow\rangle$ . What is the probability that a measurement of  $S_z$  on the  $j = \frac{3}{2}$  state gives  $+\hbar/2$ ?

KEY **C 1/3**

*B is the weight of  $|m_l = 0\rangle |\uparrow\rangle$  in the other state of the pair. Lowering the stretched state gives  $|3/2, \frac{1}{2}\rangle = \sqrt{2/3} |0\rangle |\uparrow\rangle + \sqrt{1/3} |1\rangle |\downarrow\rangle$ , because  $L_-$  acting on  $m_l = 1$  brings a factor  $\sqrt{2}$  while  $S_-$  brings 1; a candidate who stops there has found the  $j = 3/2$  state, not the  $j = \frac{1}{2}$  one. A assumes that the two uncoupled states contribute equally, which nothing in the algebra supports. D assumes that  $m_j = \frac{1}{2}$  can only mean  $m_l = 0$  with  $m_s = +\frac{1}{2}$ , ignoring the  $|m_l = 1\rangle |\downarrow\rangle$  component, which has the same  $m_l + m_s$ . C is correct:  $|\frac{1}{2}, \frac{1}{2}\rangle$  must be orthogonal to  $|3/2, \frac{1}{2}\rangle$  inside the two-dimensional  $m_j = \frac{1}{2}$  subspace, so  $|\frac{1}{2}, \frac{1}{2}\rangle = \sqrt{2/3} |1\rangle |\downarrow\rangle - \sqrt{1/3} |0\rangle |\uparrow\rangle$  in the Condon-Shortley phase, and  $P(S_z = +\hbar/2) = 1/3$ .*

U2

6

CORE  
COURSE

MULTIPLE CHOICE · DEMANDING · UQMII-06.05 · UQMII-06.06 · UQMII-06.07

[1]

A particle of mass  $m$  moves in the isotropic two-dimensional oscillator  $H_0 = (p_x^2 + p_y^2)/(2m) + \frac{1}{2}m\omega^2(x^2 + y^2)$ . Its second excited level, at  $3\hbar\omega$ , is spanned by  $|2, 0\rangle$ ,  $|1, 1\rangle$  and  $|0, 2\rangle$ , the labels counting quanta along  $x$  and along  $y$ . Here  $x = \sqrt{\hbar/(2m\omega)}(a_x + a_x^\dagger)$ , with  $y$  written likewise,  $a^\dagger|n\rangle = \sqrt{n+1}|n+1\rangle$  and  $a|n\rangle = \sqrt{n}|n-1\rangle$ . A weak perturbation  $H' = \varepsilon xy$  is added. What are the first-order shifts of this level, and which good state is left unshifted?

KEY **D  $+\varepsilon\hbar/(m\omega)$ , 0 and  $-\varepsilon\hbar/(m\omega)$ , with  $(|2, 0\rangle - |0, 2\rangle)/\sqrt{2}$  left unshifted**

*A applies the non-degenerate formula to a degenerate level. The diagonal elements do vanish, because  $xy$  changes the number of quanta along each axis by one, but  $\langle 2, 0 | H' | 1, 1 \rangle = \varepsilon \langle 2 | x | 1 \rangle \langle 0 | y | 1 \rangle$  and  $\langle 1, 1 | H' | 0, 2 \rangle = \varepsilon \langle 1 | x | 0 \rangle \langle 1 | y | 2 \rangle$  do not, and inside a degenerate subspace it is the whole matrix that must be diagonalised. C has the unshifted state right but the outer shifts too small by  $\sqrt{2}$ : it comes from dropping the  $\sqrt{2}$  in  $\langle 2 | x | 1 \rangle = \sqrt{2} \sqrt{\hbar/(2m\omega)}$ , or from diagonalising only the block of  $|2, 0\rangle$  and  $|1, 1\rangle$  and so missing the coupling of  $|1, 1\rangle$  to  $|0, 2\rangle$ . B has the right shifts but gives the middle eigenvalue to the middle label:  $|1, 1\rangle$  is coupled to both other states and is not a good state at all. The exchange  $x \leftrightarrow y$  commutes with  $H_0$  and with  $xy$ , and  $(|2, 0\rangle - |0, 2\rangle)/\sqrt{2}$  is the only state of the level that is odd under it, so it cannot mix with the other two; its shift is zero because  $H'$  has no diagonal elements and no element between  $|2, 0\rangle$  and  $|0, 2\rangle$ . D is correct: with  $\delta = \varepsilon\hbar/(2m\omega)$  the matrix in the order  $|2, 0\rangle$ ,  $|1, 1\rangle$ ,  $|0, 2\rangle$  is  $\sqrt{2}\delta \begin{bmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{bmatrix}$ , with eigenvalues  $+2\delta$ , 0 and  $-2\delta$ , the outer ones belonging to  $(|2, 0\rangle \pm \sqrt{2}|1, 1\rangle + |0, 2\rangle)/2$ . There is an exact check: in  $u = (x + y)/\sqrt{2}$  and  $v = (x - y)/\sqrt{2}$ ,  $xy = (u^2 - v^2)/2$ , so to first order the  $u$  frequency rises and the  $v$  frequency falls by  $\varepsilon/(2m\omega)$ , and the states with two  $u$  quanta, one of each, and two  $v$  quanta shift by  $+2\delta$ , 0 and  $-2\delta$ .*

U2

The ground configuration of oxygen is  $1s^2 2s^2 2p^4$ . The  $2p^4$  shell has the same terms as  $2p^2$ , namely  $^1S$ ,  $^1D$  and  $^3P$ . According to Hund's rules, which level is the ground level of oxygen?

KEY **A  $^3P_2$**

*B is the ground level of carbon,  $2p^2$ , and carrying the less-than-half-filled rule over to oxygen is the error to catch. Four electrons fill more than half of the six  $p$  spin-orbitals, the shell then behaves as two holes whose spin-orbit coupling has the opposite sign, and the largest  $J$  lies lowest. C puts the rule for  $L$  ahead of the rule for  $S$ :  $^1D$  has the larger  $L$ , but Hund's first rule, maximum  $S$ , comes first, because the antisymmetric spatial state of a triplet keeps the electrons apart and lowers their repulsion; in oxygen  $^1D$  lies about 2 eV above the ground term. D treats  $2p^4$  as a closed shell because its spins can be paired, but only a full  $p^6$  shell is obliged to be  $^1S_0$ . A is correct: the term is  $^3P$ , and  $J = L + S = 2$  because the shell is more than half full.*

U1

Three small splittings are measured in the  $n = 2$  level of hydrogen: the fine-structure splitting  $2P_{3/2} - 2P_{1/2}$ , the Lamb shift  $2S_{1/2} - 2P_{1/2}$ , and the hyperfine splitting of  $2S_{1/2}$ . Using  $mc^2 = 511$  keV,  $\alpha = 1/137$ ,  $m_e/m_p = 1/1836$ , and the powers of  $\alpha$  and of  $m_e/m_p$  that set the size of each effect, which ordering, largest first, is correct?

KEY **B fine structure, then Lamb shift, then hyperfine splitting**

*A counts powers of  $\alpha$  and nothing else. Fine and hyperfine structure both scale as  $\alpha^4 mc^2$ , but the hyperfine interaction couples the electron to the nuclear magnetic moment and so carries a further factor of about  $g_p m_e/m_p \approx 3 \times 10^{-3}$ , whereas the Lamb shift sits only one power of  $\alpha$ , softened by a logarithm, below the fine structure:  $\alpha^5 mc^2 \ln(1/\alpha)/n^3 \approx 6 \mu\text{eV}$  against  $\alpha^4 mc^2/n^3 \approx 0.2 \text{ meV}$ . C mistakes the most famous hyperfine line, the 21 cm transition of 1s hydrogen, for a large one; at 5.9  $\mu\text{eV}$  it is small, and the 2S splitting is eight times smaller again. D takes the Lamb shift's historical importance for size: it was hard to find precisely because it is ten times smaller than the fine-structure splitting it sits beside. B is correct, and the measured values bear out the estimate: 45  $\mu\text{eV}$  (10.9 GHz), 4.4  $\mu\text{eV}$  (1.06 GHz) and 0.73  $\mu\text{eV}$  (178 MHz).*

U4

On the unit sphere the angular-momentum operators act as  $L_z = -i\hbar \partial/\partial\phi$  and  $L_{\pm} = \pm\hbar e^{\pm i\phi}(\partial/\partial\theta \pm i \cot\theta \partial/\partial\phi)$ , and  $L_{\pm}Y_l^m = \hbar\sqrt{l(l+1) - m(m \pm 1)} Y_l^{m \pm 1}$ . The Condon-Shortley convention is used throughout, in which  $Y_1^1 = -\sqrt{3/(8\pi)} \sin\theta e^{i\phi}$ .

(a) DERIVE · U2

[2]

Write  $Y_2^2 = g(\theta)e^{2i\phi}$ . Starting from the condition  $L_+Y_2^2 = 0$ , derive  $g(\theta)$  up to a constant factor.

1  $L_+$  acting on  $g(\theta)e^{2i\phi}$  gives  $\hbar e^{3i\phi}[g' - 2 \cot\theta g]$ , since  $\partial/\partial\phi$  brings down  $2i$  and  $i \times 2i = -2$ , so  $L_+Y_2^2 = 0$  requires  $dg/d\theta = 2 \cot\theta g$

2 integrating,  $\ln g = 2 \ln \sin\theta + \text{constant}$ , so  $g = C \sin^2\theta$ , which is finite at both poles as a spherical harmonic must be

*The sign of the  $i \cot\theta \partial/\partial\phi$  term acting on  $e^{2i\phi}$  is where answers go wrong:  $g' = -2 \cot\theta g$  leads to  $g \propto 1/\sin^2\theta$ , which diverges at the poles. That divergence is the signal to recheck, because regularity is what the ladder route relies on.*

(b) SHOW THAT · U2

[2]

Show that normalising  $Y_2^2$  over the sphere, with  $C$  real and positive, gives  $C = (1/4)\sqrt{15/(2\pi)}$ .

1  $\int |Y_2^2|^2 d\Omega = C^2 \int_0^{2\pi} d\phi \int_0^\pi \sin^5\theta d\theta$ , and with  $u = \cos\theta$ ,  $\int_0^\pi \sin^5\theta d\theta = \int_{-1}^1 (1 - u^2)^2 du = 2 - 4/3 + 2/5 = 16/15$

2 setting  $2\pi C^2 \times 16/15 = 1$  gives  $C^2 = 15/(32\pi)$ , so  $C = \sqrt{15/(32\pi)} = (1/4)\sqrt{15/(2\pi)} = 0.386$

*Dropping the  $\sin\theta$  of the solid-angle element  $d\Omega = \sin\theta d\theta d\phi$ , and integrating  $\sin^4\theta$  instead, gives  $3\pi/8$  in place of  $16/15$ ; the answer is printed so that this slip shows.*

(c) DETERMINE · U2

[2]

Determine  $Y_2^1$  by applying  $L_-$  to  $Y_2^2$ , keeping the sign that the operator produces.

1  $L_-(\sin^2\theta e^{2i\phi}) = -\hbar e^{-i\phi}[2 \sin\theta \cos\theta - i \cot\theta (2i) \sin^2\theta]e^{2i\phi} = -4\hbar \sin\theta \cos\theta e^{i\phi}$

2 dividing by  $\hbar\sqrt{6-2} = 2\hbar$  and multiplying by  $C$ :  $Y_2^1 = -(1/2)\sqrt{15/(2\pi)} \sin\theta \cos\theta e^{i\phi} = -\sqrt{15/(8\pi)} \sin\theta \cos\theta e^{i\phi}$ , the minus sign being the Condon-Shortley phase that the lowering generates

*Candidates who drop the overall minus sign of  $L_-$ , or who normalise  $Y_2^1$  afresh and choose it positive, lose the phase that makes the  $Y_l^m$  a consistent set; every later Clebsch-Gordan coefficient or dipole matrix element inherits the error.*

(d) STATE · U1

[1]

State the parity of  $Y_2^1$  and the number of values of  $\theta$  strictly between 0 and  $\pi$  at which it vanishes.

1 even parity,  $(-1)^l = +1$ , since under  $\theta \rightarrow \pi - \theta$  and  $\phi \rightarrow \phi + \pi$  both  $\sin\theta \cos\theta$  and  $e^{i\phi}$  change sign; and one value,  $\theta = \pi/2$ , where  $\cos\theta = 0$ , a nodal plane at the equator, as  $l - |m| = 1$  requires

(e) EXPLAIN · U1

[2]

In general the recursion for  $\cos\theta Y_l^m$  gives a combination of  $Y_{l+1}^m$  and  $Y_{l-1}^m$ . Explain why  $\cos\theta Y_1^1$  is a multiple of  $Y_2^1$  alone, find the multiple, and say what this implies for a z-polarised electric-dipole transition from an  $l = 1, m = 1$  state.

1  $\cos\theta Y_1^1 = -\sqrt{3/(8\pi)} \sin\theta \cos\theta e^{i\phi} = (1/\sqrt{5})Y_2^1$ , using  $Y_2^1 = -\sqrt{15/(8\pi)} \sin\theta \cos\theta e^{i\phi}$ ; the  $l - 1$  partner would be  $Y_0$  with  $m = 1$ , which does not exist because  $|m|$  cannot exceed  $l$

2 so  $\langle l', m' | \cos\theta | 1, 1 \rangle$  is nonzero only for  $l' = 2, m' = 1$ : a z-polarised dipole transition from a p state with  $m = 1$  can reach d states but no s state, although  $\Delta l = -1$  is allowed in general

*Candidates who quote the selection rule  $\Delta l = \pm 1$  conclude that p to s is always open. The recursion makes the rule a list of what may occur, and  $m$  decides which of its two terms survives.*

In a crystal of cuprous oxide, an electron in the conduction band and a hole in the valence band bind into a hydrogen-like exciton. Model it as two particles of charges  $-e$  and  $+e$  with effective masses  $0.99m_e$  (electron) and  $0.58m_e$  (hole), interacting through the Coulomb potential screened by the relative permittivity  $\epsilon_r = 7.5$ ,  $V(r) = -e^2/(4\pi\epsilon_0\epsilon_r r)$ . Once the centre-of-mass motion is separated, the relative motion is that of one particle of reduced mass  $\mu$ , whose radial function  $u(r) = rR(r)$  obeys  $-(\hbar^2/2\mu)u'' + [V(r) + \hbar^2 l(l+1)/(2\mu r^2)]u = Eu$ . For a bound state write  $\kappa = \sqrt{(-2\mu E)/\hbar^2}$ ,  $\rho = \kappa r$ ,  $a^* = 4\pi\epsilon_0\epsilon_r \hbar^2/(\mu e^2)$  and  $\rho_0 = 2/(\kappa a^*)$ . Substituting  $u = \rho^{l+1}e^{-(\rho)}v(\rho)$  gives  $\rho v'' + 2(l+1-\rho)v' + [\rho_0 - 2(l+1)]v = 0$ . For hydrogen with an infinitely heavy nucleus,  $\hbar^2/(2m_e a_0^2) = 13.606$  eV and  $a_0 = 0.05292$  nm.

(a) DERIVE · U2

[2]

Substituting  $v(\rho) = \sum_j c_j \rho^j$ , derive the recursion relation between  $c_{j+1}$  and  $c_j$ .

- 1 with every sum re-indexed to carry  $\rho^j$ :  $\rho v''$  gives  $\sum j(j+1)c_{j+1}\rho^j$ ,  $2(l+1)v'$  gives  $\sum 2(l+1)(j+1)c_{j+1}\rho^j$ , and  $-2\rho v'$  gives  $\sum (-2j)c_j \rho^j$
- 2 equating coefficients of  $\rho^j$ :  $(j+1)(j+2l+2)c_{j+1} = [2(j+l+1) - \rho_0]c_j$ , so  $c_{j+1} = [2(j+l+1) - \rho_0]c_j / [(j+1)(j+2l+2)]$

*The index shift is where marks are lost:  $\rho v''$  and  $v'$  each lower the power of  $\rho$  by one, while  $-2\rho v'$  does not. Candidates who equate coefficients without re-indexing produce a relation that mixes three consecutive coefficients.*

(b) EXPLAIN · U1

[2]

The series solves the differential equation for any value of  $E$ . Explain why a physical solution must nevertheless have a terminating series, and why this condition fixes the energy.

- 1 for large  $j$ ,  $c_{j+1}/c_j \rightarrow 2/j$ , the ratio for  $e^{(2\rho)} = \sum (2\rho)^j/j!$ , so an unterminated  $v$  grows like  $e^{(2\rho)}$  times a power of  $\rho$ , and  $u = \rho^{l+1}e^{-(\rho)}v$  grows like  $e^{(\rho)}$  times a power of  $\rho$ : it diverges at large  $r$  and cannot be normalised
- 2 the series must therefore stop at some  $c_N$ , which needs  $2(N+l+1) - \rho_0 = 0$  for an integer  $N \geq 0$ ;  $\rho_0 = 2/(\kappa a^*)$  depends on  $E$  through  $\kappa$ , so only discrete energies satisfy the condition

*The weak answer says that an infinite series must diverge. It need not: the series converges for every  $\rho$ . What fails is normalisability, because  $e^{(2\rho)}$  overwhelms the factor  $e^{-(\rho)}$  already removed, and a candidate who cannot name the condition being imposed has not explained why the energy is quantised. The ratio test fixes the exponential but not the power of  $\rho$  in front of it; the often-written  $u \sim \rho^{l+1}e^{-(\rho)}$  has the wrong power, though the growth that matters is  $e^{(\rho)}$  either way.*

(c) SHOW THAT · U2

[2]

Show that the bound-state energies are  $E_n = -(\mu/m_e)(13.606 \text{ eV})/(\epsilon_r n^2)$ , with  $n = N + l + 1$ , where  $N$  is the degree of the terminated polynomial, and that  $l \leq n - 1$ .

- 1 termination requires  $\rho_0 = 2(N+l+1) \equiv 2n$ , and since  $N \geq 0$ ,  $n \geq l+1$ , that is  $l \leq n - 1$
- 2  $\kappa = 2/(\rho_0 a^*) = 1/(n a^*)$ , so  $E = -\hbar^2 \kappa^2 / (2\mu) = -\hbar^2 / (2\mu a^{*2} n^2)$ ; with  $a^* = a_0 \epsilon_r (m_e/\mu)$  this is  $-[\hbar^2 / (2m_e a_0^2)](\mu/m_e) / (\epsilon_r n^2) = -(\mu/m_e)(13.606 \text{ eV}) / (\epsilon_r n^2)$

*Writing  $a^*$  with  $\mu/m_e$  instead of  $m_e/\mu$ , or keeping a single factor of  $\epsilon_r$ , gives an energy that scales wrongly. One factor of  $\epsilon_r$  comes from the weaker attraction and the second from the larger orbit that results.*

(d) CALCULATE · U3

[3]

Calculate  $\mu$  as a multiple of  $m_e$ , the exciton Rydberg energy  $R^* = -E_1$  in meV, and the effective Bohr radius  $a^*$  in nm.

- 1  $\mu = (0.99 \times 0.58/1.57)m_e = 0.366m_e$
- 2  $R^* = 0.366 \times 13.606 \text{ eV} / 7.5^2 = 0.0885 \text{ eV} = 88.5 \text{ meV}$
- 3  $a^* = 0.05292 \text{ nm} \times 7.5/0.366 = 1.09 \text{ nm}$

*Using the electron's effective mass alone in place of  $\mu$  overestimates  $R^*$  by a factor of 2.7. The two masses are comparable, so neither particle can be treated as fixed, as the proton nearly can in hydrogen.*

(e) DETERMINE · U3

[2]

For these states Kramers' relation reads  $((s + 1)/n^2)\langle r^s \rangle - (2s + 1)a^*\langle r^{s-1} \rangle + (s/4)[(2l + 1)^2 - s^2]a^{*2}\langle r^{s-2} \rangle = 0$ . Absorption lines of the exciton P series ( $l = 1$ ) have been resolved up to  $n = 25$ . Determine  $\langle r \rangle$  for the  $n = 25$ ,  $l = 1$  exciton.

1  $s = 0$  gives  $\langle 1/r \rangle = 1/(n^2 a^*)$ ;  $s = 1$  then gives  $(2/n^2)\langle r \rangle - 3a^* + l(l + 1)a^*/n^2 = 0$ , so  $\langle r \rangle = (a^*/2)[3n^2 - l(l + 1)]$

2  $\langle r \rangle = (1.09 \text{ nm}/2)(3 \times 625 - 2) = 1.02 \times 10^3 \text{ nm}$ , about  $1.0 \mu\text{m}$

*The error to catch is using the  $s = 1$  relation without first finding  $\langle 1/r \rangle$  from  $s = 0$ . Candidates who take  $n^2 a^*$  as the size get  $0.68 \mu\text{m}$ ; the P-state mean radius is half as large again, because  $\langle r \rangle \approx (3/2)n^2 a^*$  when  $l \ll n$ .*

## 11 CORE COURSE

STRUCTURED · DEMANDING · UQMII-03.01 · UQMII-03.02 · UQMII-03.03 · UQMII-03.04 · UQMII-05.02

[10]

The neutron is a spin- $\frac{1}{2}$  particle whose magnetic moment is  $\mu = \gamma S$ , with  $\gamma = -1.832 \times 10^8 \text{ rad s}^{-1} \text{ T}^{-1}$ , so the moment points opposite to the spin. In a magnetic field  $B$  its spin Hamiltonian is  $H = -\mu \cdot B = -\gamma B \cdot S$ , and the spin operators obey  $[S_x, S_y] = i\hbar S_z$  and its cyclic permutations. In every part the neutrons travel at  $2200 \text{ m/s}$ , and their motion through the apparatus is treated classically, so that a neutron spends a time  $L/v$  in a region of length  $L$ .

(a) DERIVE · U2

[2]

For a uniform static field  $B = B\hat{z}$ , derive from the Heisenberg equation of motion the equations of motion of  $S_x$ ,  $S_y$  and  $S_z$ , written as one vector equation, and hence the angular frequency  $\omega_L$  at which  $\langle S \rangle$  precesses about  $B$  and the sense of the precession.

1  $dS_x/dt = (i/\hbar)[H, S_x] = (i/\hbar)(-\gamma B)[S_z, S_x] = (i/\hbar)(-\gamma B)(i\hbar S_y) = \gamma B S_y$ ; likewise  $dS_y/dt = -\gamma B S_x$  and  $dS_z/dt = 0$ , which together are  $dS/dt = \gamma S \times B$

2 taking expectation values,  $\langle S_z \rangle$  is constant while  $\langle S_x \rangle$  and  $\langle S_y \rangle$  rotate about  $B$  at  $\omega_L = |\gamma|B$ ; because  $\gamma < 0$ ,  $dS/dt = |\gamma|B \times S$ , a right-handed rotation about  $B$

*A sign slip in  $[S_z, S_x] = i\hbar S_y$  reverses the sense of precession while leaving  $|\gamma|B$  intact, which is why the part asks for the vector equation rather than the frequency alone.*

(b) CALCULATE · U3

[2]

In one arm of a neutron interferometer the neutrons cross a region  $2.0 \text{ cm}$  long in which a uniform field  $B$  is applied perpendicular to their path. Calculate the time each neutron spends in the field, and the field  $B_2\pi$  for which its spin precesses through exactly one turn.

1  $t = 0.020 \text{ m}/(2200 \text{ m s}^{-1}) = 9.09 \times 10^{-6} \text{ s}$

2  $B_2\pi = 2\pi/(|\gamma|t) = 2\pi/(1.832 \times 10^8 \text{ rad s}^{-1} \text{ T}^{-1} \times 9.09 \times 10^{-6} \text{ s}) = 3.77 \times 10^{-3} \text{ T}$  (3.77 mT)

*Treating  $\gamma$  as a frequency in hertz per tesla, or dropping the  $2\pi$ , gives a field wrong by a factor of  $2\pi$ ; with  $\gamma$  in  $\text{rad s}^{-1} \text{ T}^{-1}$  the precession angle is  $|\gamma|Bt$  in radians.*

(c) PREDICT · U1

[2]

The two arms are recombined, and the count rate at one output port is recorded as  $B$  is raised from zero; at  $B = 0$  this port is at an interference maximum. In the field the spin state is acted on by the rotation operator  $\exp(-i\phi\hat{n}\cdot\sigma/2)$ , where  $\phi$  is the precession angle and  $\hat{n}$  the field direction. Predict the count rate at  $B = B_2\pi$ , and the smallest nonzero field at which the port returns to its  $B = 0$  count rate.

1 the recombined intensity is proportional to  $|\chi + e^{(-i\phi\hat{n}\cdot\sigma/2)}\chi|^2 = 2 + 2\cos(\phi/2)$  for any spin state  $\chi$ , since  $\langle\chi|\hat{n}\cdot\sigma|\chi\rangle$  is real and contributes only to the imaginary part of the overlap; at  $\phi = 2\pi$  the operator is  $-I$ , so the port is at an interference minimum, ideally dark, although every spin points as it did at  $B = 0$

2 the count rate first returns to its  $B = 0$  value at  $\phi = 4\pi$ , that is  $B = 2B_2\pi = 7.55 \text{ mT}$

*The expected answer is that a spin turned through a full circle is unchanged, so the count rate recovers at  $3.77 \text{ mT}$ . The prediction must rest on the rotation operator for spin  $\frac{1}{2}$ , which is  $-I$  at  $2\pi$ ; the sign is invisible in a single beam and becomes observable only against the unrotated arm.*

(d) DESCRIBE · U2

[2]

A resonance spin flipper is a region with a static field  $B_0$  along  $z$  and a field of magnitude  $B_1 \ll B_0$  rotating in the  $xy$ -plane at angular frequency  $\omega$ , in the same sense as the precession. Describe how transforming to the frame that rotates with  $B_1$  reduces the problem to precession about a static effective field, giving that field's components and the flip probability that follows.

- 1 in the frame rotating at  $\omega$  about  $z$ ,  $B_1$  is static along an axis  $x'$ , and the transformation adds  $-\omega S_z$  to the Hamiltonian, which acts as a fictitious field  $\omega/|\gamma|$  opposing  $B_0$ :  $B_{\text{eff}} = (B_0 - \omega/|\gamma|)\hat{z} + B_1\hat{x}'$
- 2 the spin precesses about  $B_{\text{eff}}$  at  $\Omega = \sqrt{(\Delta^2 + \omega_1^2)}$ , with  $\omega_0 = |\gamma|B_0$ ,  $\omega_1 = |\gamma|B_1$  and  $\Delta = \omega - \omega_0$ , so a spin starting along  $z$  flips with probability  $P = (\omega_1^2/\Omega^2) \sin^2(\Omega t/2)$ ; on resonance  $B_{\text{eff}} = B_1\hat{x}'$  and  $P = \sin^2(\omega_1 t/2)$

*Candidates who stay in the laboratory frame face a time-dependent Hamiltonian they cannot integrate. Going to the frame that turns with  $B_1$  makes the field static whichever way  $B_1$  rotates; the sense decides only the sign of the fictitious field, which cancels  $B_0$  at  $\omega = \omega_0$  when  $B_1$  turns with the precession. A field turning the other way sees  $B_0 + \omega/|\gamma|$  and never comes to resonance, which is why the counter-rotating half of an oscillating field is what the rotating-wave approximation discards.*

(e) CALCULATE · U3

[2]

The flipper is 5.0 cm long and  $B_0 = 10.0$  mT. Calculate the frequency  $\omega/2\pi$  at which  $B_1$  must rotate, and the smallest value of  $B_1$  that turns a neutron spin polarised along  $+z$  into one polarised along  $-z$ .

- 1 on resonance,  $\omega/2\pi = |\gamma|B_0/2\pi = 1.832 \times 10^8 \text{ rad s}^{-1} \text{ T}^{-1} \times 0.0100 \text{ T}/2\pi = 2.92 \times 10^5 \text{ Hz}$  (292 kHz)
- 2  $t = 0.050 \text{ m}/(2200 \text{ m s}^{-1}) = 2.27 \times 10^{-5} \text{ s}$ , and a flip needs  $\omega_1 t = \pi$ , so  $B_1 = \pi/(|\gamma|t) = 7.55 \times 10^{-4} \text{ T}$  (0.755 mT)

*Setting  $\omega_1 t = 2\pi$ , a full Rabi cycle, returns the spin to where it started; a flip needs half a cycle. For a truly rotating  $B_1$  the rotating-frame result is exact at any strength; the smallness of 0.755 mT against  $B_0 = 10.0$  mT matters when the flipper is driven by an oscillating field instead, whose counter-rotating half is then far enough off resonance to neglect.*

12  
CORE  
COURSE

STRUCTURED · DEMANDING · UQMII-06.02 · UQMII-06.05 · UQMII-06.06 · UQMII-07.01 · UQMII-07.02 · UQMII-07.03 · UQMII-07.04 · UQMII-07.05

[11]

Two atoms of mass  $m$  are held in a narrow one-dimensional box trap, modelled as an infinite square well on  $0 < x < L$ . The single-particle states are  $\psi_n(x) = \sqrt{2/L} \sin(n\pi x/L)$ , with energies  $E_n = n^2 E_1$ , where  $E_1 = \pi^2 \hbar^2 / (2mL^2)$ . The atoms interact weakly through a short-range repulsion  $H' = g\delta(x_1 - x_2)$ , with  $g > 0$ , which is treated as a perturbation of  $H_0 = H_1 + H_2$ .  $P_{12}$  exchanges every label of the two atoms, coordinates and internal states alike. You may use  $\int_0^L \psi_1(x)^4 dx = 3/(2L)$ .

(a) EXPLAIN · U1

[2]

$P_{12}$  commutes with  $H_0 + H'$ . Explain why this alone does not require the two-atom state to be symmetric or antisymmetric under exchange, and state what does.

- 1  $[P_{12}, H] = 0$  means only that exchange symmetry, if a state has it, is conserved in time; states with no exchange symmetry, such as  $\psi_1(x_1)\psi_2(x_2)$ , are perfectly good states of the two-particle space, as they are for distinguishable atoms
- 2 the symmetrisation postulate: identical particles must be in states symmetric under  $P_{12}$  (bosons, integer spin) or antisymmetric (fermions, half-integer spin), the link to spin being the spin-statistics connection, quoted from relativistic field theory rather than derived

*The error to catch is the argument that a symmetric Hamiltonian forces symmetric eigenstates. A commuting operator allows the eigenstates to be chosen symmetric or antisymmetric; only the postulate makes the choice compulsory, and only for identical particles.*

- (b) **SHOW THAT** · U2 [2]
- Show that  $\int_0^L \psi_1(x)^2 \psi_2(x)^2 dx = 1/L$ .
- 1 with  $u = \pi x/L$ ,  $\sin^2 u \sin^2 2u = \frac{1}{4}(1 - \cos 2u)(1 - \cos 4u) = \frac{1}{4}[1 - \frac{1}{2}\cos 2u - \cos 4u + \frac{1}{2}\cos 6u]$ , using  $\cos 2u \cos 4u = \frac{1}{2}(\cos 2u + \cos 6u)$
  - 2 each cosine integrates to zero over  $0 < u < \pi$ , leaving  $(2/L)^2 \times \frac{1}{4} \times L = 1/L$   
*Replacing each  $\sin^2$  by its average of  $\frac{1}{2}$  happens to give  $1/L$  here, but the same shortcut gives  $1/L$  for  $\int \psi_1^4 dx$ , whose true value is  $3/(2L)$ ; the marks are for the product expansion, which is what makes the result reliable.*
- (c) **DETERMINE** · U2 [3]
- For two distinguishable atoms the unperturbed level  $5E_1$  is twofold degenerate, spanned by  $|12\rangle = \psi_1(x_1)\psi_2(x_2)$  and  $|21\rangle = \psi_2(x_1)\psi_1(x_2)$ . Determine the matrix of  $H'$  in this subspace, its first-order energy shifts and the corresponding good states.
- 1 diagonal (direct) elements:  $\langle 12|H'|12\rangle = \langle 21|H'|21\rangle = g \int \psi_1(x)^2 \psi_2(x)^2 dx = g/L$ , the delta function setting  $x_1 = x_2 = x$
  - 2 off-diagonal (exchange) element:  $\langle 12|H'|21\rangle = g \int \psi_1 \psi_2 \psi_2 \psi_1 dx = g/L$ , the same integral, because a contact interaction samples both orderings at the same point
  - 3 the matrix  $(g/L)[[1, 1], [1, 1]]$  has eigenvalues  $2g/L$  and  $0$ , with good states  $(|12\rangle + |21\rangle)/\sqrt{2}$  and  $(|12\rangle - |21\rangle)/\sqrt{2}$ , the eigenstates of  $P_{12}$  with eigenvalues  $+1$  and  $-1$   
*Applying the non-degenerate formula gives both states the single shift  $g/L$  and misses the splitting. The equality of the exchange and direct integrals is special to a contact interaction; for a finite-range repulsion the exchange integral is smaller, but  $P_{12}$  still fixes the good states.*
- (d) **CALCULATE** · U3 [2]
- Take  $g = 0.10E_1L$ . Calculate, to first order in  $g$  and in units of  $E_1$ , the ground-state energy of two identical spinless bosons, and of two identical fermions in the same internal state.
- 1 bosons: both atoms in  $\psi_1$ , so  $E = 2E_1 + g \int \psi_1^4 dx = 2E_1 + 3g/(2L) = 2.15E_1$
  - 2 fermions: antisymmetry forbids both in  $\psi_1$ , so the lowest state is  $(|12\rangle - |21\rangle)/\sqrt{2}$  at  $5E_1$  with shift  $J - K = 0$ , giving  $E = 5.00E_1$ , which is exact to all orders because every antisymmetric spatial state vanishes at  $x_1 = x_2$ , where the delta function acts  
*Candidates give the fermions the direct shift  $g/L$  alone, forgetting the exchange term that cancels it. First order is safe for the bosons: the largest coupling of the ground state to another level,  $\langle 11|H'|22\rangle = g/L = 0.10E_1$ , is small against the gap of  $6E_1$ .*
- (e) **COMPARE** · U1 [2]
- Two spin- $\frac{1}{2}$  fermions, for example atoms in two internal states labelled  $\uparrow$  and  $\downarrow$ , occupy  $\psi_1$  and  $\psi_2$  in the same trap,  $H'$  does not act on spin, and  $g = 0.10E_1L$  as in (d). Compare the first-order energies of the states with total spin  $S = 0$  and  $S = 1$ , and account for the difference.
- 1 the whole state must be antisymmetric, so  $S = 0$  (antisymmetric spin singlet) goes with the symmetric spatial state, at  $5E_1 + 2g/L = 5.20E_1$ , and  $S = 1$  (symmetric spin triplet) goes with the antisymmetric spatial state and stays at  $5.00E_1$ : the triplet lies lower by  $2g/L = 0.20E_1$
  - 2 the splitting is an exchange correlation, not a spin-dependent force: the triplet's spatial wavefunction vanishes where the atoms meet, so the repulsion never acts, just as orthohelium lies below parahelium and as Hund's first rule favours maximum  $S$   
*The error to catch is placing the singlet lower because paired spins seem to attract, or giving the two states one energy because  $H'$  ignores spin. The energy depends on spin only through the spatial symmetry that antisymmetry imposes.*

A source emits pairs of spin- $\frac{1}{2}$  particles intended to be in the singlet state. Alice measures the spin component of one particle along a direction at angle  $a$  in the  $xz$ -plane and Bob that of the other along angle  $b$ , each recording  $+1$  or  $-1$ . For each setting the correlation  $E$  is the mean of the product of the two results; for the ideal singlet  $E(a, b) = -\cos(a - b)$ . Every local hidden-variable model obeys  $|S| \leq 2$ , where  $S = E(a, b) - E(a, b') + E(a', b) + E(a', b')$ . The run used  $a = 0^\circ$ ,  $a' = 90^\circ$ ,  $b = 45^\circ$  and  $b' = 135^\circ$ , and the table gives the number of detected pairs with each combination of results, Alice's sign first. Treat each detected pair as an independent trial.

**(a)** CALCULATE · U4

[2]

Calculate  $E$  for each of the four settings.

1  $E = (N_{++} + N_{--} - N_{+-} - N_{-+})/N$ , with  $N$  the total for that setting:  $E(a, b) = -327/513 = -0.637$  and  $E(a, b') = +294/482 = +0.610$

2  $E(a', b) = -300/520 = -0.577$  and  $E(a', b') = -288/482 = -0.598$

*Dividing every row by one round total, such as 500, introduces errors of up to 4% that survive into  $S$ ; each correlation must be divided by its own number of pairs, which here runs from 482 to 520.*

**(b)** DETERMINE · U4

[2]

Determine  $S$ , and the fraction of the ideal-singlet value that it reaches.

1  $S = -0.637 - 0.610 - 0.577 - 0.598 = -2.42$ , the minus sign in front of the positive  $E(a, b')$  making all four terms negative

2 for the ideal singlet each  $|E| = \cos 45^\circ = 0.707$  and  $S = -2\sqrt{2} = -2.83$ , so the data reach  $2.42/2.83 = 0.86$  of it, as for a singlet mixed with uncorrelated noise,  $E = -V \cos(a - b)$  with visibility  $V \approx 0.86$

*Adding  $E(a, b')$  instead of subtracting it gives  $S = -1.20$  and an apparent agreement with local realism. The combination is fixed by the inequality, and the angles were chosen so that every term pushes  $S$  the same way.*

**(c)** ESTIMATE · U4

[2]

Estimate the standard uncertainty in  $S$  from counting statistics, stating the assumptions you make.

1 assumes that each pair is an independent trial whose product  $\pm 1$  has mean  $E$  and variance  $1 - E^2$ , and that the four settings are sampled independently, so  $\sigma_E = \sqrt{(1 - E^2)/N} \approx \sqrt{((1 - 0.37)/500)} \approx 0.036$  for each setting

2  $\sigma_S = \sqrt{(\sum \sigma_E^2)} \approx 2 \times 0.036 = 0.071$

*Adding the four  $\sigma_E$  linearly gives 0.14 and halves the apparent significance; independent errors add in quadrature. Taking the spread of the four  $|E|$  values as the uncertainty is no better, since four numbers fix a spread only roughly and any real difference between settings would be mistaken for noise.*

**(d)** EVALUATE · U4

[2]

Evaluate whether these data rule out every local hidden-variable model, and say what else a conclusive test must secure.

1  $|S| - 2 = 0.42$ , about  $5.9\sigma$  with  $\sigma_S = 0.071$ : statistically decisive, far beyond what counting fluctuations about any  $|S| \leq 2$  could produce

2 but the conclusion also needs a large enough fraction of pairs detected, or a fair-sampling assumption (the detection loophole), setting choices made at random and at space-like separation from the other side's measurement (the locality loophole), and a check of systematic errors such as analyser-angle calibration, which counting statistics do not include

*Strong answers separate statistical significance from the assumptions behind the inequality. A violation by many standard deviations shows that no local model reproduces these counts only if the detected pairs are a fair sample and neither side's setting could influence the other.*

(e) JUSTIFY · U4

[2]

Quantum mechanics predicts that Alice's results alone cannot reveal which setting Bob chose. Justify this from the singlet's reduced density operator, and test it against the data for Alice's setting a.

- 1 tracing Bob's particle out of the singlet gives  $\rho_A = I/2$ , and Bob's measurement, averaged over his results, which Alice does not know, leaves  $\rho_A$  unchanged, so Alice obtains +1 with probability  $1/2$  at every a, whatever b is
- 2 from the data,  $P_{A(+1)} = (43 + 215)/513 = 0.503$  with Bob at b and  $(192 + 48)/482 = 0.498$  with Bob at b'; each has standard uncertainty  $\sqrt{(0.25/N)} \approx 0.022$ , so both agree with  $1/2$  and with each other: no signal

*Candidates look for the no-signalling test in the correlations E, which do depend on both settings. It lies in the marginal counts, which the table gives only implicitly, and the comparison means nothing without an uncertainty.*

14  
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FREE RESPONSE · EXTENDED DERIVATION · DISCRIMINATING · UQMII-05.07 · UQMII-06.02 · UQMII-08.02 · UQMII-08.03 · UQMII-08.04 · UQMII-08.05 · UQMII-08.06 · UQMII-08.08

[15]

A hydrogen-like ion has one electron of mass m bound to a point nucleus of charge Ze, treated as infinitely heavy, so that  $V(r) = -Ze^2/(4\pi\epsilon_0 r)$  and the unperturbed energies  $E_n = -(Z\alpha)^2 mc^2/(2n^2)$  are degenerate in l,  $m_l$  and  $m_s$ . With  $a = a_0/Z$ , so that  $\hbar^2/(ma) = Ze^2/(4\pi\epsilon_0)$  and  $E_n = -Ze^2/(8\pi\epsilon_0 a n^2)$ , the unperturbed states give  $\langle 1/r \rangle = 1/(n^2 a)$ ,  $\langle 1/r^2 \rangle = 1/[n^3(l + 1/2)a^2]$ ,  $\langle 1/r^3 \rangle = 1/[n^3(l + 1/2)(l + 1)a^3]$  for  $l \geq 1$ , and  $|\psi_{n00}(0)|^2 = 1/(\pi n^3 a^3)$ . The fine-structure Hamiltonian is  $H_{\text{rel}} + H_{\text{SO}} + H_{\text{D}}$ , with  $H_{\text{rel}} = -p^4/(8m^3 c^2)$ ;  $H_{\text{SO}} = [1/(2m^2 c^2)](1/r)(dV/dr) L \cdot S$ , which already contains the Thomas factor of  $1/2$ , quoted from relativistic kinematics; and the Darwin term  $H_{\text{D}} = [\pi \hbar^2/(2m^2 c^2)][Ze^2/(4\pi\epsilon_0)]\delta^3(r)$ , quoted from the Dirac equation. Take  $mc^2 = 0.5110$  MeV,  $\alpha = 1/137.04$  and  $\hbar = 4.136 \times 10^{-15}$  eV s.

(a) JUSTIFY · U1

[2]

Each level n is degenerate, yet each fine-structure term can be evaluated with the non-degenerate formula  $E^{(1)} = \langle H' \rangle$  in the coupled basis  $|n, l, j, m_j\rangle$ . Justify this, naming the operators each term commutes with.

- 1  $H_{\text{rel}}$  and  $H_{\text{D}}$  are spin-independent scalars: they commute with  $L^2$ ,  $L_z$ ,  $S^2$  and  $S_z$ , so they have no matrix elements between states of different l,  $m_l$  or  $m_s$ , and are diagonal in the uncoupled basis and equally in the coupled one
- 2  $H_{\text{SO}} \propto L \cdot S = (J^2 - L^2 - S^2)/2$  commutes with  $J^2$ ,  $J_z$ ,  $L^2$  and  $S^2$  but not with  $L_z$  or  $S_z$ , so it is diagonal only in the coupled basis; there all three terms are diagonal, the degenerate states are already the good states, and  $E^{(1)} = \langle H' \rangle$  holds state by state

*Answers that call the coupled basis conventional miss the point: it is forced by  $H_{\text{SO}}$ . The argument is complete only when it also shows that  $H_{\text{rel}}$  cannot mix different l inside the degenerate level, which a less symmetric perturbation could.*

(b) SHOW THAT · U2

[3]

Starting from  $p^2/(2m) = H_0 - V$ , show that the relativistic shift is  $E_{\text{rel}} = -[E_n^2/(2mc^2)][4n/(l + 1/2) - 3]$ .

- 1  $H_{\text{rel}} = -(1/(2mc^2))(p^2/2m)^2$ , and because  $p^2$  is Hermitian ( $p^4$  is the squared norm of  $p^2|\psi\rangle$ ), so  $E_{\text{rel}} = -(1/(2mc^2))\langle (E_n - V)^2 \rangle = -(1/(2mc^2))\langle E_n^2 - 2E_n V + V^2 \rangle$
- 2  $\langle V \rangle = -[Ze^2/(4\pi\epsilon_0)]\langle 1/r \rangle = -Ze^2/(4\pi\epsilon_0 n^2 a) = 2E_n$ , and  $\langle V^2 \rangle = [Ze^2/(4\pi\epsilon_0)]^2 \langle 1/r^2 \rangle = [Ze^2/(4\pi\epsilon_0 a)]^2/[n^3(l + 1/2)] = 4nE_n^2/(l + 1/2)$ , using  $Ze^2/(4\pi\epsilon_0 a) = -2n^2 E_n$
- 3 so  $E_{\text{rel}} = -(1/(2mc^2))\langle E_n^2 - 4E_n^2 + 4nE_n^2/(l + 1/2) \rangle = -[E_n^2/(2mc^2)][4n/(l + 1/2) - 3]$

*Candidates who expand  $p^4$  in coordinates meet derivatives of the Coulomb singularity; the route through  $(E_n - V)^2$  avoids them, and it is legitimate only because  $p^2$  can act to the left on the bra. The sign of  $\langle V \rangle = 2E_n$ , which is negative, is the slip that turns  $-3$  into  $+5$ , and since the result is printed, a candidate who forces agreement without it earns nothing for the last line.*

(c) DERIVE · U2

[3]

Derive the first-order spin-orbit shift  $E_{SO}$  of a state with  $l \geq 1$ , expressed in terms of  $E_n$ ,  $mc^2$ ,  $n$ ,  $l$  and  $j$ .

- 1  $(1/r)dV/dr = [Ze^2/(4\pi\epsilon_0)]/r^3$ , so  $H_{SO} = [Ze^2/(4\pi\epsilon_0)] L \cdot S / (2m^2c^2r^3)$
- 2 in the coupled basis  $L \cdot S = (J^2 - L^2 - S^2)/2$  has eigenvalue  $(\hbar^2/2)[j(j+1) - l(l+1) - 3/4]$ , and  $\langle 1/r^3 \rangle = 1/[n^3l(l+1/2)(l+1)a^3]$
- 3  $E_{SO} = [Ze^2/(4\pi\epsilon_0)](\hbar^2/(ma))[j(j+1) - l(l+1) - 3/4]/[4mc^2a^2n^3l(l+1/2)(l+1)]$ , and with  $\hbar^2/(ma) = Ze^2/(4\pi\epsilon_0)$  and  $[Ze^2/(4\pi\epsilon_0a)]^2 = 4n^4E_n^2$  this is  $[E_n^2/(mc^2)] n[j(j+1) - l(l+1) - 3/4]/[l(l+1/2)(l+1)]$

*Evaluating  $\langle L \cdot S \rangle$  in the uncoupled basis as  $m_l m_s \hbar^2$  takes the diagonal elements of a matrix that is not diagonal there, and gives a shift that depends on  $m_l$ ; the result must depend on  $j$  instead.*

(d) SHOW THAT · U2

[3]

Show that, once the Darwin term is included for  $l = 0$ , the three terms sum to  $E_{fs} = [E_n^2/(2mc^2)][3 - 4n/(j + 1/2)]$  for every state, so that the energy depends on  $n$  and  $j$  only.

- 1  $j = l + 1/2$ : the bracket in  $E_{SO}$  is  $l$ , so  $E_{SO} = nE_n^2/[mc^2(l + 1/2)(l + 1)]$ , and  $E_{rel} + E_{SO} = [E_n^2/(2mc^2)][3 - 4n/(l + 1/2) + 2n/((l + 1/2)(l + 1))] = [E_n^2/(2mc^2)][3 - 4n/(l + 1)]$ , with  $l + 1 = j + 1/2$
- 2  $j = l - 1/2$ : the bracket is  $-(l + 1)$ , so  $E_{SO} = -nE_n^2/[mc^2l(l + 1/2)]$ , and  $E_{rel} + E_{SO} = [E_n^2/(2mc^2)][3 - 4n/(l + 1/2) - 2n/(l(l + 1/2))] = [E_n^2/(2mc^2)][3 - 4n/l]$ , with  $l = j + 1/2$
- 3  $l = 0$ :  $H_{SO}$  contributes nothing,  $E_D = [\pi\hbar^2/(2m^2c^2)][Ze^2/(4\pi\epsilon_0)]/(\pi n^3a^3) = 2nE_n^2/(mc^2)$ , and  $E_{rel} = -[E_n^2/(2mc^2)](8n - 3)$ , so the sum is  $[E_n^2/(2mc^2)](3 - 4n)$ , the formula with  $j = 1/2$

*This part catches candidates who apply the spin-orbit formula at  $l = 0$ , where it is  $0/0$ , instead of recognising that  $L \cdot S$  vanishes there and that the Darwin term, a contact term acting only where  $|\psi(0)|^2$  is nonzero, takes its place. Because the result is printed, each case must be carried to it explicitly.*

(e) SKETCH · U1

[2]

For  $\text{He}^+$  ( $Z = 2$ ), sketch the fine structure of the  $n = 2$  level: draw the unperturbed level and the fine-structure levels labelled  $2S_{(1/2)}$ ,  $2P_{(1/2)}$  and  $2P_{(3/2)}$ , marking each shift in  $\mu\text{eV}$  and the  $2P_{(3/2)} - 2P_{(1/2)}$  splitting in GHz.

- 1  $E_2 = -(2\alpha)^2 mc^2/8 = -13.6 \text{ eV}$  and  $E_2^2/(2mc^2) = 181.1 \mu\text{eV}$ , so  $2S_{(1/2)}$  and  $2P_{(1/2)}$  are drawn as one level  $5 \times 181.1 = 906 \mu\text{eV}$  below the unperturbed level and  $2P_{(3/2)}$  as a level  $181 \mu\text{eV}$  below it: every state lies below  $E_2$
- 2 the  $2P_{(3/2)} - 2P_{(1/2)}$  splitting is marked as  $4 \times 181.1 \mu\text{eV} = 724 \mu\text{eV}$ , which is  $724 \times 10^{-6} \text{ eV} / (4.136 \times 10^{-15} \text{ eV s}) = 175 \text{ GHz}$ , sixteen times hydrogen's  $10.9 \text{ GHz}$

*Common sketches put  $2P_{(3/2)}$  above the unperturbed level, as a spin-orbit-only picture would because its  $E_{SO}$  is positive, or separate  $2S_{(1/2)}$  from  $2P_{(1/2)}$ . The relativistic term lowers every state, and in this theory the two  $j = 1/2$  states coincide exactly.*

The measured  $2S_{1/2}$ – $2P_{1/2}$  Lamb shifts are 1.058 GHz in hydrogen and 14.04 GHz in  $\text{He}^+$ . Welton's argument gives, for an  $nS$  level,  $\Delta E \propto \alpha(Z\alpha)^4 mc^2 \ln[1/(Z\alpha)]/n^3$ , with a prefactor, and an argument of the logarithm, that it fixes only roughly. Evaluate how well this scaling accounts for the ratio of the two shifts.

- 1 the scaling predicts a ratio  $2^4 \ln[1/(2\alpha)]/\ln(1/\alpha) = 16 \times 4.23/4.92 = 13.7$ , below the  $Z^4 = 16$  of the fine structure because the logarithm falls with  $Z$ ; the measured ratio is  $14.04/1.058 = 13.3$
- 2 judgement: agreement to about 4%, so the scaling captures the physics, a correction proportional to  $Z|\psi(0)|^2 \propto Z^4$  that acts on  $s$  states only; but the argument of the logarithm is fixed only to an order of magnitude, so agreement at a few per cent is partly fortunate, since the ratio cancels the prefactor but not that uncertainty

*Scaling the hydrogen value by  $Z^4$  alone predicts 16.9 GHz, 20% too high. A strong answer shows the logarithm doing measurable work, then limits its claim to what an order-of-magnitude argument can support.*

## What the command words are asking for

Examiners mark to the command word as well as to the physics. An answer that explains where the question said state has spent time earning one mark; one that states a result where the question said derive has earned none, however correct the result.

|                  |                                                                                                                                                                  |
|------------------|------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| <b>State</b>     | Give the result, definition or law concisely. No justification is required.                                                                                      |
| <b>Describe</b>  | Give the relevant features of a situation or process in words, precisely enough that someone else could reproduce it.                                            |
| <b>Explain</b>   | Give the physical reason a result or behaviour occurs, connecting it explicitly to the principle that governs it.                                                |
| <b>Calculate</b> | Obtain a numerical value, showing the relation used, the substitution and the units of the result.                                                               |
| <b>Determine</b> | Obtain a result by any valid route the problem allows — analytic, graphical or numerical — with enough working to be followed.                                   |
| <b>Derive</b>    | Start from a named fundamental law or definition and reach the required result by explicit, justified steps.                                                     |
| <b>Show that</b> | Establish a result the question gives you. Every step must be shown, because the stated answer earns nothing on its own.                                         |
| <b>Estimate</b>  | Reach an order-of-magnitude value from stated, reasonable assumptions, and say what those assumptions are.                                                       |
| <b>Sketch</b>    | Draw the shape of a graph or field with axes labelled and its key features marked — intercepts, asymptotes, turning points, limits. Exact scale is not required. |
| <b>Justify</b>   | Support a claim or a choice with evidence, and with the reasoning that connects that evidence to the claim.                                                      |
| <b>Evaluate</b>  | Weigh a model, argument or result against criteria, including its assumptions and domain of validity, and reach a stated judgement.                              |
| <b>Compare</b>   | Identify the similarities and differences between two situations, models or results, relating each difference to its cause.                                      |
| <b>Predict</b>   | Say what will happen when a condition changes, reasoning from a principle rather than guessing, and give the reason.                                             |

### WHAT IS BEING TESTED

## University assessment objectives

Each course has the two papers a university course is examined by: a midterm on the first half of its units, and a cumulative final weighted towards the second half. Every paper combines short conceptual multiple-choice items with structured problems, a data or estimation question, and at least one extended derivation. Constants are given where a question needs them; a calculator and your own formula sheet are assumed.

|                             |                                                                                                                                                                                                                                             |
|-----------------------------|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| <b>U1</b><br>18 MARKS · 24% | <b>Conceptual understanding</b><br>Identify the governing principle and the conditions under which it holds, and reason qualitatively about what a result must look like before calculating it.                                             |
| <b>U2</b><br>31 MARKS · 42% | <b>Mathematical modelling and derivation</b><br>Translate a physical situation into mathematics: choose coordinates and approximations, set up the governing equations, solve them symbolically, and derive stated results from named laws. |

**U3**

12 MARKS · 16%

**Quantitative problem solving**

Carry a multi-step calculation to a numerical result with correct units and sensible precision, and check it against dimensions, limiting cases and orders of magnitude.

**U4**

13 MARKS · 18%

**Data, estimation and experimental reasoning**

Analyse measurements and their uncertainties, linearise and fit data, estimate orders of magnitude from stated assumptions, and judge whether evidence supports a model.

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