

University Quantum Mechanics II · Final Examination

The whole of Quantum Mechanics II, weighted towards the second half of the course: external fields and hyperfine structure, the variational principle, WKB, time-dependent perturbation theory and radiation, Berry's phase, and scattering. The spherical harmonics, hydrogen, spin in fields, density operators, angular momentum, perturbation theory and identical particles from the first half are sampled throughout.

SUGGESTED TIME 150 minutes	TOTAL MARKS 118	QUESTIONS 19	MULTIPLE CHOICE 10
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SECTION	UQMII · Final · University Quantum Mechanics II — Final examination
IN THE FORMAT OF	A cumulative university final: conceptual multiple choice, structured problems, a data-analysis question and two extended derivations
DEMAND	Recall 1 · Routine 8 · Demanding 7 · Discriminating 3 <i>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.</i>
COURSE UNITS	UQMII-01 · UQMII-02 · UQMII-03 · UQMII-04 · UQMII-05 · UQMII-06 · UQMII-07 · UQMII-08 · UQMII-09 · UQMII-10 · UQMII-11 · UQMII-12 · UQMII-13 · UQMII-14 · UQMII-15

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.

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University Quantum Mechanics II · Final Examination

Answer all questions. 118 marks in 150 minutes.

1 MULTIPLE CHOICE · RECALL · UQMII-01.02 [1]
CORE COURSE

A linear molecule attached by one end to a flat surface is modelled as a rigid rotor, of moment of inertia I about the attached end, that turns freely except that its axis cannot point into the surface. The polar angle θ of the axis, measured from the outward normal to the surface, is therefore confined to $0 \leq \theta \leq \pi/2$, and the surface acts as a hard wall: the wavefunction must vanish at $\theta = \pi/2$, where the axis would lie in the surface. The rotor's Hamiltonian is $H = L^2/(2I)$. For $m = 0$, with $x = \cos \theta$ and $\lambda = 2IE/\hbar^2$, the angular equation is Legendre's equation, and of its power-series solutions about $x = 0$ only the series of odd powers of x vanishes at $x = 0$, as the wall requires. Which values of λ are allowed?

- A** $\lambda = l(l+1)$ with $l = 0, 1, 2, \dots$, the free rotor's values, because the wall changes a boundary condition but not Legendre's equation.
- B** $\lambda = l(l+1)$ with $l = 0, 2, 4, \dots$, because only the even polynomials are symmetric about the equator, where the wall lies.
- C** $\lambda = l(l+1)$ with $l = 1, 3, 5, \dots$, because the odd series must still terminate to stay finite at $\theta = 0$, where the axis lies along the surface normal.
- D** Any $\lambda \geq 0$, because the series need only be finite for $0 \leq \theta \leq \pi/2$, and the pole $\theta = \pi$, where an unterminated series diverges, lies outside that range.

Answer

2 MULTIPLE CHOICE · ROUTINE · UQMII-02.09 · UQMII-07.07 [1]
CORE COURSE

A crude model of a valence electron outside a closed-shell core replaces the Coulomb potential by $V(r) = -k/r - \beta/r^2$, where $k = e^2/(4\pi\epsilon_0)$ and β is a small positive constant representing the extra attraction felt by an electron that penetrates the core. Compared with hydrogen, which statement about the bound-state spectrum is correct?

- A** The degeneracy in m is lifted, because the extra term breaks the symmetry that protected it.
- B** Levels of the same n but different l separate, with the lowest l pushed down most, while each keeps its $(2l+1)$ -fold degeneracy in m ; the quantum Runge-Lenz vector is no longer conserved.
- C** No degeneracy is lifted: the extra term simply adds to the centrifugal term $\hbar^2 l(l+1)/(2mr^2)$, and so shifts every level of a given n by the same amount.
- D** The l -degeneracy survives at first order in β , because $\langle 1/r^2 \rangle$ is the same for every state of a given n , and is lifted only at second order.

Answer

3CORE
COURSE

MULTIPLE CHOICE · ROUTINE · UQMII-03.01 · UQMII-03.03

[1]

In a nuclear magnetic resonance magnet whose field B points along $+z$, the spins of protons at rest precess at 400.0 MHz. A particle at rest whose magnetic moment is $\mu = \gamma S$ has the Hamiltonian $H = -\gamma B S_z$, and each spin component obeys the Heisenberg equation $dS/dt = (i/\hbar)[H, S]$; $\gamma = +2.675 \times 10^8 \text{ rad s}^{-1} \text{ T}^{-1}$ for the proton and $\gamma = -1.761 \times 10^{11} \text{ rad s}^{-1} \text{ T}^{-1}$ for the electron. A free electron is now held at rest in the same magnet. Which statement about the precession of its spin is correct?

- A** It precesses at 400.0 MHz, in the same sense as the proton spins, because the Larmor frequency is set by the field alone.
- B** It precesses at 263.3 GHz, in the same sense as the proton spins, because every moment precesses in the sense fixed by the direction of B .
- C** It precesses at 131.7 GHz, in the opposite sense to the proton spins, because the two spinor components acquire phases of only $\pm \gamma B t/2$.
- D** It precesses at 263.3 GHz, in the opposite sense to the proton spins, while S_z , which commutes with H , stays constant.

Answer

4CORE
COURSE

MULTIPLE CHOICE · ROUTINE · UQMII-08.01 · UQMII-08.06

[1]

In hydrogen the fine-structure shifts are $E_{fs} = -[E_n^2/(2mc^2)][4n/(j + \frac{1}{2}) - 3]$, where $E_n = -13.6 \text{ eV}/n^2$, so they are smaller than the Bohr energies by a factor of order α^2 and depend on n and j only. The $2p_{3/2}$ - $2p_{1/2}$ splitting is measured to be 10.97 GHz. What splitting does the formula then predict between the $3d_{5/2}$ and $3d_{3/2}$ levels?

- A** 1.08 GHz
- B** 3.25 GHz
- C** 4.88 GHz
- D** 0.722 GHz

Answer

5CORE
COURSE

MULTIPLE CHOICE · ROUTINE · UQMII-09.01 · UQMII-09.02

[1]

A hydrogen atom in the $2p_{1/2}$ level is placed in a magnetic field of 0.10 T, which is weak compared with the 10.97 GHz fine-structure splitting of $n = 2$. By what frequency are its two m_j sublevels split? Take $\mu_B = 5.788 \times 10^{-5} \text{ eV T}^{-1}$ and $h = 4.136 \times 10^{-15} \text{ eV s}$.

- A** 2.80 GHz
- B** 1.40 GHz
- C** 0.933 GHz
- D** 1.87 GHz

Answer

6

CORE
COURSE

MULTIPLE CHOICE · ROUTINE · UQMII-10.01

[1]

A system has exact ground and first excited energies $E_0 = -1.00$ eV and $E_1 = -0.25$ eV, with normalised eigenstates ψ_0 and ψ_1 . A normalised trial state is $\phi = \sqrt{(1 - \epsilon^2)} \psi_0 + \epsilon \psi_1$ with $\epsilon = 0.10$, so that 1% of its weight lies in the wrong state. What is $\langle \phi | H | \phi \rangle$?

- A -1.020 eV
- B -0.9925 eV
- C -0.925 eV
- D -1.000 eV

Answer

7

CORE
COURSE

MULTIPLE CHOICE · DEMANDING · UQMII-11.06 · UQMII-11.07

[1]

A cold atom of mass m is held along x in a harmonic trap whose angular frequency ω satisfies $\omega/2\pi = 2.0$ kHz. A thin repulsive light sheet is then switched on at the trap centre and is modelled as an impenetrable wall at $x = 0$, so that the atom moves in $V(x) = \frac{1}{2}m\omega^2 x^2$ for $x > 0$ only. WKB quantisation is applied using the connection-formula phase at the smooth turning point and the condition $\psi = 0$ at the wall. What energy does it predict for the first excited state of this half-trap, expressed as the frequency E/h and measured from the bottom of the trap?

- A 3.0 kHz
- B 5.0 kHz
- C 6.0 kHz
- D 7.0 kHz

Answer

8

CORE
COURSE

MULTIPLE CHOICE · ROUTINE · UQMII-14.04

[1]

A two-level system is swept at a constant rate through an avoided crossing. The probability of a diabatic passage, in which the system stays in its initial diabatic state and so jumps the gap, is measured to be 0.20. According to the Landau-Zener formula, what is this probability when the sweep rate is doubled?

- A 0.45
- B 0.40
- C 0.10
- D 0.040

Answer

9CORE
COURSE

MULTIPLE CHOICE · DEMANDING · UQMII-12.09 · UQMII-13.05 · UQMII-13.08

[1]

A hydrogen atom is prepared in the $2s_{1/2}$ state, isolated and in zero field. It lives for about 0.12 s, whereas $2p$ lives for 1.6 ns. Which process is responsible for its decay?

- A** Emission of one electric-dipole photon to $1s$, slowed because the $2s$ radial function has a node.
- B** Emission of one electric-dipole photon to $2p_{1/2}$, which lies 1.06 GHz below $2s_{1/2}$ because of the Lamb shift.
- C** Emission of two electric-dipole photons together, through virtual intermediate p states, sharing the 10.2 eV between them.
- D** Emission of one magnetic-dipole photon to $1s$, allowed because parity is unchanged and $\Delta l = 0$.

Answer

10CORE
COURSE

MULTIPLE CHOICE · ROUTINE · UQMII-15.04 · UQMII-15.07

[1]

Slow electrons scatter from atoms of a noble gas, which are modelled as spherically symmetric attractive wells. At the energies of interest only the s wave is appreciably scattered, and at one energy its phase shift passes through $\delta_0 = \pi$. What is observed near that energy?

- A** A peak in the total cross-section, reaching the unitarity limit $4\pi/k^2$.
- B** A deep minimum in the total cross-section, because $(4\pi/k^2)\sin^2\delta_0$ vanishes, so the gas becomes nearly transparent to the electrons.
- C** A new bound state appearing at exactly that energy, because Levinson's theorem requires one whenever δ_0 reaches π .
- D** A cross-section equal to the geometric value πR^2 , because a phase shift of π reflects the wave as a hard sphere of the well's radius would.

Answer

Two electrons, each held in one of a pair of neighbouring quantum dots, interact through the exchange Hamiltonian $H = (J/\hbar^2) \mathbf{S}_1 \cdot \mathbf{S}_2$, with $J = 2.0 \mu\text{eV}$. Their orbital states are frozen, so only the spins evolve. Write $|\uparrow\downarrow\rangle$ for spin 1 up and spin 2 down along z , and similarly for the other product states. Take $\hbar = 1.055 \times 10^{-34} \text{ J s}$ and $1 \text{ eV} = 1.602 \times 10^{-19} \text{ J}$.

(a) SHOW THAT

[2]

Show that the eigenvalues of H are $J/4$ for each of the three triplet states and $-3J/4$ for the singlet.

(b) DETERMINE

[3]

At $t = 0$ the spins are prepared in $|\uparrow\downarrow\rangle$. By expressing this state in the coupled basis, determine the probability $P(t)$ that a measurement at time t finds the spins in $|\downarrow\uparrow\rangle$.

(c) CALCULATE

[1]

Calculate the shortest time after which the two spins have completely exchanged their states.

(d) DETERMINE

[3]

Determine the reduced density matrix of spin 1 at time t and its purity $\text{Tr } \rho_1^2$, and hence the earliest time at which spin 1 is maximally mixed.

(e) EXPLAIN

[2]

At that time an experimenter measures spin 1 alone, along any axis they choose. Explain why no such measurement can distinguish it from a spin drawn from an ensemble prepared half in $|\uparrow\rangle$ and half in $|\downarrow\rangle$, and what kind of measurement would reveal the difference.

An electron in a cubic InAs nanocrystal is modelled as a particle of charge $-e$ and effective mass $m^* = 0.023m_e$ in a cubical infinite well of side $L = 20$ nm centred on the origin, $-L/2 < x, y, z < L/2$. Spin is ignored, since its Zeeman energy is the same for every orbital state. The unperturbed states are $\psi_{(n_1 n_2 n_3)} = u_{(n_1)}(x)u_{(n_2)}(y)u_{(n_3)}(z)$, with energies $(n_1^2 + n_2^2 + n_3^2)\epsilon$, where $\epsilon = \pi^2 \hbar^2 / (2m^* L^2)$, $u_1(x) = \sqrt{2/L} \cos(\pi x/L)$ and $u_2(x) = \sqrt{2/L} \sin(2\pi x/L)$. A uniform magnetic field $B = 1.5$ T is applied along z . In the symmetric gauge, and to first order in B , it adds $H' = (\mu^* B / \hbar) L_z$, where $\mu^* = e\hbar / (2m^*)$ is the effective magneton and $L_z = -i\hbar(x \partial/\partial y - y \partial/\partial x)$; the term in B^2 is neglected. You may use $\int u_1(x) \times u_2(x) dx = 16L/(9\pi^2)$ and $\int u_1(du_2/dx) dx = 8/(3L) = -\int u_2(du_1/dx) dx$, each integral running from $-L/2$ to $L/2$. Take $m_e = 9.109 \times 10^{-31}$ kg, $\hbar = 1.055 \times 10^{-34}$ J s, $e = 1.602 \times 10^{-19}$ C and $1 \text{ eV} = 1.602 \times 10^{-19}$ J.

(a) CALCULATE

[2]

Calculate ϵ in meV, and the energies and degeneracies of the ground level and of the first excited level.

(b) CALCULATE

[2]

Calculate $\mu^* B$ in meV, and its ratio to the spacing 3ϵ that separates the first excited level from the levels on either side of it.

(c) DETERMINE

[3]

Using the integrals given, determine the matrix of H' in the first excited level, its eigenvalues in meV, and the good states.

(d) EXPLAIN

[2]

Explain how the rotation through 90° about the z -axis identifies these good states without any diagonalisation.

(e) SHOW THAT

[2]

The field is turned, at the same strength, to lie along the body diagonal $\hat{n} = (1, 1, 1)/\sqrt{3}$, so that $H' = (\mu^* B / \hbar) \hat{n} \cdot \mathbf{L}$. Show that the first excited level splits in exactly the same way, into shifts of $+3.63$ meV, 0 and -3.63 meV.

A hydrogen atom in the $n = 2$ shell is placed in a uniform static electric field F along z ; hyperfine structure is ignored. Without the field, $2s_{1/2}$ lies above $2p_{1/2}$ by the Lamb shift, $L = h \times 1057.8$ MHz, and $2p_{3/2}$ lies $h \times 10.97$ GHz above $2p_{1/2}$. The perturbation is $H' = eFz$. In the uncoupled basis $\langle 2s|z|2p, m_l = 0 \rangle = -3a_0$, with $a_0 = 5.29 \times 10^{-11}$ m, and in the convention used here $|2p_{1/2}, m_j = +1/2\rangle = \sqrt{(2/3)}|m_l = 1\rangle|\downarrow\rangle - \sqrt{(1/3)}|m_l = 0\rangle|\uparrow\rangle$ and $|2s_{1/2}, m_j = +1/2\rangle = |2s\rangle|\uparrow\rangle$. The $2p$ lifetime is 1.60 ns, and an isolated $2s$ atom lives for 0.122 s. Take $h = 6.626 \times 10^{-34}$ J s and $e = 1.602 \times 10^{-19}$ C.

(a) SHOW THAT

[2]

Show that H' couples $|2s_{1/2}, +1/2\rangle$ to $|2p_{1/2}, +1/2\rangle$ and to no other $2p_{1/2}$ state, with a matrix element of magnitude $\sqrt{3} ea_0 F$.

(b) EXPLAIN

[2]

Explain why the $2s_{1/2}$ level has no linear Stark shift in a weak field, although the $n = 2$ level of hydrogen is often said to show a linear Stark effect of $\pm 3ea_0 F$.

(c) DETERMINE

[3]

Neglecting $2p_{3/2}$, determine the energies of the two $m_j = +1/2$ states as functions of F , measured from the midpoint between $2s_{1/2}$ and $2p_{1/2}$, and the field at which the coupling equals half the Lamb shift.

(d) CALCULATE

[3]

The $2s$ -like state decays through the $2p_{1/2}$ component that the field mixes into it. Calculate its lifetime in a field of 2.0 V cm^{-1} .

(e) JUSTIFY

[2]

Justify the neglect in (d) of the $2p_{3/2}$ level and of the natural width of the $2p$ state.

A heavy quark and antiquark bound in a meson are modelled non-relativistically as one particle of reduced mass μ , with $\mu c^2 = 0.75 \text{ GeV}$, in the linear confining potential $V(r) = \sigma r$, with $\sigma = 0.90 \text{ GeV fm}^{-1}$. Only $l = 0$ is considered. The exact ground-state energy is $E_0 = 2.3381\epsilon_0$, where $\epsilon_0 = (\hbar^2 \sigma^2 / 2\mu)^{1/3}$ and -2.3381 is the first zero of the Airy function Ai ; for any s state of this potential it can also be shown that $|\psi(0)|^2 = \mu\sigma / (2\pi\hbar^2)$ exactly. Take $\hbar c = 0.1973 \text{ GeV fm}$, and $\int_0^\infty r^n e^{-\beta r} dr = n! / \beta^{n+1}$.

(a) SHOW THAT

[2]

Show that for the normalised trial function $\psi_\beta(r) = \sqrt{(\beta^3/\pi)} e^{-\beta r}$, $\langle H \rangle = \hbar^2 \beta^2 / (2\mu) + 3\sigma / (2\beta)$.

(b) DETERMINE

[3]

Determine the value of β that minimises $\langle H \rangle$, and show that the resulting bound is $E_{\text{exp}} = 3(3/4)^{2/3} \epsilon_0 = 2.476 \epsilon_0$.

(c) CALCULATE

[2]

Calculate ϵ_0 , the exponential bound and the exact ground-state energy in GeV, and the percentage by which the bound exceeds the exact value.

(d) EXPLAIN

[2]

A Gaussian trial function $e^{-\alpha r^2}$, optimised in the same way, gives $2.3448 \epsilon_0$, within 0.3% of the exact value, although an exponential is the exact ground state of hydrogen. Explain why the Gaussian does so much better in this potential.

(e) EVALUATE

[3]

The meson's decay rate to a lepton pair is proportional to $|\psi(0)|^2$. The optimal Gaussian trial, $\psi = (2\alpha/\pi)^{3/4} e^{-\alpha r^2}$, has $\alpha^{3/2} = (\mu\sigma/3\hbar^2)\sqrt{2/\pi}$. A student proposes using it to predict $|\psi(0)|^2$, arguing that an energy within 0.3% of the exact value shows the trial state to be accurate. Evaluate this proposal.

For spontaneous emission by an electron from an upper state $|b\rangle$ to a lower state $|a\rangle$ at angular frequency ω , Einstein's detailed-balance argument with the Planck spectrum gives $A = \omega^3 |\langle a|e|r|b\rangle|^2 / (3\pi\epsilon_0\hbar c^3)$. The absorption oscillator strength from a non-degenerate state $|a\rangle$ to a level b is $f = (2m_e\omega/3\hbar)\Sigma |\langle b|r|a\rangle|^2$, summed over the degenerate states of b , and for one electron the Thomas-Reiche-Kuhn sum rule gives $\Sigma f = 1$ over all levels b . As a model, take an electron bound in the isotropic three-dimensional harmonic potential $\frac{1}{2}m_e\omega^2 r^2$, with states $|n_x, n_y, n_z\rangle$ and $\langle 0|x|1\rangle = \sqrt{\hbar/2m_e\omega}$ for each Cartesian direction. Take $e = 1.602 \times 10^{-19}$ C, $m_e = 9.109 \times 10^{-31}$ kg, $\epsilon_0 = 8.854 \times 10^{-12}$ F m $^{-1}$, $c = 2.998 \times 10^8$ m s $^{-1}$, $k_B = 1.381 \times 10^{-23}$ J K $^{-1}$ and $1 \text{ u} = 1.661 \times 10^{-27}$ kg.

(a) EXPLAIN

[2]

Explain why an atom treated by perturbation theory in a classical field would, in an excited state with no applied field, never decay, and how Einstein's argument nevertheless fixes A .

(b) SHOW THAT

[2]

Show that for the oscillator the rate from $|1, 0, 0\rangle$ to $|0, 0, 0\rangle$ is $A = e^2\omega^2/(6\pi\epsilon_0 m_e c^3)$, and comment on the absence of $\hbar$.

(c) DETERMINE

[2]

Determine the absorption oscillator strength from $|0, 0, 0\rangle$ to the first excited level, and state what the Thomas-Reiche-Kuhn sum rule then implies for every other transition from the ground state.

(d) CALCULATE

[3]

The sodium resonance lines near 589.0 nm (3s to 3p) have statistical weights in the same 1 : 3 ratio as the oscillator's, so for them $A = f \times e^2\omega^2/(6\pi\epsilon_0 m_e c^3)$. The measured 3p lifetime is 16.2 ns. Calculate the oscillator's lifetime at 589.0 nm, and hence the oscillator strength of the sodium resonance transition.

(e) COMPARE

[2]

Compare the natural linewidth of the sodium line with its Doppler width in a vapour at 500 K, for which the full width at half maximum is $\Delta\nu_D = (v/c)\sqrt{8k_BT \ln 2/M}$, with $M = 22.99 \text{ u}$.

A superconducting qubit is driven close to resonance. In the frame rotating with the drive its Hamiltonian is $H(\phi) = (\hbar/2)[\Delta\sigma_z + \Omega(\cos\phi\sigma_x + \sin\phi\sigma_y)]$, where the detuning is $\Delta/2\pi = 3.0$ MHz, the Rabi frequency is $\Omega/2\pi = 4.0$ MHz, and ϕ is the phase of the drive, which can be ramped. Equivalently $H = (\hbar\Omega_{\text{eff}}/2)\hat{n} \cdot \sigma$, with $\Omega_{\text{eff}} = \sqrt{\Delta^2 + \Omega^2}$ and $\hat{n} = (\sin\theta\cos\phi, \sin\theta\sin\phi, \cos\theta)$. In the experiment ϕ is ramped at a constant rate from 0 to 2π in a time $T = 4.0\ \mu\text{s}$, so that $\hat{n}$ traces a circle on a cone about the z-axis.

(a) STATE

[2]

State the eigenvalues of H , and the angle θ between $\hat{n}$ and the z-axis.

(b) SHOW THAT

[2]

Show that the adiabatic condition for the ramp becomes $T \gg \pi\Omega/(\Delta^2 + \Omega^2)$, and evaluate the right-hand side.

(c) CALCULATE

[3]

Calculate the geometric phase acquired in one circuit by each of the two eigenstates, and the difference between their dynamic phases.

(d) PREDICT

[2]

In a spin-echo version, the qubit starts in an equal superposition of the two eigenstates at $\phi = 0$, is taken once round the circuit, has its two eigenstates exchanged by a π pulse, and is then taken round the circuit in the opposite sense in the same time T . Predict the relative phase between the two components at the end, and how it changes if T is doubled or if $\Delta/2\pi$ is raised to 6.0 MHz with Ω unchanged.

(e) EXPLAIN

[2]

The same circuit also bounds the rest of the sphere, a cap of solid angle 4π minus the one used in (c). Explain why that cap gives the same phase factor, and what this has to do with the degeneracy of H at $\Delta = \Omega = 0$.

A hydrogen maser oscillates on the transition from $F = 1, m_F = 0$ to $F = 0$ in the hyperfine structure of the ground state, whose zero-field frequency is ν_{hfs} . A small static field B along z is applied by a solenoid around the storage bulb, but the ambient field is not fully cancelled. The field inside the bulb is measured by the Zeeman frequency f_Z , the low-frequency transition between neighbouring $F = 1$ sublevels, which in these weak fields is $f_Z = \mu_B B/h$. For each solenoid current the maser's output is compared with a reference oscillator, giving a frequency offset $\delta\nu$ that also contains a constant but unknown contribution from the reference and from collisions with the bulb wall. With $g_e = 2$ and the proton's magnetic moment neglected, the ground-state Hamiltonian is $H = A S_e \cdot S_p/\hbar^2 + (2\mu_B B/\hbar)S_{ez}$, where $A = h\nu_{\text{hfs}}$. Take $\mu_B = 9.274 \times 10^{-24} \text{ J T}^{-1}$ and $h = 6.626 \times 10^{-34} \text{ J s}$.

Maser frequency offset and in-situ Zeeman frequency for six solenoid currents

Run	Solenoid current I / mA	Zeeman frequency f_Z / kHz	Frequency offset $\delta\nu$ / mHz
1	1.0	0.40	3.74
2	2.0	0.70	4.17
3	3.0	1.00	4.92
4	4.0	1.30	5.87
5	5.0	1.60	7.13
6	6.0	1.90	8.57

(a) **SHOW THAT**

[3]

Working in the $m_F = 0$ subspace spanned by $|\uparrow\downarrow\rangle$ and $|\downarrow\uparrow\rangle$ (electron spin first), show that the frequency of the $F = 1, m_F = 0$ to $F = 0$ transition is $\nu_c = \sqrt{(\nu_{\text{hfs}}^2 + 4f_Z^2)} \approx \nu_{\text{hfs}} + 2f_Z^2/\nu_{\text{hfs}}$.

(b) **DESCRIBE**

[2]

Describe how the readings should be plotted to test this model and to extract ν_{hfs} , and explain why the solenoid current should not be used as the measure of the field.

(c) **DETERMINE**

[3]

Determine the gradient of your graph and hence a value of ν_{hfs} , and comment on its agreement with the accepted 1420.406 MHz.

- (d) **ESTIMATE** [2]
- The maser is normally operated at $f_Z = 0.80$ kHz. Estimate how constant f_Z , and hence the field, must be kept if field fluctuations are to change the maser frequency by less than 1 part in 10^{15} , stating your assumptions.

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18
CORE
COURSE

FREE RESPONSE · EXTENDED DERIVATION · DISCRIMINATING · UQMII-12.06 · UQMII-15.02 · UQMII-15.05 · UQMII-15.08 · UQMII-15.09

[15]

A particle of mass m and energy $E = \hbar^2 k^2 / 2m$ is scattered elastically by a potential $V(r)$ that vanishes at large r . To apply Fermi's golden rule, the system is placed in a cubic box of side L with periodic boundary conditions, so that the plane-wave states $\langle r | k \rangle = e^{i(k \cdot r)} / L^{3/2}$ are normalised and the incident state carries a probability current density $\hbar k / (mL^3)$. The golden rule gives the rate $\Gamma = (2\pi/\hbar) |\langle f | V | i \rangle|^2 \rho(E)$ into a group of final states whose density per unit energy is $\rho(E)$. Write $\tilde{V}(q) = \int e^{-i(q \cdot r)} V(r) d^3r$. Take $m_e = 9.109 \times 10^{-31}$ kg, $e = 1.602 \times 10^{-19}$ C, $c = 2.998 \times 10^8$ m s $^{-1}$ and $\alpha = 1/137.0$.

- (a) **DERIVE** [3]
- Derive, from the periodic boundary conditions, the density of final states per unit energy $\rho(E)$ for plane waves whose wavevectors point into a small solid angle $d\Omega$.

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- (b) **DERIVE** [3]
- Using the golden rule, derive the differential cross-section $d\sigma/d\Omega$ for elastic scattering in terms of $\tilde{V}(q)$, where $q = k_f - k_i$, and confirm that it does not depend on L .

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- (c) **SHOW THAT** [2]
- For the screened Coulomb potential $V(r) = (g/r)e^{-r/a}$, show that $\tilde{V}(q) = 4\pi g / (q^2 + 1/a^2)$.

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- (d) **DETERMINE** [2]
- Take the limit $a \rightarrow \infty$ with $g = Z_1 Z_2 e^2 / (4\pi\epsilon_0)$. Determine $d\sigma/d\Omega$ as a function of the scattering angle θ , and compare it with Rutherford's classical result, $d\sigma/d\Omega = g^2 / (16E^2 \sin^4(\theta/2))$.

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- (e) **EXPLAIN** [2]
- The first Born amplitude, $f(\theta) = -(\frac{m}{2\pi\hbar^2})\tilde{V}(q)$, is real for this potential, so $\text{Im } f(0) = 0$, yet the total cross-section it gives is positive. Explain why this does not contradict the optical theorem, $\sigma = (4\pi/k) \text{Im } f(0)$.

- (f) **ESTIMATE** [3]
- For a Coulomb-like potential of strength $g = Ze^2/(4\pi\epsilon_0)$, the first Born approximation is reliable when $g/(\hbar v) = Z\alpha c/v \ll 1$, where v is the speed of the incident particle. Estimate whether the Born cross-section can be trusted for electrons of kinetic energy 2.0 keV scattered by neutral helium ($Z = 2$) and by neutral iron ($Z = 26$), stating your assumptions.

19

CORE COURSE

FREE RESPONSE · MODEL, SOLVE AND CHECK THE LIMITS · DISCRIMINATING · UQMII-11.04 · UQMII-11.09

[15]

A particle of mass m moves in one dimension in the potential $V(x) = \frac{1}{2}m\omega^2x^2(1 - x/L)$, the model used for the phase of a current-biased Josephson junction. V has a minimum at $x = 0$ and a barrier beyond which, for $x > L$, it falls without limit, so the ground state of the well is metastable and escapes by tunnelling. For the numerical parts take $\omega/2\pi = 8.0$ GHz, with L such that the barrier height is $V_b = 3.0\hbar\omega$. A full treatment, matching the Gaussian ground state of the well onto the decaying WKB solution under the barrier, gives the escape rate $\Gamma = (\omega/2\pi)\sqrt{(864\pi V_b/\hbar\omega)} \exp(-36V_b/5\hbar\omega)$, which is quoted here. You may use $\int_0^1 u\sqrt{1-u} du = 4/15$. Take $\hbar = 1.055 \times 10^{-34}$ J s and $k_B = 1.381 \times 10^{-23}$ J K⁻¹.

- (a) **SHOW THAT** [2]
- Show that the top of the barrier lies at $x = 2L/3$ and that $V_b = (2/27)m\omega^2L^2$.

- (b) **SKETCH** [2]
- Sketch $V(x)$ from $x = -L/3$ to $x = 4L/3$, marking V_b , the ground-state energy $\frac{1}{2}\hbar\omega$ and the classical turning points at that energy, and on the same axes sketch the magnitude of the metastable ground-state wavefunction.

(c) **DERIVE** [3]

Starting from the WKB tunnelling exponent $2S/\hbar = (2/\hbar)\int\sqrt{2m(V-E)} dx$ taken across the barrier, derive its value for an energy $E \rightarrow 0$ at the bottom of the well, and express it in terms of $V_b/\hbar\omega$.

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(d) **CALCULATE** [2]

Calculate, for $V_b = 3.0\hbar\omega$, the naive escape rate $\Gamma_0 = (\omega/2\pi)\exp(-2S/\hbar)$, which pictures the particle striking the barrier once per classical period, and the quoted rate Γ .

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(e) **EVALUATE** [3]

Evaluated between its turning points at the actual ground-state energy $E = \frac{1}{2}\hbar\omega$, the barrier integral gives $2S/\hbar = 17.15$ for these parameters. Evaluate the naive estimate in the light of this: identify which of its approximations causes most of the discrepancy, and explain why the difficulty is worst for the lowest state.

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(f) **ESTIMATE** [3]

Thermal activation over the barrier occurs at a rate of order $(\omega/2\pi)\exp(-V_b/k_BT)$. Estimate the temperature below which escape is dominated by tunnelling, stating your assumptions, and say what an experiment would observe below it.

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University Quantum Mechanics II · Final 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.

1 MULTIPLE CHOICE · RECALL · UQMII-01.02 **[1]**

CORE
COURSE

A linear molecule attached by one end to a flat surface is modelled as a rigid rotor, of moment of inertia I about the attached end, that turns freely except that its axis cannot point into the surface. The polar angle θ of the axis, measured from the outward normal to the surface, is therefore confined to $0 \leq \theta \leq \pi/2$, and the surface acts as a hard wall: the wavefunction must vanish at $\theta = \pi/2$, where the axis would lie in the surface. The rotor's Hamiltonian is $H = L^2/(2I)$. For $m = 0$, with $x = \cos \theta$ and $\lambda = 2IE/\hbar^2$, the angular equation is Legendre's equation, and of its power-series solutions about $x = 0$ only the series of odd powers of x vanishes at $x = 0$, as the wall requires. Which values of λ are allowed?

KEY C $\lambda = l(l + 1)$ with $l = 1, 3, 5, \dots$, because the odd series must still terminate to stay finite at $\theta = 0$, where the axis lies along the surface normal.

C is correct. With the even series excluded, the solution is a series of odd powers alone, and unless it stops, its coefficients fall off only as $1/k$ at large k , so it diverges at $x = +1$ just as at $x = -1$. The pole $\theta = 0$, where the molecule stands straight up, lies inside the allowed region, so the series must terminate, and a series of odd powers terminates only when $\lambda = l(l + 1)$ with l odd. The allowed states are P_1, P_3, P_5 and so on, each of which vanishes at $x = 0$, with $E = \hbar^2 l(l + 1)/(2I)$ for odd l only. D is the tempting error. On the full sphere, for any λ , one combination of the even and odd series stays finite at $\theta = 0$ and diverges only at $\theta = \pi$, so excluding $\theta = \pi$ seems to lift the restriction. But unless $\lambda = l(l + 1)$ with l odd, that combination does not vanish at the wall, and the odd series the wall does allow has definite parity, so it diverges at both poles or at neither. A keeps the free rotor's spectrum, forgetting that the new boundary condition removes solutions: the even polynomials P_0, P_2, P_4 and so on are nonzero at $x = 0$, so half of the free rotor's $m = 0$ levels are lost. B mistakes a node for a symmetry. The wall allows only solutions that vanish at $x = 0$, which for polynomials of definite parity means the odd ones, with $P_l(-x) = -P_l(x)$; the even polynomials, symmetric about the equator, are nonzero there and are exactly the ones the wall excludes.

U1

2 MULTIPLE CHOICE · ROUTINE · UQMII-02.09 · UQMII-07.07 **[1]**

CORE
COURSE

A crude model of a valence electron outside a closed-shell core replaces the Coulomb potential by $V(r) = -k/r - \beta/r^2$, where $k = e^2/(4\pi\epsilon_0)$ and β is a small positive constant representing the extra attraction felt by an electron that penetrates the core. Compared with hydrogen, which statement about the bound-state spectrum is correct?

KEY B Levels of the same n but different l separate, with the lowest l pushed down most, while each keeps its $(2l + 1)$ -fold degeneracy in m ; the quantum Runge-Lenz vector is no longer conserved.

B is correct. The potential is still central, so L^2 and L_z commute with H and the $2l + 1$ states of each l stay degenerate. The extra term can be absorbed into the centrifugal term, $\hbar^2 l(l + 1)/(2mr^2) - \beta/r^2 = \hbar^2 l'(l' + 1)/(2mr^2)$, with $l - l' \approx (2m\beta/\hbar^2)/(2l + 1)$, so the radial equation is still hydrogenic but with a non-integer l' , and $E = -Ry/(n_r + l' + 1)^2 = -Ry/(n - \delta_l)^2$: the quantum-defect form, with δ_l largest for s states. The extra symmetry of the pure $1/r$ potential, generated by the Runge-Lenz vector, is gone, and the l -degeneracy with it. A mistakes a change in the radial form of the potential for a loss of spherical symmetry; only a non-central term, such as an external field, can split m . C starts from the right observation, that the term adds to the centrifugal barrier, but how far it moves the effective l depends on l itself, so the shift differs from one l to the next. D uses the wrong expectation value: by the Feynman-Hellmann route of Unit 6, $\langle 1/r^2 \rangle = 1/[n^3(l + 1/2)a_0^2]$ depends on l , so the first-order shifts $-\beta\langle 1/r^2 \rangle$ already differ, and are largest for $l = 0$.

U1

3

CORE
COURSE

MULTIPLE CHOICE · ROUTINE · UQMII-03.01 · UQMII-03.03

[1]

In a nuclear magnetic resonance magnet whose field B points along $+z$, the spins of protons at rest precess at 400.0 MHz. A particle at rest whose magnetic moment is $\mu = \gamma S$ has the Hamiltonian $H = -\gamma B S_z$, and each spin component obeys the Heisenberg equation $dS/dt = (i/\hbar)[H, S]$; $\gamma = +2.675 \times 10^8 \text{ rad s}^{-1} \text{ T}^{-1}$ for the proton and $\gamma = -1.761 \times 10^{11} \text{ rad s}^{-1} \text{ T}^{-1}$ for the electron. A free electron is now held at rest in the same magnet. Which statement about the precession of its spin is correct?

KEY D It precesses at 263.3 GHz, in the opposite sense to the proton spins, while S_z , which commutes with H , stays constant.

The Heisenberg equation gives $dS_x/dt = (i/\hbar)(-\gamma B)[S_z, S_x] = \gamma B S_y$ and $dS_y/dt = -\gamma B S_x$, while $[H, S_z] = 0$, so S_z is conserved and the transverse components rotate about z at the rate $|\gamma|B$, in a sense set by the sign of γ . The proton data fix $B = 2\pi(400.0 \text{ MHz})/\gamma_p = 9.395 \text{ T}$, and the electron then precesses at $|\gamma_e|B/2\pi = 400.0 \text{ MHz} \times (1.761 \times 10^{11})/(2.675 \times 10^8) = 263.3 \text{ GHz}$; because γ_e and γ_p have opposite signs, it turns the other way: D. A treats the Larmor frequency as a property of the field alone, but $\omega = |\gamma|B$, and the electron's gyromagnetic ratio is 658 times the proton's, which is why electron-spin resonance in this magnet needs microwaves rather than radio waves. B has the right rate but drops the sign of γ : the electron's moment is antiparallel to its spin and the proton's parallel, so the torque turns the two spins in opposite senses. C is the half-angle trap. The two spinor components do acquire phases $e^{\pm i\gamma B t/2}$, but $\langle S \rangle$ is turned by their relative phase, $\gamma B t$, so a vector operator precesses at the full rate $|\gamma|B$.

U2

4

CORE
COURSE

MULTIPLE CHOICE · ROUTINE · UQMII-08.01 · UQMII-08.06

[1]

In hydrogen the fine-structure shifts are $E_{fs} = -[E_n^2/(2mc^2)][4n/(j + \frac{1}{2}) - 3]$, where $E_n = -13.6 \text{ eV}/n^2$, so they are smaller than the Bohr energies by a factor of order α^2 and depend on n and j only. The $2p_{3/2}-2p_{1/2}$ splitting is measured to be 10.97 GHz. What splitting does the formula then predict between the $3d_{5/2}$ and $3d_{3/2}$ levels?

KEY A 1.08 GHz

Between two levels of the same n the formula gives a splitting $[E_n^2/(2mc^2)] \times 4n[1/(j_1 + \frac{1}{2}) - 1/(j_2 + \frac{1}{2})]$, which falls as n^{-3} times the bracket in j . For $2p$ it is $(E_2^2/2mc^2) \times 8 \times (1 - \frac{1}{2}) = 4E_2^2/(2mc^2)$, and for $3d$ it is $(E_3^2/2mc^2) \times 12 \times (\frac{1}{2} - \frac{1}{3}) = 2E_3^2/(2mc^2)$, so the ratio is $\frac{1}{2} \times (E_3/E_2)^2 = \frac{1}{2} \times 16/81 = 8/81$, and the $3d$ splitting is $10.97 \text{ GHz} \times 8/81 = 1.08 \text{ GHz}$ (A). B, 3.25 GHz, is the $3p_{3/2}-3p_{1/2}$ splitting: it treats every fine-structure doublet as a $j = \frac{1}{2}, 3/2$ pair, when the d levels have $j = 3/2$ and $5/2$. C scales the $2p$ splitting by $(2/3)^2$, as the Bohr energies scale, treating fine structure as a fixed fraction of $|E_n|$; the factor $4n$ makes it fall as n^{-3} , and the j values change the bracket as well. D drops the factor n from $4n/(j + \frac{1}{2})$, so it scales as n^{-4} and is too small by a factor $3/2$. Because the energies depend on n and j only, $3d_{3/2}$ coincides with $3p_{3/2}$, so this 1.08 GHz is also the gap between that pair and the highest $n = 3$ level.

U3

5

CORE
COURSE

MULTIPLE CHOICE · ROUTINE · UQMII-09.01 · UQMII-09.02

[1]

A hydrogen atom in the $2p_{1/2}$ level is placed in a magnetic field of 0.10 T, which is weak compared with the 10.97 GHz fine-structure splitting of $n = 2$. By what frequency are its two m_j sublevels split? Take $\mu_B = 5.788 \times 10^{-5} \text{ eV T}^{-1}$ and $h = 4.136 \times 10^{-15} \text{ eV s}$.

KEY C 0.933 GHz

In a weak field j and m_j stay good and the shift is $g_j \mu_B B m_j$, with the Landé factor given by the projection theorem, $g_j = 1 + [j(j+1) + s(s+1) - l(l+1)]/[2j(j+1)]$. For $l = 1$ and $j = \frac{1}{2}$ this is $1 + (\frac{3}{4} + \frac{3}{4} - 2)/(3/2) = 2/3$, so the $m_j = \pm \frac{1}{2}$ sublevels are split by $(2/3)\mu_B B = (2/3)(5.788 \times 10^{-5} \text{ eV T}^{-1})(0.10 \text{ T}) = 3.86 \times 10^{-6} \text{ eV}$, or 0.933 GHz (C). A takes the spin g -factor of 2, which is right for $2s_{1/2}$ but not for a state whose spin is partly antiparallel to its orbital angular momentum. B takes the orbital g -factor of 1 and ignores the spin altogether. D uses $4/3$, the factor for $2p_{3/2}$, reached by taking $j = l + \frac{1}{2}$ or by a sign slip in the projection formula. The splitting is comparable with the 1.06 GHz Lamb shift, but that does not matter here: the Zeeman term commutes with L^2 , so it cannot mix $2p_{1/2}$ with $2s_{1/2}$, and the splitting it must be weak against is the 10.97 GHz separation from $2p_{3/2}$.

U3

6

CORE
COURSE

MULTIPLE CHOICE · ROUTINE · UQMII-10.01

[1]

A system has exact ground and first excited energies $E_0 = -1.00$ eV and $E_1 = -0.25$ eV, with normalised eigenstates ψ_0 and ψ_1 . A normalised trial state is $\phi = \sqrt{1 - \varepsilon^2} \psi_0 + \varepsilon \psi_1$ with $\varepsilon = 0.10$, so that 1% of its weight lies in the wrong state. What is $\langle \phi | H | \phi \rangle$?

KEY **B** **-0.9925 eV**

Orthogonality removes the cross terms, so $\langle H \rangle = (1 - \varepsilon^2)E_0 + \varepsilon^2 E_1 = 0.99(-1.00 \text{ eV}) + 0.01(-0.25 \text{ eV}) = -0.9925 \text{ eV}$ (B). The error, $\varepsilon^2(E_1 - E_0) = 0.0075 \text{ eV}$, is second order in the 10% admixture of amplitude, which is why a variational energy is far more accurate than the trial state that produced it. A weights the energies by the amplitudes rather than their squares, $\sqrt{0.99} E_0 + 0.10 E_1 = -1.020 \text{ eV}$. It lies below E_0 , which the variational theorem forbids for any admissible trial state, so it should be rejected on sight. C also weights by amplitudes, as $(1 - \varepsilon)E_0 + \varepsilon E_1$, and so makes the error first order: 0.075 eV , ten times too large. D supposes that a 1% admixture is too small to register. The energy is insensitive to it, but not blind, and the shift is always upwards.

U3

7

CORE
COURSE

MULTIPLE CHOICE · DEMANDING · UQMII-11.06 · UQMII-11.07

[1]

A cold atom of mass m is held along x in a harmonic trap whose angular frequency ω satisfies $\omega/2\pi = 2.0$ kHz. A thin repulsive light sheet is then switched on at the trap centre and is modelled as an impenetrable wall at $x = 0$, so that the atom moves in $V(x) = \frac{1}{2}m\omega^2 x^2$ for $x > 0$ only. WKB quantisation is applied using the connection-formula phase at the smooth turning point and the condition $\psi = 0$ at the wall. What energy does it predict for the first excited state of this half-trap, expressed as the frequency E/h and measured from the bottom of the trap?

KEY **D** **7.0 kHz**

A smooth turning point contributes a phase of $\pi/4$ to the WKB condition and a hard wall, where ψ must vanish, contributes $\pi/2$, so $(1/\hbar) \int_0^x p \, dx = (n + \frac{3}{4})\pi$ with $n = 0, 1, 2, \dots$. For the half-trap the integral is a quarter of the area $2\pi E/\omega$ enclosed by the full oscillator's phase-space ellipse, $\pi E/(2\omega)$, so $E = (2n + 3/2)\hbar\omega$, and the first excited state, $n = 1$, has $E = 3.5\hbar\omega$, or $E/h = 3.5 \times 2.0 \text{ kHz} = 7.0 \text{ kHz}$ (D). The result is exact: the allowed states are the odd states of the full oscillator, the ones that vanish at $x = 0$. A, 3.0 kHz, is tempting in two ways. It is the full trap's first excited state, $(n + \frac{1}{2})\hbar\omega$ with $n = 1$, found by ignoring the wall, and it is also the correct formula applied to the ground state, $n = 0$, instead of the first excited state. C, 6.0 kHz, applies the rule $(n + \frac{1}{2})\pi$, correct between two smooth turning points, to a region bounded by one smooth turning point and one wall, and so gives $(2n + 1)\hbar\omega$. B, 5.0 kHz, uses $(n + \frac{3}{4})\pi$, which treats the wall as contributing no phase at all; it gives $(2n + \frac{1}{2})\hbar\omega$, the even states of the full oscillator, which satisfy $\psi'(0) = 0$ rather than $\psi(0) = 0$. These phase corrections matter most for the lowest states, where they are a large fraction of the total.

U2

8

CORE
COURSE

MULTIPLE CHOICE · ROUTINE · UQMII-14.04

[1]

A two-level system is swept at a constant rate through an avoided crossing. The probability of a diabatic passage, in which the system stays in its initial diabatic state and so jumps the gap, is measured to be 0.20. According to the Landau-Zener formula, what is this probability when the sweep rate is doubled?

KEY **A** **0.45**

The Landau-Zener probability is $P = \exp(-2\pi|H_{12}|^2/(\hbar\alpha))$, where α is the rate at which the diabatic energies cross, so the exponent is inversely proportional to the rate. Doubling α halves the exponent, and P becomes $\sqrt{0.20} = 0.45$ (A). B doubles the probability, treating it as proportional to the rate, which would soon carry it past 1. C halves it, the answer of a candidate who expects a faster sweep to be more adiabatic when the opposite is true: a faster sweep gives the system less time to follow its instantaneous eigenstate. D squares the probability, which is what halving the sweep rate would do. The exponential dependence on $1/\alpha$ is what makes a modest slowing of the sweep so effective at suppressing the jump.

U3

9

CORE
COURSE

MULTIPLE CHOICE · DEMANDING · UQMII-12.09 · UQMII-13.05 · UQMII-13.08

[1]

A hydrogen atom is prepared in the $2s_{1/2}$ state, isolated and in zero field. It lives for about 0.12 s, whereas $2p$ lives for 1.6 ns. Which process is responsible for its decay?

KEY C Emission of two electric-dipole photons together, through virtual intermediate p states, sharing the 10.2 eV between them.

C is correct: the dominant decay is two-photon emission, a second-order process through virtual p states, with a rate of about 8 s^{-1} ; because the energy can be shared in any proportion, the photons form a continuum rather than a line. A is ruled out exactly, not merely slowed. The dipole operator is odd, $1s$ and $2s$ are both even, and $\Delta l = \pm 1$ is required, so the matrix element vanishes whatever the radial functions look like. B names an allowed transition, but its rate carries a factor ω^3 , and at 1.06 GHz rather than the $2.47 \times 10^{15}\text{ Hz}$ of Lyman- α that factor is smaller by about 10^{19} , leaving a rate of order 10^{-9} s^{-1} . D is the subtle one. Parity and angular momentum do permit a magnetic-dipole transition, but its operator, $-(\mu_B/\hbar)(L + 2S)$, does not act on r , so between $2s$ and $1s$ it is multiplied by the overlap of two orthogonal radial functions and vanishes; relativistic corrections restore a rate of only about $2.5 \times 10^{-6}\text{ s}^{-1}$. A state with no allowed one-photon decay is emptied by the fastest of the slower processes, and for hydrogen $2s$ that is two-photon emission.

U1

10

CORE
COURSE

MULTIPLE CHOICE · ROUTINE · UQMII-15.04 · UQMII-15.07

[1]

Slow electrons scatter from atoms of a noble gas, which are modelled as spherically symmetric attractive wells. At the energies of interest only the s wave is appreciably scattered, and at one energy its phase shift passes through $\delta_0 = \pi$. What is observed near that energy?

KEY B A deep minimum in the total cross-section, because $(4\pi/k^2)\sin^2\delta_0$ vanishes, so the gas becomes nearly transparent to the electrons.

The s -wave cross-section is $\sigma_0 = (4\pi/k^2)\sin^2\delta_0$, which vanishes when $\delta_0 = \pi$: a well that pulls the wave in by exactly half a wavelength leaves the outgoing wave indistinguishable from an unscattered one. With the higher partial waves small, the total cross-section has a deep minimum, the Ramsauer-Townsend effect (B). A describes $\delta_0 = \pi/2$, where $\sin^2\delta_0 = 1$ and the s wave scatters as strongly as unitarity allows. C misreads Levinson's theorem, which relates the phase shift at zero energy to the number of bound states; bound states have negative energy, and a phase shift passing through π at a positive energy creates none. D borrows a classical picture that fails twice over: phase shifts of 0 and π are physically identical for scattering, and even a genuine hard sphere at low energy scatters $4\pi R^2$, not πR^2 .

U1

11

CORE
COURSE

STRUCTURED · ROUTINE · UQMII-04.04 · UQMII-04.07 · UQMII-05.04

[11]

Two electrons, each held in one of a pair of neighbouring quantum dots, interact through the exchange Hamiltonian $H = (J/\hbar^2)S_1 \cdot S_2$, with $J = 2.0\text{ }\mu\text{eV}$. Their orbital states are frozen, so only the spins evolve. Write $|\uparrow\downarrow\rangle$ for spin 1 up and spin 2 down along z , and similarly for the other product states. Take $\hbar = 1.055 \times 10^{-34}\text{ J s}$ and $1\text{ eV} = 1.602 \times 10^{-19}\text{ J}$.

(a) SHOW THAT · U2

[2]

Show that the eigenvalues of H are $J/4$ for each of the three triplet states and $-3J/4$ for the singlet.

1 $S^2 = (S_1 + S_2)^2 = S_1^2 + S_2^2 + 2S_1 \cdot S_2$, so $S_1 \cdot S_2 = (S^2 - S_1^2 - S_2^2)/2 = (\hbar^2/2)[s(s+1) - 3/2]$ on states of total spin s

2 $s = 1$ (the three triplet states) gives $S_1 \cdot S_2 = \hbar^2/4$ and $E = J/4$; $s = 0$ (the singlet) gives $S_1 \cdot S_2 = -3\hbar^2/4$ and $E = -3J/4$, a triplet-singlet splitting of J

Candidates who diagonalise a 4×4 matrix spend ten minutes on what the identity for S^2 does in one line. Those who drop the $1/2$ from $S_1 \cdot S_2 = (S^2 - S_1^2 - S_2^2)/2$ find eigenvalues twice too large.

- (b) DETERMINE · U2 [3]
- At $t = 0$ the spins are prepared in $|\uparrow\downarrow\rangle$. By expressing this state in the coupled basis, determine the probability $P(t)$ that a measurement at time t finds the spins in $|\downarrow\uparrow\rangle$.
- $|\uparrow\downarrow\rangle = (|T_0\rangle + |S\rangle)/\sqrt{2}$, with $|T_0\rangle = (|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle)/\sqrt{2}$ and $|S\rangle = (|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)/\sqrt{2}$
 - each coupled state evolves with its own energy: $|\psi(t)\rangle = [e^{(-ijt/4\hbar)}|T_0\rangle + e^{(3ijt/4\hbar)}|S\rangle]/\sqrt{2}$, so $\langle\downarrow\uparrow|\psi(t)\rangle = [e^{(-ijt/4\hbar)} - e^{(3ijt/4\hbar)}]/2$
 - $P(t) = |1 - e^{(ijt/\hbar)}|^2/4 = \sin^2(Jt/2\hbar)$, oscillating between 0 and 1
- The relative sign of $|\downarrow\uparrow\rangle$ in the singlet decides everything. A candidate who adds probabilities, a half from each coupled state, instead of amplitudes finds P constant at $1/2$ and misses the swap entirely.*
- (c) CALCULATE · U3 [1]
- Calculate the shortest time after which the two spins have completely exchanged their states.
- $P = 1$ first when $Jt/2\hbar = \pi/2$, at $t = \pi\hbar/J = \pi \times 1.055 \times 10^{-34} \text{ J s} / (2.0 \times 10^{-6} \times 1.602 \times 10^{-19} \text{ J}) = 1.03 \times 10^{-9} \text{ s}$, about 1.0 ns
- Using h instead of $\hbar$ gives 6.5 ns. The swap takes half a period of the triplet-singlet beat, whose angular frequency is $J/\hbar$.*
- (d) DETERMINE · U2 [3]
- Determine the reduced density matrix of spin 1 at time t and its purity $\text{Tr } \rho_1^2$, and hence the earliest time at which spin 1 is maximally mixed.
- $|\psi(t)\rangle = a|\uparrow\downarrow\rangle + b|\downarrow\uparrow\rangle$ with $|a|^2 = \cos^2(Jt/2\hbar)$ and $|b|^2 = \sin^2(Jt/2\hbar)$; tracing over spin 2 removes the cross terms because they carry $\langle\downarrow\uparrow\rangle = 0$ for spin 2, so $\rho_1 = \cos^2(Jt/2\hbar)|\uparrow\rangle\langle\uparrow| + \sin^2(Jt/2\hbar)|\downarrow\rangle\langle\downarrow|$
 - $\text{Tr } \rho_1^2 = \cos^4(Jt/2\hbar) + \sin^4(Jt/2\hbar) = 1 - \frac{1}{2}\sin^2(Jt/\hbar)$, which reaches its minimum of $1/2$ when $Jt/\hbar = \pi/2$
 - $t = \pi\hbar/(2J) = 0.52 \text{ ns}$, half the swap time: $\rho_1 = I/2$, its Bloch vector $(0, 0, \cos(Jt/\hbar))$ is at the centre of the ball, and the pair is in the maximally entangled pure state $(|\uparrow\downarrow\rangle - i|\downarrow\uparrow\rangle)/\sqrt{2}$, up to an overall phase, with entanglement entropy $\ln 2$
- The cross terms vanish because the two components carry orthogonal states of spin 2, not because the coefficients happen to be real. At the moment of maximal mixing the pair as a whole is in a pure state: a mixed part does not mean a mixed whole.*
- (e) EXPLAIN · U1 [2]
- At that time an experimenter measures spin 1 alone, along any axis they choose. Explain why no such measurement can distinguish it from a spin drawn from an ensemble prepared half in $|\uparrow\rangle$ and half in $|\downarrow\rangle$, and what kind of measurement would reveal the difference.
- every outcome probability for a measurement on spin 1 alone is $\text{Tr}(\rho_1\Pi)$ for the projector Π of that outcome, and both preparations have $\rho_1 = I/2$, so every axis gives $1/2$ and $1/2$: preparations with the same density operator cannot be told apart by any measurement on that system
 - the difference lies only in correlations between the two spins, which need joint measurements: the entangled state has $\langle\sigma_x \otimes \sigma_y\rangle = +1$, whereas a mixture of $|\uparrow\downarrow\rangle$ and $|\downarrow\uparrow\rangle$ has zero transverse correlations (a measurement in the Bell basis would also distinguish them)
- The answer that the spin is secretly up or down, and simply not yet known, is the error this part catches. The randomness of spin 1 comes from its entanglement with spin 2, and no measurement on one side can reveal it.*

An electron in a cubic InAs nanocrystal is modelled as a particle of charge $-e$ and effective mass $m^* = 0.023m_e$ in a cubical infinite well of side $L = 20$ nm centred on the origin, $-L/2 < x, y, z < L/2$. Spin is ignored, since its Zeeman energy is the same for every orbital state. The unperturbed states are $\psi_{(n_1 n_2 n_3)} = u_{(n_1)}(x)u_{(n_2)}(y)u_{(n_3)}(z)$, with energies $(n_1^2 + n_2^2 + n_3^2)\epsilon$, where $\epsilon = \pi^2 \hbar^2 / (2m^* L^2)$, $u_1(x) = \sqrt{2/L} \cos(\pi x/L)$ and $u_2(x) = \sqrt{2/L} \sin(2\pi x/L)$. A uniform magnetic field $B = 1.5$ T is applied along z . In the symmetric gauge, and to first order in B , it adds $H' = (\mu^* B / \hbar) L_z$, where $\mu^* = e\hbar / (2m^*)$ is the effective magneton and $L_z = -i\hbar(x \partial/\partial y - y \partial/\partial x)$; the term in B^2 is neglected. You may use $\int u_1(x) \times u_2(x) dx = 16L / (9\pi^2)$ and $\int u_1(du_2/dx) dx = 8/(3L) = -\int u_2(du_1/dx) dx$, each integral running from $-L/2$ to $L/2$. Take $m_e = 9.109 \times 10^{-31}$ kg, $\hbar = 1.055 \times 10^{-34}$ J s, $e = 1.602 \times 10^{-19}$ C and $1 \text{ eV} = 1.602 \times 10^{-19}$ J.

(a) CALCULATE · U3

[2]

Calculate ϵ in meV, and the energies and degeneracies of the ground level and of the first excited level.

1 $\epsilon = \pi^2 \hbar^2 / (2m^* L^2) = \pi^2 (1.055 \times 10^{-34} \text{ J s})^2 / (2 \times 0.023 \times 9.109 \times 10^{-31} \text{ kg} \times (20 \times 10^{-9} \text{ m})^2) = 6.55 \times 10^{-21} \text{ J} = 40.9 \text{ meV}$

2 the ground level ψ_{111} lies at $3\epsilon = 123 \text{ meV}$ and is non-degenerate; the first excited level lies at $6\epsilon = 245 \text{ meV}$ and is threefold degenerate, spanned by ψ_{211} , ψ_{121} and ψ_{112}

Omitting the effective mass gives $\epsilon = 0.94 \text{ meV}$, over forty times too small. The threefold degeneracy of the first excited level, on which the rest of the question turns, should be noticed here.

(b) CALCULATE · U3

[2]

Calculate $\mu^* B$ in meV, and its ratio to the spacing 3ϵ that separates the first excited level from the levels on either side of it.

1 $\mu^* B = e\hbar B / (2m^*) = (1.602 \times 10^{-19} \text{ C})(1.055 \times 10^{-34} \text{ J s})(1.5 \text{ T}) / (2 \times 0.023 \times 9.109 \times 10^{-31} \text{ kg}) = 6.05 \times 10^{-22} \text{ J} = 3.78 \text{ meV}$

2 $\mu^* B / 3\epsilon = 3.78 \text{ meV} / 123 \text{ meV} = 0.031 \ll 1$, so admixtures from outside the level are at most a few per cent and second-order shifts at most about $(\mu^* B)^2 / 3\epsilon \approx 0.1 \text{ meV}$: first-order theory within the degenerate level is adequate

The free-electron Bohr magneton gives $\mu_B B = 0.087 \text{ meV}$, too small by the factor $m_e/m^* \approx 43$; the small effective mass is why orbital magnetic effects are so large in InAs. The ratio should be taken to the gap, not to the level energy.

(c) DETERMINE · U2

[3]

Using the integrals given, determine the matrix of H' in the first excited level, its eigenvalues in meV, and the good states.

1 the diagonal elements vanish because each ψ is real, and ψ_{112} is uncoupled because L_z leaves the z factor alone and $\langle u_2 | u_1 \rangle = 0$; the one independent element is $\langle \psi_{211} | L_z | \psi_{121} \rangle = -i\hbar [\langle u_2 | x | u_1 \rangle \langle u_1 | u_2' \rangle - \langle u_2 | u_1' \rangle \langle u_1 | y | u_2 \rangle] = -i\hbar \times 2 \times (16L/9\pi^2)(8/3L) = -i\hbar(256/27\pi^2) = -0.961i\hbar$

2 in the basis $(\psi_{211}, \psi_{121}, \psi_{112})$, $H' = 0.961\mu^* B \begin{bmatrix} 0 & -i & 0 \\ i & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}$, with eigenvalues $+0.961\mu^* B = +3.63 \text{ meV}$, 0 and -3.63 meV

3 the good states are $(\psi_{211} + i\psi_{121})/\sqrt{2}$, raised by 3.63 meV , $(\psi_{211} - i\psi_{121})/\sqrt{2}$, lowered by 3.63 meV , and ψ_{112} , unshifted, so the level at 245 meV splits into three levels spanning 7.26 meV

The sign of the second term is the trap: $\int u_2 u_1' dx = -8/(3L)$, so the two contributions add rather than cancel. A candidate who finds the element zero, or who applies the non-degenerate formula to ψ_{211} alone and finds no shift, concludes wrongly that the level does not split.

(d) EXPLAIN · U1

[2]

Explain how the rotation through 90° about the z-axis identifies these good states without any diagonalisation.

- 1 the rotation R , which sends $\psi(x, y, z)$ to $\psi(y, -x, z)$, maps the cube onto itself and so commutes with H_0 , and it commutes with L_z , the generator of rotations about z , and so with H' ; because u_1 is even and u_2 odd, it takes ψ_{211} to ψ_{121} , ψ_{121} to $-\psi_{211}$ and ψ_{112} to itself
- 2 within the level its eigenstates are $(\psi_{211} \pm i\psi_{121})/\sqrt{2}$, with eigenvalues $\mp i$, and ψ_{112} , with eigenvalue 1; the three eigenvalues are distinct, so H' has no element between these states and they are the good states, the analogues of $m = +1, -1$ and 0

The symmetry used must belong to the cube as well as to the field. The walls break full rotational symmetry about z , so L_z does not commute with H_0 and m is not an exact quantum number; a candidate who labels the states by exact $m = \pm 1$ cannot explain why the splitting is $0.961\mu_B$ rather than μ_B .

(e) SHOW THAT · U2

[2]

The field is turned, at the same strength, to lie along the body diagonal $\hat{n} = (1, 1, 1)/\sqrt{3}$, so that $H' = (\mu_B/\hbar)\hat{n}\cdot\mathbf{L}$. Show that the first excited level splits in exactly the same way, into shifts of +3.63 meV, 0 and -3.63 meV.

- 1 the cube is unchanged by the cyclic relabelling $x \rightarrow y \rightarrow z$, so L_x couples only ψ_{121} and ψ_{112} , and L_y only ψ_{112} and ψ_{211} , with the same magnitude as L_z ; in the basis $(\psi_{211}, \psi_{121}, \psi_{112})$ every element is $(L_k)_{ij} = -i\hbar c \epsilon_{kij}$, with $c = 256/27\pi^2 = 0.961$
- 2 these are c times the matrices of an $l = 1$ angular momentum in the Cartesian basis, so $\hat{n}\cdot\mathbf{L}$ has the characteristic equation $\lambda(\lambda^2 - c^2\hbar^2) = 0$ and the eigenvalues 0 and $\pm c\hbar$ for every unit vector $\hat{n}$: the shifts are 0 and $\pm 0.961\mu_B = \pm 3.63$ meV whatever the direction of $\mathbf{B}$

The expected error is to suppose that a cube, being less symmetric than a sphere, must split differently for different field directions. At first order within a threefold level of a cube the splitting is isotropic; the anisotropy appears only at higher order in B .

13 CORE COURSE

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[12]

A hydrogen atom in the $n = 2$ shell is placed in a uniform static electric field F along z ; hyperfine structure is ignored. Without the field, $2s_{1/2}$ lies above $2p_{1/2}$ by the Lamb shift, $L = h \times 1057.8$ MHz, and $2p_{3/2}$ lies $h \times 10.97$ GHz above $2p_{1/2}$. The perturbation is $H' = eFz$. In the uncoupled basis $|2s|z|2p, m_l = 0\rangle = -3a_0$, with $a_0 = 5.29 \times 10^{-11}$ m, and in the convention used here $|2p_{1/2}, m_j = +1/2\rangle = \sqrt{(2/3)}|m_l = 1\rangle| \downarrow \rangle - \sqrt{(1/3)}|m_l = 0\rangle| \uparrow \rangle$ and $|2s_{1/2}, m_j = +1/2\rangle = |2s\rangle| \uparrow \rangle$. The $2p$ lifetime is 1.60 ns, and an isolated $2s$ atom lives for 0.122 s. Take $h = 6.626 \times 10^{-34}$ J s and $e = 1.602 \times 10^{-19}$ C.

(a) SHOW THAT · U2

[2]

Show that H' couples $|2s_{1/2}, +1/2\rangle$ to $|2p_{1/2}, +1/2\rangle$ and to no other $2p_{1/2}$ state, with a matrix element of magnitude $\sqrt{3} ea_0 F$.

- 1 z does not act on spin and, being proportional to rY_1^0 , cannot change m_l , so it conserves m_j : $|2s_{1/2}, +1/2\rangle$ couples only to $m_j = +1/2$, and within $|2p_{1/2}, +1/2\rangle$ only the $|m_l = 0\rangle| \uparrow \rangle$ component contributes
- 2 $\langle 2s_{1/2}, +1/2 | eFz | 2p_{1/2}, +1/2 \rangle = eF \times (-\sqrt{(1/3)}) \times (-3a_0) = \sqrt{3} ea_0 F$

Candidates who include the $m_l = 1$ component have forgotten that z cannot change m_l . The $\sqrt{3}$ is the Clebsch-Gordan weight $\sqrt{(1/3)}$ multiplying the $3a_0$ of the uncoupled element.

- (b) EXPLAIN · U1 [2]**
- Explain why the $2s_{1/2}$ level has no linear Stark shift in a weak field, although the $n = 2$ level of hydrogen is often said to show a linear Stark effect of $\pm 3ea_0F$.
- 1 the Lamb shift separates $2s_{1/2}$ from $2p_{1/2}$, so in a weak field the two $2s_{1/2}$ states ($m_j = \pm 1/2$) are degenerate only with each other and both have definite (even) parity; every first-order matrix element between them, $\langle 2s_{1/2} | eFz | 2s_{1/2} \rangle$, vanishes because z is odd, so the leading shift is second order and, dominated by $2p_{1/2}$, about $3e^2a_0^2F^2/L$
 - 2 the linear effect $\pm 3ea_0F$ assumes $2s$ and $2p_0$ exactly degenerate, so that the field mixes them at first order; with the Lamb shift present the shift becomes linear only once $\sqrt{3}ea_0F$ is large compared with L , and reaches $\pm 3ea_0F$ only when the field also overwhelms the 10.97 GHz fine structure
- The textbook linear Stark effect belongs to a hydrogen atom without fine structure or Lamb shift. A state of definite parity has no first-order shift in any field too weak to overcome the splitting that isolates it.*
- (c) DETERMINE · U2 [3]**
- Neglecting $2p_{3/2}$, determine the energies of the two $m_j = +1/2$ states as functions of F , measured from the midpoint between $2s_{1/2}$ and $2p_{1/2}$, and the field at which the coupling equals half the Lamb shift.
- 1 in the basis $\{|2s_{1/2}, +1/2\rangle, |2p_{1/2}, +1/2\rangle\}$ the Hamiltonian is $[[L/2, V], [V, -L/2]]$, with $V = \sqrt{3}ea_0F$
 - 2 $E_{\pm} = \pm\sqrt{(L^2/4 + 3e^2a_0^2F^2)}$: for $\sqrt{3}ea_0F \ll L$ the $2s$ -like level rises quadratically, by $3e^2a_0^2F^2/L$, and for $\sqrt{3}ea_0F \gg L$ the shifts become linear, $\pm\sqrt{3}ea_0F$
 - 3 $V = L/2$ at $F = L/(2\sqrt{3}ea_0) = (6.626 \times 10^{-34} \times 1057.8 \times 10^6 \text{ J})/(2\sqrt{3} \times 1.602 \times 10^{-19} \text{ C} \times 5.29 \times 10^{-11} \text{ m}) = 2.39 \times 10^4 \text{ V m}^{-1}$, about 240 V cm^{-1}
- Non-degenerate perturbation theory used at every field gives a quadratic shift that grows without limit. The 2×2 solution shows the crossover from quadratic to linear, near 240 V cm^{-1} , which is the scale the word 'weak' refers to.*
- (d) CALCULATE · U3 [3]**
- The $2s$ -like state decays through the $2p_{1/2}$ component that the field mixes into it. Calculate its lifetime in a field of 2.0 V cm^{-1} .
- 1 with $F = 200 \text{ V m}^{-1}$, $V/h = \sqrt{3}ea_0F/h = \sqrt{3} \times 1.602 \times 10^{-19} \times 5.29 \times 10^{-11} \times 200 / (6.626 \times 10^{-34}) \text{ Hz} = 4.43 \text{ MHz}$
 - 2 the admixed $2p$ probability is $(V/L)^2 = (4.43/1057.8)^2 = 1.75 \times 10^{-5}$, so the decay rate is $1.75 \times 10^{-5} / (1.60 \times 10^{-9} \text{ s}) = 1.10 \times 10^4 \text{ s}^{-1}$, beside which the field-free rate $1/(0.122 \text{ s}) = 8.2 \text{ s}^{-1}$ is negligible
 - 3 $\tau = 1/(1.10 \times 10^4 \text{ s}^{-1}) = 91 \mu\text{s}$, about 1300 times shorter than the field-free lifetime: a field of a few V cm^{-1} quenches the metastable state
- The admixture is a probability, $(V/L)^2$, not an amplitude. A candidate who multiplies the $2p$ rate by V/L finds $0.38 \mu\text{s}$, some 240 times too short; one who mixes angular frequency for L with ordinary frequency for V is out by $(2\pi)^2$.*
- (e) JUSTIFY · U4 [2]**
- Justify the neglect in (d) of the $2p_{3/2}$ level and of the natural width of the $2p$ state.
- 1 $|2p_{3/2}, +1/2\rangle = \sqrt{1/3}|m_l = 1\rangle|\downarrow\rangle + \sqrt{2/3}|m_l = 0\rangle|\uparrow\rangle$, orthogonal to the $2p_{1/2}$ state, is coupled by $\sqrt{6}ea_0F$, twice as strongly in square, but it lies $10.97 - 1.06 = 9.91 \text{ GHz}$ from $2s_{1/2}$, so its admixture is $2 \times (1.058/9.91)^2 \approx 0.023$ of the $2p_{1/2}$ one: it adds about 2% to the rate
 - 2 the $2p$ natural width is $\Gamma/2\pi = 1/(2\pi \times 1.60 \text{ ns}) = 99.5 \text{ MHz}$; including it replaces L^2 by $L^2 + (\hbar\Gamma/2)^2$, a fractional change of $(49.7/1057.8)^2 \approx 0.2\%$, so neither neglect changes the $91 \mu\text{s}$ by more than a few per cent
- A justification must size what it neglects. 'The $2p_{3/2}$ level is far away' earns nothing until the larger matrix element has been set against the larger detuning.*

A heavy quark and antiquark bound in a meson are modelled non-relativistically as one particle of reduced mass μ , with $\mu c^2 = 0.75 \text{ GeV}$, in the linear confining potential $V(r) = \sigma r$, with $\sigma = 0.90 \text{ GeV fm}^{-1}$. Only $l = 0$ is considered. The exact ground-state energy is $E_0 = 2.3381\epsilon_0$, where $\epsilon_0 = (\hbar^2 \sigma^2 / 2\mu)^{1/3}$ and -2.3381 is the first zero of the Airy function Ai ; for any s state of this potential it can also be shown that $|\psi(0)|^2 = \mu\sigma / (2\pi\hbar^2)$ exactly. Take $\hbar c = 0.1973 \text{ GeV fm}$, and $\int_0^\infty r^n e^{-\beta r} dr = n!/\beta^{n+1}$.

(a) SHOW THAT · U2

[2]

Show that for the normalised trial function $\psi_\beta(r) = \sqrt{(\beta^3/\pi)} e^{(-\beta r)}$, $\langle H \rangle = \hbar^2 \beta^2 / (2\mu) + 3\sigma / (2\beta)$.

- 1 $\langle T \rangle = (\hbar^2 / 2\mu) \int |\nabla \psi|^2 d^3r$, and $|\nabla \psi|^2 = \beta^2 |\psi|^2$ for this function, so $\langle T \rangle = \hbar^2 \beta^2 / (2\mu)$ (equivalently, from the full radial Laplacian with the integrals given)
- 2 $\langle r \rangle = (\beta^3 / \pi) \times 4\pi \int_0^\infty r^3 e^{(-2\beta r)} dr = 4\beta^3 \times 3! / (2\beta)^4 = 3 / (2\beta)$, so $\langle V \rangle = 3\sigma / (2\beta)$

Candidates who use $-(\hbar^2 / 2\mu) d^2 \psi / dr^2$ alone, dropping the $(2/r) d\psi / dr$ term of the three-dimensional Laplacian, find a negative kinetic energy, which should stop them at once.

(b) DETERMINE · U2

[3]

Determine the value of β that minimises $\langle H \rangle$, and show that the resulting bound is $E_{\text{exp}} = 3(3/4)^{2/3} \epsilon_0 = 2.476 \epsilon_0$.

- 1 $d\langle H \rangle / d\beta = \hbar^2 \beta / \mu - 3\sigma / (2\beta^2) = 0$ gives $\beta^3 = 3\mu\sigma / (2\hbar^2)$
- 2 at the minimum $3\sigma / (2\beta) = \hbar^2 \beta^2 / \mu$, twice the kinetic term (the virial theorem for a linear potential), so $\langle H \rangle = 3\hbar^2 \beta^2 / (2\mu)$
- 3 substituting $\beta^2 = (3\mu\sigma / 2\hbar^2)^{2/3}$ gives $E_{\text{exp}} = 3(\hbar^2 / 2\mu)^{1/3} (3\sigma / 4)^{2/3} = 3(3/4)^{2/3} \epsilon_0 = 2.476 \epsilon_0$

Checking $\langle V \rangle = 2\langle T \rangle$ at the minimum catches an arithmetic slip before the bound is quoted. A candidate who substitutes a wrong β into $\langle H \rangle$ still obtains an upper bound, only a poorer one, so the check matters.

(c) CALCULATE · U3

[2]

Calculate ϵ_0 , the exponential bound and the exact ground-state energy in GeV, and the percentage by which the bound exceeds the exact value.

- 1 $\epsilon_0 = [(\hbar c)^2 \sigma^2 / (2\mu c^2)]^{1/3} = [(0.1973 \text{ GeV fm})^2 \times (0.90 \text{ GeV fm}^{-1})^2 / (1.50 \text{ GeV})]^{1/3} = 0.276 \text{ GeV}$
- 2 $E_{\text{exp}} = 2.476 \times 0.276 \text{ GeV} = 0.683 \text{ GeV}$ against $E_0 = 2.3381 \times 0.276 \text{ GeV} = 0.645 \text{ GeV}$: the bound is 5.9% high, and above the exact value, as it must be

A bound below 0.645 GeV would signal an error: the theorem allows a trial energy only above the exact one. It says nothing about how far above, which is why the exact value is needed to judge the trial function.

(d) EXPLAIN · U1

[2]

A Gaussian trial function $e^{(-\alpha r^2)}$, optimised in the same way, gives $2.3448\epsilon_0$, within 0.3% of the exact value, although an exponential is the exact ground state of hydrogen. Explain why the Gaussian does so much better in this potential.

- 1 for a potential that is finite at $r = 0$, the s -wave equation gives $u = r\psi = c_1 r + c_3 r^3 + \dots$ with no r^2 term, so ψ has zero slope at the origin; the exponential's cusp, $\psi \approx 1 - \beta r$, is right only where a $1/r$ singularity balances it, and here it costs kinetic energy for nothing, whereas the Gaussian is smooth at the origin
- 2 the energy is decided by the shape of ψ where $|\psi|^2 r^2$ is large; the exact function decays as $\exp[-(2/3)(r/l)^{3/2}]$ with $l = (\hbar^2 / 2\mu\sigma)^{1/3}$, between the two trials, and the Gaussian's smooth, rounded peak matches the bulk of the exact function far better than the exponential's cusp

The tempting answer is that a Gaussian is 'more like an oscillator'. The decisive difference is at $r = 0$: a cusp belongs to a $1/r$ potential, and paying for one where the potential is smooth wastes kinetic energy.

(e) EVALUATE · U3

[3]

The meson's decay rate to a lepton pair is proportional to $|\psi(0)|^2$. The optimal Gaussian trial, $\psi = (2\alpha/\pi)^{3/4} e^{-(\alpha r^2)}$, has $\alpha^{3/2} = (\mu\sigma/3\hbar^2)\sqrt{(2/\pi)}$. A student proposes using it to predict $|\psi(0)|^2$, arguing that an energy within 0.3% of the exact value shows the trial state to be accurate. Evaluate this proposal.

- 1 $|\psi(0)|^2 = (2\alpha/\pi)^{3/2} = (2/\pi)^{3/2}(\mu\sigma/3\hbar^2)\sqrt{(2/\pi)} = 4\mu\sigma/(3\pi^2\hbar^2)$
- 2 against the exact $\mu\sigma/(2\pi\hbar^2)$ the ratio is $8/(3\pi) = 0.85$, so the Gaussian predicts a decay rate 15% too low; the exponential trial, with $\beta^3 = 3\mu\sigma/(2\hbar^2)$, gives $\beta^3/\pi = 3\mu\sigma/(2\pi\hbar^2)$, three times too high
- 3 the proposal should be rejected: $\langle H \rangle$ is stationary under variations of ψ , so a first-order error in ψ gives only a second-order error in E , while $|\psi(0)|^2$ has no such protection and is wrong at first order; an accurate energy certifies an upper bound on E , not the wavefunction, least of all its value at one point, where the weight $r^2|\psi|^2$ contributes nothing to E

This is the sentence that separates the answers: a variational energy certifies an upper bound and nothing else. A 0.3% energy can accompany a 15% error in a local property of the state.

15
CORE
COURSE

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[11]

For spontaneous emission by an electron from an upper state $|b\rangle$ to a lower state $|a\rangle$ at angular frequency ω , Einstein's detailed-balance argument with the Planck spectrum gives $A = \omega^3 | \langle a | \mathbf{r} | b \rangle |^2 / (3\pi\epsilon_0\hbar c^3)$. The absorption oscillator strength from a non-degenerate state $|a\rangle$ to a level b is $f = (2m_e\omega/3\hbar)\Sigma | \langle b | \mathbf{r} | a \rangle |^2$, summed over the degenerate states of b , and for one electron the Thomas-Reiche-Kuhn sum rule gives $\Sigma f = 1$ over all levels b . As a model, take an electron bound in the isotropic three-dimensional harmonic potential $\frac{1}{2}m_e\omega^2 r^2$, with states $|n_x, n_y, n_z\rangle$ and $\langle 0 | x | 1 \rangle = \sqrt{\hbar/(2m_e\omega)}$ for each Cartesian direction. Take $e = 1.602 \times 10^{-19}$ C, $m_e = 9.109 \times 10^{-31}$ kg, $\epsilon_0 = 8.854 \times 10^{-12}$ F m $^{-1}$, $c = 2.998 \times 10^8$ m s $^{-1}$, $k_B = 1.381 \times 10^{-23}$ J K $^{-1}$ and $1 \text{ u} = 1.661 \times 10^{-27}$ kg.

(a) EXPLAIN · U1

[2]

Explain why an atom treated by perturbation theory in a classical field would, in an excited state with no applied field, never decay, and how Einstein's argument nevertheless fixes A .

- 1 with no applied field the perturbation $\mathbf{e} \cdot \mathbf{r}$ is zero, and the excited state is an eigenstate of the atomic Hamiltonian, so it is stationary: the semiclassical theory has no spontaneous emission
- 2 in equilibrium with thermal radiation, absorption at the rate $B\rho(\omega)$ must balance stimulated emission plus spontaneous emission, $A + B\rho(\omega)$, between Boltzmann-populated levels; with Planck's $\rho(\omega)$ this forces $A = (\hbar\omega^3/\pi^2c^3)B$, and B is computed from the golden rule in a classical field (the quantum-electrodynamic derivation, which gives the same A , is quoted)

Candidates often say the excited state decays because it is unstable. In this theory it is an eigenstate and nothing makes it decay; the marks are for seeing that A is borrowed from equilibrium with Planck's law.

(b) SHOW THAT · U2

[2]

Show that for the oscillator the rate from $|1, 0, 0\rangle$ to $|0, 0, 0\rangle$ is $A = e^2\omega^2/(6\pi\epsilon_0m_e c^3)$, and comment on the absence of $\hbar$.

- 1 only the x component connects the two states: $| \langle 0,0,0 | \mathbf{r} | 1,0,0 \rangle |^2 = | \langle 0 | x | 1 \rangle |^2 = \hbar/(2m_e\omega)$, the y and z components vanishing because they would have to change n_y or n_z
- 2 $A = \omega^3 e^2 (\hbar/(2m_e\omega)) / (3\pi\epsilon_0\hbar c^3) = e^2\omega^2/(6\pi\epsilon_0m_e c^3)$; $\hbar$ cancels, and the result is exactly the classical radiation-damping rate of a charged oscillator, as the correspondence principle requires

Candidates who include y and z components, or take $| \langle 0 | x | 1 \rangle |^2 = \hbar/(m_e\omega)$ without the 2, double the rate. The disappearance of $\hbar$ is the check: a harmonically bound charge radiates as it does classically.

(c) DETERMINE · U2

[2]

Determine the absorption oscillator strength from $|0, 0, 0\rangle$ to the first excited level, and state what the Thomas-Reiche-Kuhn sum rule then implies for every other transition from the ground state.

- 1 the first excited level has three states, $|1,0,0\rangle$, $|0,1,0\rangle$ and $|0,0,1\rangle$, each with $|\langle b|r|0,0,0\rangle|^2 = \hbar/(2m_e\omega)$, so $f = (2m_e\omega/3\hbar) \times 3\hbar/(2m_e\omega) = 1$
- 2 this one transition exhausts the sum rule, so every other transition from the ground state has $f = 0$, consistent with the dipole operator changing a single quantum number by one

A sum rule exhausted by one line is a strong statement. Candidates who expect the oscillator to absorb at 2ω as well have forgotten what the dipole operator can do in one step.

(d) CALCULATE · U3

[3]

The sodium resonance lines near 589.0 nm (3s to 3p) have statistical weights in the same 1 : 3 ratio as the oscillator's, so for them $A = f \times e^2\omega^2/(6\pi\epsilon_0 m_e c^3)$. The measured 3p lifetime is 16.2 ns. Calculate the oscillator's lifetime at 589.0 nm, and hence the oscillator strength of the sodium resonance transition.

- 1 $\omega = 2\pi c/\lambda = 2\pi \times 2.998 \times 10^8 \text{ m s}^{-1}/(589.0 \times 10^{-9} \text{ m}) = 3.198 \times 10^{15} \text{ rad s}^{-1}$
- 2 $A = e^2\omega^2/(6\pi\epsilon_0 m_e c^3) = 6.41 \times 10^7 \text{ s}^{-1}$, so the oscillator lifetime is 15.6 ns
- 3 $f = A_{\text{Na}}/A_{\text{osc}} = 15.6 \text{ ns}/16.2 \text{ ns} = 0.96$: the single 3s-3p transition carries about 96% of the one-electron sum, the rest going to 3s-np with $n \geq 4$ and to the continuum

The ratio of the two lifetimes is the oscillator strength. A value above 1 would contradict the sum rule and signals a slip in ω , most often a wavelength left in nanometres or a frequency used in place of an angular frequency.

(e) COMPARE · U3

[2]

Compare the natural linewidth of the sodium line with its Doppler width in a vapour at 500 K, for which the full width at half maximum is $\Delta\nu_D = (v/c)\sqrt{8k_{\text{BT}} \ln 2/M}$, with $M = 22.99 \text{ u}$.

- 1 natural width $\Delta\nu = 1/(2\pi\tau) = 1/(2\pi \times 16.2 \times 10^{-9} \text{ s}) = 9.8 \text{ MHz}$, a Lorentzian full width
- 2 $\Delta\nu_D = [1/(589.0 \times 10^{-9} \text{ m})] \times \sqrt{(8 \times 1.381 \times 10^{-23} \text{ J K}^{-1} \times 500 \text{ K} \times \ln 2)/(22.99 \times 1.661 \times 10^{-27} \text{ kg}))} = (1.698 \times 10^6 \text{ m}^{-1})(1.00 \times 10^3 \text{ m s}^{-1}) = 1.70 \text{ GHz}$, about 170 times wider, so the vapour line is Doppler-dominated and the natural width shows only in the far wings or in Doppler-free or cold-atom measurements

Candidates who quote $1/\tau$ as the width in hertz are out by 2π . The comparison is the reason the natural width of an allowed optical line is seen only once the Doppler width has been removed.

16 CORE COURSE

STRUCTURED · DISCRIMINATING · UQMII-14.02 · UQMII-14.05 · UQMII-14.06 · UQMII-14.07

[11]

A superconducting qubit is driven close to resonance. In the frame rotating with the drive its Hamiltonian is $H(\varphi) = (\hbar/2)[\Delta\sigma_z + \Omega(\cos\varphi\sigma_x + \sin\varphi\sigma_y)]$, where the detuning is $\Delta/2\pi = 3.0 \text{ MHz}$, the Rabi frequency is $\Omega/2\pi = 4.0 \text{ MHz}$, and φ is the phase of the drive, which can be ramped. Equivalently $H = (\hbar\Omega_{\text{eff}}/2)\hat{n} \cdot \sigma$, with $\Omega_{\text{eff}} = \sqrt{\Delta^2 + \Omega^2}$ and $\hat{n} = (\sin\theta\cos\varphi, \sin\theta\sin\varphi, \cos\theta)$. In the experiment φ is ramped at a constant rate from 0 to 2π in a time $T = 4.0 \mu\text{s}$, so that $\hat{n}$ traces a circle on a cone about the z-axis.

(a) STATE · U1

[2]

State the eigenvalues of H , and the angle θ between $\hat{n}$ and the z-axis.

- 1 $E_{\pm} = \pm\hbar\Omega_{\text{eff}}/2 = \pm(\hbar/2)\sqrt{\Delta^2 + \Omega^2}$, that is $\pm\hbar \times 2.5 \text{ MHz}$, a gap of $\hbar \times 5.0 \text{ MHz}$; the two levels meet only at $\Delta = \Omega = 0$
- 2 $\cos\theta = \Delta/\Omega_{\text{eff}} = 3/5$ ($\sin\theta = 4/5$), so $\theta = 53.1^\circ$

The drive is part of the Hamiltonian in this frame, so the eigenvalues are $\pm\hbar\Omega_{\text{eff}}/2$, not $\pm\hbar\Delta/2$. A candidate who forgets it places $\hat{n}$ along z and finds no geometric phase at all.

(b) SHOW THAT · U2

[2]

Show that the adiabatic condition for the ramp becomes $T \gg \pi\Omega/(\Delta^2 + \Omega^2)$, and evaluate the right-hand side.

- 1 $dH/dt = (2\pi/T)\partial H/\partial\phi = (2\pi/T)(\hbar\Omega/2)(-\sin\phi\sigma_x + \cos\phi\sigma_y)$; the unit vector $(-\sin\phi, \cos\phi, 0)$ is perpendicular to $\hat{n}$, so its matrix element between the eigenstates along $\pm\hat{n}$ has magnitude 1, and $|(-dH/dt)| = \pi\hbar\Omega/T$
- 2 the condition $\hbar|(-dH/dt)| \ll (E_+ - E_-)^2$ becomes $\pi\hbar^2\Omega/T \ll \hbar^2(\Delta^2 + \Omega^2)$, so $T \gg \pi\Omega/(\Delta^2 + \Omega^2) = \pi(2\pi \times 4.0 \times 10^6 \text{ s}^{-1})/(2\pi \times 5.0 \times 10^6 \text{ s}^{-1})^2 = 80 \text{ ns}$, and the $4.0 \mu\text{s}$ ramp is fifty times longer

The rate of change must be compared with the square of the gap divided by $\hbar$, not with the gap. Candidates who compare $2\pi/T$ with Ω_{eff} reach a condition of the right order but cannot show where the factor $\Omega/\Omega_{\text{eff}}$ comes from.

(c) CALCULATE · U3

[3]

Calculate the geometric phase acquired in one circuit by each of the two eigenstates, and the difference between their dynamic phases.

- 1 $\hat{n}$ sweeps a cone of half-angle θ , enclosing a solid angle $2\pi(1 - \cos\theta) = 2\pi \times 2/5 = 0.8\pi \text{ sr}$
- 2 the geometric phase is minus half the solid angle, $-0.4\pi \text{ rad}$ (-72°), for the state along $+\hat{n}$ (the upper level) and $+0.4\pi \text{ rad}$ for the state along $-\hat{n}$, so the two differ by 0.8π
- 3 the dynamic phases differ by $\Omega_{\text{eff}}T = 2\pi \times 5.0 \text{ MHz} \times 4.0 \mu\text{s} = 40\pi \text{ rad}$, twenty full turns, proportional to both T and Ω_{eff} : a 1% error in Ω_{eff} shifts it by 0.4π , as much as the geometric phase itself

The solid angle of a cone is $2\pi(1 - \cos\theta)$, not $\pi\theta^2$. A candidate who notes that 40π is zero modulo 2π misses the point: it is the drift of the dynamic phase with Ω_{eff} and T that has to be removed before the geometric phase can be seen.

(d) PREDICT · U1

[2]

In a spin-echo version, the qubit starts in an equal superposition of the two eigenstates at $\phi = 0$, is taken once round the circuit, has its two eigenstates exchanged by a π pulse, and is then taken round the circuit in the opposite sense in the same time T . Predict the relative phase between the two components at the end, and how it changes if T is doubled or if $\Delta/2\pi$ is raised to 6.0 MHz with Ω unchanged.

- 1 each component spends time T in each eigenstate, so the dynamic phases cancel, while exchanging the eigenstates and reversing the sense of the circuit each reverse the sign of a component's geometric phase, so the geometric phases add: the relative phase is $2 \times 0.8\pi = 1.6\pi \text{ rad}$ (288° , equivalently -0.4π), unchanged when T is doubled as long as the ramp stays adiabatic
- 2 with $\Delta/2\pi = 6.0 \text{ MHz}$, $\cos\theta = 6/\sqrt{52} = 0.832$ and the relative phase becomes $4\pi(1 - 0.832) = 0.67\pi \text{ rad}$ (121°): it depends only on the geometry of the circuit

Candidates who expect the echo to cancel both phases have not seen that the two reversals, of the eigenstate labels and of the circuit, together leave the geometric phase adding. Independence of T is the experimental signature that the phase is geometric.

(e) EXPLAIN · U1

[2]

The same circuit also bounds the rest of the sphere, a cap of solid angle 4π minus the one used in (c). Explain why that cap gives the same phase factor, and what this has to do with the degeneracy of H at $\Delta = \Omega = 0$.

- 1 seen from the other cap the circuit runs in the opposite sense, so for the $+\hat{n}$ state $\gamma = +\frac{1}{2}(4\pi - 0.8\pi) = 2\pi - 0.4\pi$, which equals -0.4π modulo 2π : $e^{i\gamma}$ is the same whichever surface is used
- 2 the Berry curvature is the field of a monopole at the degeneracy, the origin of the space of $(\Omega \cos \phi, \Omega \sin \phi, \Delta)$, where the two eigenvalues meet; its total flux for a spin-half is 2π in magnitude, a multiple of 2π , which is why the phase of a closed circuit, the flux through it, is unambiguous

Surface-dependent Berry phases are the error this part is set to catch. The phase is defined modulo 2π only because the flux of the monopole at the degeneracy is quantised.

17

CORE
COURSE

DATA ANALYSIS · DEMANDING · UQMII-09.07 · UQMII-09.08 · UQMII-09.09

[10]

A hydrogen maser oscillates on the transition from $F = 1$, $m_F = 0$ to $F = 0$ in the hyperfine structure of the ground state, whose zero-field frequency is ν_{hfs} . A small static field B along z is applied by a solenoid around the storage bulb, but the ambient field is not fully cancelled. The field inside the bulb is measured by the Zeeman frequency f_Z , the low-frequency transition between neighbouring $F = 1$ sublevels, which in these weak fields is $f_Z = \mu_B B/h$. For each solenoid current the maser's output is compared with a reference oscillator, giving a frequency offset $\delta\nu$ that also contains a constant but unknown contribution from the reference and from collisions with the bulb wall. With $g_e = 2$ and the proton's magnetic moment neglected, the ground-state Hamiltonian is $H = A S_e \cdot S_p/\hbar^2 + (2\mu_B B/\hbar) S_{ez}$, where $A = h\nu_{\text{hfs}}$. Take $\mu_B = 9.274 \times 10^{-24} \text{ J T}^{-1}$ and $h = 6.626 \times 10^{-34} \text{ J s}$.

(a) SHOW THAT · U2

[3]

Working in the $m_F = 0$ subspace spanned by $|\uparrow\downarrow\rangle$ and $|\downarrow\uparrow\rangle$ (electron spin first), show that the frequency of the $F = 1$, $m_F = 0$ to $F = 0$ transition is $\nu_c = \sqrt{(\nu_{\text{hfs}})^2 + 4f_Z^2} \approx \nu_{\text{hfs}} + 2f_Z^2/\nu_{\text{hfs}}$.

- 1 $S_e \cdot S_p = S_{ez} S_{pz} + \frac{1}{2}(S_{e+} S_{p-} + S_{e-} S_{p+})$ has diagonal elements $-\hbar^2/4$ and off-diagonal elements $\hbar^2/2$ in this subspace, while the Zeeman term adds $+\mu_B B$ to $|\uparrow\downarrow\rangle$ and $-\mu_B B$ to $|\downarrow\uparrow\rangle$
- 2 the matrix $\begin{bmatrix} -A/4 + \mu_B B & A/2 \\ A/2 & -A/4 - \mu_B B \end{bmatrix}$ has eigenvalues $-A/4 \pm \sqrt{(A^2/4 + \mu_B^2 B^2)}$, which at $B = 0$ are $A/4$ ($F = 1$) and $-3A/4$ ($F = 0$)
- 3 $h\nu_c = 2\sqrt{(A^2/4 + \mu_B^2 B^2)}$, so $\nu_c = \sqrt{(\nu_{\text{hfs}})^2 + 4f_Z^2} \approx \nu_{\text{hfs}} + 2f_Z^2/\nu_{\text{hfs}}$ when $f_Z \ll \nu_{\text{hfs}}$: the clock transition has no term linear in B

Candidates who keep only the diagonal elements find ν_c independent of B ; those who use the weak-field linear result find a shift proportional to $m_F = 0$, which is zero, and miss the quadratic term the maser has to control.

(b) DESCRIBE · U4

[2]

Describe how the readings should be plotted to test this model and to extract ν_{hfs} , and explain why the solenoid current should not be used as the measure of the field.

- 1 plot $\delta\nu$ against f_Z^2 : the model predicts a straight line $\delta\nu = c + (2/\nu_{\text{hfs}})f_Z^2$, the unknown constant offset c appearing only in the intercept and the gradient being $2/\nu_{\text{hfs}}$
- 2 B is not proportional to I , because the uncanceled ambient field adds to the solenoid's (here $f_Z = 0.10 \text{ kHz} + 0.30 \text{ kHz mA}^{-1} \times I$, a residual of about 7 nT), and the solenoid's calibration inside the bulb is not known; f_Z measures the field the atoms actually experience

A plot against I^2 gives a gradient in mHz mA^{-2} , which cannot yield ν_{hfs} without an independent calibration of the solenoid, and the residual field makes it curve slightly. The Zeeman frequency is the atoms' own magnetometer.

(c) DETERMINE · U4

[3]

Determine the gradient of your graph and hence a value of ν_{hfs} , and comment on its agreement with the accepted 1420.406 MHz.

- 1 $f_Z^2 = 0.160, 0.490, 1.00, 1.69, 2.56$ and 3.61 kHz^2 , and the six points lie on a straight line with intercept $c \approx 3.50 \text{ mHz}$
- 2 gradient = $1.41 \text{ mHz kHz}^{-2}$ (accept 1.39 to $1.42 \text{ mHz kHz}^{-2}$), which is $1.41 \times 10^{-9} \text{ Hz}^{-1}$
- 3 $\nu_{\text{hfs}} = 2/\text{gradient} = 2/(1.41 \times 10^{-9} \text{ Hz}^{-1}) = 1.42 \times 10^9 \text{ Hz}$ (accept 1.41 to 1.44 GHz), agreeing with 1420.406 MHz within the half-per-cent uncertainty of the gradient, which confirms the quadratic Zeeman model; the neglected proton moment would change the gradient by only about 0.6%

Candidates who keep f_Z in kilohertz and $\delta\nu$ in millihertz must carry the factor of 10^{-9} through; an answer near 1.4 MHz or 1.4 THz signals a lost 10^3 . That a millihertz shift of the maser returns the gigahertz hyperfine frequency is a strong test of the model.

(d) ESTIMATE · U4

[2]

The maser is normally operated at $f_Z = 0.80 \text{ kHz}$. Estimate how constant f_Z , and hence the field, must be kept if field fluctuations are to change the maser frequency by less than 1 part in 10^{15} , stating your assumptions.

- 1 $d\nu_c/df_Z = 4f_Z/\nu_{\text{hfs}} = 4 \times 800 \text{ Hz}/(1.4204 \times 10^9 \text{ Hz}) = 2.25 \times 10^{-6}$, and the tolerance $10^{-15} \times 1.42 \times 10^9 \text{ Hz} = 1.4 \times 10^{-6} \text{ Hz}$ allows a change in f_Z of about 0.63 Hz
- 2 that is a fractional stability of $\delta f_Z/f_Z \approx 8 \times 10^{-4}$: the field of about 57 nT must be held to about 0.05 nT , assuming the quadratic law of (a) holds and every other frequency shift stays constant

Candidates who require the whole quadratic shift, rather than its change, to stay below 10^{-15} conclude that the field must be almost zero. It is the fluctuation that matters, and the derivative $4f_Z/\nu_{\text{hfs}}$ converts a field fluctuation into a frequency fluctuation.

18
CORE
COURSE

FREE RESPONSE · EXTENDED DERIVATION · DISCRIMINATING · UQMII-12.06 · UQMII-15.02 · UQMII-15.05 · UQMII-15.08 · UQMII-15.09

[15]

A particle of mass m and energy $E = \hbar^2 k^2/2m$ is scattered elastically by a potential $V(r)$ that vanishes at large r . To apply Fermi's golden rule, the system is placed in a cubic box of side L with periodic boundary conditions, so that the plane-wave states $\langle r|k \rangle = e^{i(k \cdot r)}/L^{3/2}$ are normalised and the incident state carries a probability current density $\hbar k/(mL^3)$. The golden rule gives the rate $\Gamma = (2\pi/\hbar)|\langle f|V|i \rangle|^2 \rho(E)$ into a group of final states whose density per unit energy is $\rho(E)$. Write $\tilde{V}(q) = \int e^{-i(q \cdot r)} V(r) d^3r$. Take $m_e = 9.109 \times 10^{-31} \text{ kg}$, $e = 1.602 \times 10^{-19} \text{ C}$, $c = 2.998 \times 10^8 \text{ m s}^{-1}$ and $\alpha = 1/137.0$.

(a) DERIVE · U2

[3]

Derive, from the periodic boundary conditions, the density of final states per unit energy $\rho(E)$ for plane waves whose wavevectors point into a small solid angle $d\Omega$.

- 1 periodic boundary conditions allow $k = (2\pi/L)(n_x, n_y, n_z)$ with integer n_x, n_y and n_z , one state for each volume $(2\pi/L)^3 = (2\pi)^3/L^3$ of k -space
- 2 the states with wavevectors in a shell k to $k + dk$ inside $d\Omega$ number $dN = L^3 k^2 dk d\Omega / (2\pi)^3$
- 3 with $E = \hbar^2 k^2/2m$, $dE = \hbar^2 k dk/m$, so $\rho(E) = dN/dE = L^3 m k d\Omega / (8\pi^3 \hbar^2)$

Candidates who count states on the whole sphere of radius k lose the $d\Omega$, and those who use $2\pi/L$ rather than $(2\pi/L)^3$ for the k -space volume per state lose a factor of L^2 . Either leaves the cross-section depending on the box.

- (b) **DERIVE** · U2 [3]
- Using the golden rule, derive the differential cross-section $d\sigma/d\Omega$ for elastic scattering in terms of $\tilde{V}(q)$, where $q = k_f - k_i$, and confirm that it does not depend on L .
- 1 $\langle k_f | V | k_i \rangle = L^{-3} \int e^{-i(k_f - k_i) \cdot r} V(r) d^3r = \tilde{V}(q)/L^3$, with $|k_f| = |k_i| = k$ by energy conservation
 - 2 the rate into $d\Omega$ is $d\Gamma = (2\pi/\hbar)(|\tilde{V}|^2/L^6)(L^3 mk d\Omega/8\pi^3 \hbar^2) = mk |\tilde{V}(q)|^2 d\Omega/(4\pi^2 \hbar^3 L^3)$
 - 3 dividing by the incident current density $\hbar k/(mL^3)$ gives $d\sigma/d\Omega = (m/2\pi \hbar^2)^2 |\tilde{V}(q)|^2$, in which L^3 has cancelled between the matrix element, the density of states and the flux
- The box must cancel. A candidate whose cross-section still contains L has mishandled one of the three places L enters: the normalisation of the states, the density of states, or the flux.*
- (c) **SHOW THAT** · U2 [2]
- For the screened Coulomb potential $V(r) = (g/r)e^{(-r/a)}$, show that $\tilde{V}(q) = 4\pi g/(q^2 + 1/a^2)$.
- 1 for a central potential, integrating over the angle between q and r with $\int_{-1}^1 e^{(-iqru)} du = 2 \sin(qr)/(qr)$ gives $\tilde{V}(q) = (4\pi/q) \int_0^\infty r V(r) \sin(qr) dr$
 - 2 $\tilde{V}(q) = (4\pi g/q) \int_0^\infty e^{(-r/a)} \sin(qr) dr = (4\pi g/q) \times q/(q^2 + 1/a^2) = 4\pi g/(q^2 + 1/a^2)$
- Candidates who expand $e^{(-iq \cdot r)}$ in partial waves spend a page on what the angular integral does in a line. $\int_0^\infty e^{(-\lambda r)} \sin(qr) dr = q/(q^2 + \lambda^2)$ is the whole of the radial work.*
- (d) **DETERMINE** · U2 [2]
- Take the limit $a \rightarrow \infty$ with $g = Z_1 Z_2 e^2/(4\pi\epsilon_0)$. Determine $d\sigma/d\Omega$ as a function of the scattering angle θ , and compare it with Rutherford's classical result, $d\sigma/d\Omega = g^2/(16E^2 \sin^4(\theta/2))$.
- 1 for elastic scattering through θ , $q = |k_f - k_i| = 2k \sin(\theta/2)$, so $d\sigma/d\Omega = (m/2\pi \hbar^2)^2 (4\pi g)^2/q^4 = 4m^2 g^2/(\hbar^4 q^4) = m^2 g^2/(4\hbar^4 k^4 \sin^4(\theta/2))$
 - 2 with $\hbar^2 k^2 = 2mE$ this is $g^2/(16E^2 \sin^4(\theta/2))$, identical to Rutherford's result; the total cross-section diverges at small θ , which a finite screening length a removes
- That the first Born approximation reproduces Rutherford's formula exactly is a special property of the Coulomb potential, not evidence that the approximation is good. The divergence of the total cross-section without screening is why a finite a was needed.*
- (e) **EXPLAIN** · U1 [2]
- The first Born amplitude, $f(\theta) = -(m/2\pi \hbar^2) \tilde{V}(q)$, is real for this potential, so $\text{Im } f(0) = 0$, yet the total cross-section it gives is positive. Explain why this does not contradict the optical theorem, $\sigma = (4\pi/k) \text{Im } f(0)$.
- 1 the Born cross-section is of second order in V , so the optical theorem relates it to the imaginary part of the forward amplitude at second order; the first-order amplitude is real for a real potential, and $\text{Im } f(0)$ first appears in the second Born term
 - 2 the theorem holds order by order in V : the first Born approximation conserves probability only to first order, and its failure to satisfy the optical theorem on its own is a statement about the order of the approximation, not a violation of unitarity
- Candidates who conclude that the optical theorem fails in the Born approximation have compared quantities of different order in V . The real amplitude is consistent with a positive cross-section once each side is taken at the same order.*

(f) ESTIMATE · U4

[3]

For a Coulomb-like potential of strength $g = Ze^2/(4\pi\epsilon_0)$, the first Born approximation is reliable when $g/(\hbar v) = Z\alpha c/v \ll 1$, where v is the speed of the incident particle. Estimate whether the Born cross-section can be trusted for electrons of kinetic energy 2.0 keV scattered by neutral helium ($Z = 2$) and by neutral iron ($Z = 26$), stating your assumptions.

- 1 $v = \sqrt{2E/m_e} = \sqrt{(2 \times 2.0 \times 10^3 \times 1.602 \times 10^{-19} \text{ J})/9.109 \times 10^{-31} \text{ kg}} = 2.65 \times 10^7 \text{ m s}^{-1}$, so $v/c = 0.088$ and non-relativistic kinematics are adequate
- 2 $Z\alpha c/v = Z \times (1/137.0)/0.0885 = 0.0825Z$, which is 0.17 for helium and 2.1 for iron
- 3 the Born cross-section is adequate for helium, with corrections of order $Z\alpha c/v$, about 17%, but fails for iron, where partial waves or an exact treatment are needed; the estimate assumes that the scattering that matters happens close to the nucleus, where screening is weak, and ignores exchange with, and excitation of, the atomic electrons

The criterion compares the strength of the potential with $\hbar v$, not the range with the wavelength; high energy helps only because v grows. Iron fails at 2 keV because Z enters linearly.

19
CORE
COURSE

FREE RESPONSE · MODEL, SOLVE AND CHECK THE LIMITS · DISCRIMINATING · UQMII-11.04 · UQMII-11.09

[15]

A particle of mass m moves in one dimension in the potential $V(x) = \frac{1}{2}m\omega^2 x^2(1 - x/L)$, the model used for the phase of a current-biased Josephson junction. V has a minimum at $x = 0$ and a barrier beyond which, for $x > L$, it falls without limit, so the ground state of the well is metastable and escapes by tunnelling. For the numerical parts take $\omega/2\pi = 8.0 \text{ GHz}$, with L such that the barrier height is $V_b = 3.0\hbar\omega$. A full treatment, matching the Gaussian ground state of the well onto the decaying WKB solution under the barrier, gives the escape rate $\Gamma = (\omega/2\pi)\sqrt{(864\pi V_b/\hbar\omega)} \exp(-36V_b/5\hbar\omega)$, which is quoted here. You may use $\int_0^1 u\sqrt{1-u} du = 4/15$. Take $\hbar = 1.055 \times 10^{-34} \text{ J s}$ and $k_B = 1.381 \times 10^{-23} \text{ J K}^{-1}$.

(a) SHOW THAT · U2

[2]

Show that the top of the barrier lies at $x = 2L/3$ and that $V_b = (2/27)m\omega^2 L^2$.

- 1 $dV/dx = m\omega^2(x - 3x^2/2L) = m\omega^2 x(1 - 3x/2L)$, which vanishes at $x = 0$, the minimum, and at $x = 2L/3$, the maximum
- 2 $V(2L/3) = \frac{1}{2}m\omega^2(4L^2/9)(1/3) = (2/27)m\omega^2 L^2$

Candidates who look for the barrier at the zeros of V confuse $x = L$, where V returns to zero, with the top. The barrier height grows as L^2 , which is why the escape rate is so sensitive to the parameters that set L .

(b) SKETCH · U1

[2]

Sketch $V(x)$ from $x = -L/3$ to $x = 4L/3$, marking V_b , the ground-state energy $\frac{1}{2}\hbar\omega$ and the classical turning points at that energy, and on the same axes sketch the magnitude of the metastable ground-state wavefunction.

- 1 V : a parabolic minimum at $x = 0$ with V rising for $x < 0$, a maximum V_b at $x = 2L/3$, back to zero at $x = L$ and falling without limit beyond; the line $E = \frac{1}{2}\hbar\omega = V_b/6$ meets V at two points inside the well, near $x \approx -0.15L$ and $x \approx 0.17L$, and once more on the outer slope just inside $x = L$ (near $0.97L$)
- 2 $|\psi|$: a Gaussian-like hump centred in the well, decaying roughly exponentially through the barrier by several orders of magnitude, then emerging beyond the outer turning point as a small outgoing oscillatory wave that does not decay, with a wavelength that shortens as V falls

The sketch must show that the wavefunction beyond the barrier does not decay: an outgoing wave carries probability away, which is what makes the state metastable rather than bound.

(c) DERIVE · U2

[3]

Starting from the WKB tunnelling exponent $2S/\hbar = (2/\hbar) \int \sqrt{2m(V - E)} dx$ taken across the barrier, derive its value for an energy $E \rightarrow 0$ at the bottom of the well, and express it in terms of $V_b/\hbar\omega$.

- 1 at $E \rightarrow 0$ the turning points bounding the barrier are $x = 0$ and $x = L$, where $V = 0$, and between them $\sqrt{2mV} = m\omega x \sqrt{1 - x/L}$
- 2 $\int_0^L m\omega x \sqrt{1 - x/L} dx = m\omega L^2 \int_0^1 u \sqrt{1 - u} du = (4/15)m\omega L^2$, so $2S/\hbar = (8/15)m\omega L^2/\hbar$
- 3 from (a), $m\omega^2 L^2 = (27/2)V_b$, so $m\omega L^2/\hbar = (27/2)V_b/\hbar\omega$ and $2S/\hbar = (8/15)(27/2)V_b/\hbar\omega = 36V_b/(5\hbar\omega) = 7.2V_b/\hbar\omega$, the exponent of the quoted result

Candidates who integrate from $x = 0$ to $2L/3$ treat the top of the barrier as a turning point. The WKB integral runs between the two points where $V = E$, which at $E = 0$ are $x = 0$ and $x = L$.

(d) CALCULATE · U3

[2]

Calculate, for $V_b = 3.0\hbar\omega$, the naive escape rate $\Gamma_0 = (\omega/2\pi)\exp(-2S/\hbar)$, which pictures the particle striking the barrier once per classical period, and the quoted rate Γ .

- 1 $2S/\hbar = 7.2 \times 3.0 = 21.6$ and $e^{(-21.6)} = 4.2 \times 10^{-10}$, so $\Gamma_0 = 8.0 \times 10^9 \text{ s}^{-1} \times 4.2 \times 10^{-10} = 3.3 \text{ s}^{-1}$
- 2 $\sqrt{(864\pi \times 3.0)} = 90$, so $\Gamma = 90 \times 3.3 \text{ s}^{-1} = 3.0 \times 10^2 \text{ s}^{-1}$, a lifetime of 3.3 ms: the naive estimate is too low by a factor of about 90

An exponent of 21.6 gives a factor of 4×10^{-10} , so a candidate who writes $e^{(-7.2)}$ has dropped $V_b/\hbar\omega = 3.0$. The factor of 90 in the prefactor is equivalent to changing the exponent by 4.5, a large correction for a method whose exponent is right.

(e) EVALUATE · U1

[3]

Evaluated between its turning points at the actual ground-state energy $E = \frac{1}{2}\hbar\omega$, the barrier integral gives $2S/\hbar = 17.15$ for these parameters. Evaluate the naive estimate in the light of this: identify which of its approximations causes most of the discrepancy, and explain why the difficulty is worst for the lowest state.

- 1 $(\omega/2\pi)e^{(-17.15)} = 8.0 \times 10^9 \text{ s}^{-1} \times 3.6 \times 10^{-8} = 2.9 \times 10^2 \text{ s}^{-1}$, within about 5% of the quoted $3.0 \times 10^2 \text{ s}^{-1}$
- 2 so most of the factor of 90 comes from setting $E = 0$ in the exponent: $E_0 = \frac{1}{2}\hbar\omega = V_b/6$ is not small compared with V_b , and lowering the exponent by 4.45 multiplies the rate by about 86; the $\sqrt{(V_b/\hbar\omega)}$ in the quoted prefactor is this energy dependence of the exponent, expanded about $E = 0$
- 3 near the bottom of the well the classically allowed region is only about one zero-point width across, so neither the WKB wavefunction nor the classical attempt frequency is valid there, and the slope of the exponent, $d(2S/\hbar)/dE$, grows logarithmically as E falls towards the bottom of the well, so the exponent cannot simply be taken at $E = 0$; for highly excited states the Gamow form with the true energy works, but the ground state needs its Gaussian matched onto the WKB tail

The 'failure of the prefactor' for the lowest state is the energy dependence of the exponent near the bottom of the well. Candidates who blame the attempt frequency alone miss that a shift of $\frac{1}{2}\hbar\omega$ in E changes the exponent by more than 4.

Thermal activation over the barrier occurs at a rate of order $(\omega/2\pi)\exp(-V_b/k_BT)$. Estimate the temperature below which escape is dominated by tunnelling, stating your assumptions, and say what an experiment would observe below it.

- 1 comparing exponents, and assuming the prefactors are of comparable size, tunnelling wins when $V_b/k_BT > 7.2V_b/\hbar\omega$, that is below $k_BT^* = \hbar\omega/7.2$
- 2 $\hbar\omega = 1.055 \times 10^{-34} \text{ J s} \times 2\pi \times 8.0 \times 10^9 \text{ s}^{-1} = 5.30 \times 10^{-24} \text{ J}$, so $\hbar\omega/k_B = 0.384 \text{ K}$ and $T^* \approx 53 \text{ mK}$ (a fuller treatment gives $\hbar\omega/(2\pi k_B) = 61 \text{ mK}$, the same order)
- 3 below T^* the escape rate stops falling with temperature and levels off at the tunnelling rate, the signature of macroscopic quantum tunnelling; at 53 mK, $k_BT \approx 0.14\hbar\omega$, so the excited levels of the well are scarcely populated, justifying the ground-state treatment, and dissipation is neglected throughout

An estimate without its assumptions earns two of the three marks. Comparing exponents ignores the prefactors, which move the crossover only logarithmically.

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.

State	Give the result, definition or law concisely. No justification is required.
Describe	Give the relevant features of a situation or process in words, precisely enough that someone else could reproduce it.
Explain	Give the physical reason a result or behaviour occurs, connecting it explicitly to the principle that governs it.
Calculate	Obtain a numerical value, showing the relation used, the substitution and the units of the result.
Determine	Obtain a result by any valid route the problem allows — analytic, graphical or numerical — with enough working to be followed.
Derive	Start from a named fundamental law or definition and reach the required result by explicit, justified steps.
Show that	Establish a result the question gives you. Every step must be shown, because the stated answer earns nothing on its own.
Estimate	Reach an order-of-magnitude value from stated, reasonable assumptions, and say what those assumptions are.
Sketch	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.
Justify	Support a claim or a choice with evidence, and with the reasoning that connects that evidence to the claim.
Evaluate	Weigh a model, argument or result against criteria, including its assumptions and domain of validity, and reach a stated judgement.
Compare	Identify the similarities and differences between two situations, models or results, relating each difference to its cause.
Predict	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.

U1 27 MARKS · 23%	Conceptual understanding Identify the governing principle and the conditions under which it holds, and reason qualitatively about what a result must look like before calculating it.
U2 49 MARKS · 42%	Mathematical modelling and derivation 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

27 MARKS · 23%

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

15 MARKS · 13%

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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