

University Advanced Quantum Mechanics · Final Examination

The whole of Advanced Quantum Mechanics, weighted towards the second half: quantised fields and spin-statistics, second quantisation, the radiation field and spontaneous emission, Bethe's Lamb shift, open systems and the Bose gas. Symmetries, identical-particle scattering, the Klein-Gordon and Dirac equations, $g = 2$ and exact Dirac hydrogen are sampled from the first half.

SUGGESTED TIME 150 minutes	TOTAL MARKS 114	QUESTIONS 18	MULTIPLE CHOICE 10
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SECTION **UAQM · Final · University Advanced Quantum Mechanics — 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 2**

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

COURSE UNITS UAQM-01 · UAQM-02 · UAQM-03 · UAQM-04 · UAQM-05 · UAQM-06 · UAQM-07 · UAQM-08 · UAQM-09 · UAQM-10 · UAQM-11 · UAQM-12 · UAQM-13 · UAQM-14 · UAQM-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 Advanced Quantum Mechanics · Final Examination

Answer all questions. 114 marks in 150 minutes.

1 MULTIPLE CHOICE · ROUTINE · UAQM-01.06 · UAQM-01.07 [1]

CORE
COURSE

A metallic grain a few nanometres across holds an odd number N of conduction electrons. Its shape is irregular, its impurities are random, and strong spin-orbit scattering mixes spin with orbital motion, so that no spatial symmetry and no component of the total spin is conserved. No magnetic field is applied, so every term in the grain's Hamiltonian H is even under time reversal, and for N spin-half particles the time-reversal operator satisfies $\Theta^2 = (-1)^N$. Which statement about the energy levels of the grain is correct?

- A** Every level is non-degenerate: once spin-orbit scattering has mixed the spin states, only a spatial symmetry could force two states to share an energy.
- B** Every level is at least twofold degenerate: for an eigenstate $|\psi\rangle$, $\Theta|\psi\rangle$ has the same energy, and $\Theta^2 = -1$ makes it orthogonal to $|\psi\rangle$.
- C** The levels are twofold degenerate only while the spin-orbit scattering is weak, because the pairs are the spin-up and spin-down states of each orbital, which strong spin-orbit coupling mixes.
- D** Every level is twofold degenerate, and stays so when one more electron is added, because each electron's states still come in time-reversed pairs.

Answer

2 MULTIPLE CHOICE · DEMANDING · UAQM-02.05 · UAQM-02.08 [1]

CORE
COURSE

The elastic scattering of ^{16}O by ^{16}O is followed at a fixed centre-of-mass angle $\theta = 60^\circ$ while the centre-of-mass energy is stepped down from 8.0 MeV to 3.0 MeV, below the Coulomb barrier of about 10 MeV; at this angle the nuclei never come closer than about 17 fm, so only the Coulomb interaction acts. ^{16}O nuclei are identical spin-0 bosons. The Coulomb amplitude the pair would have if the nuclei were distinguishable is, up to a phase that does not depend on θ , $f(\theta) = -[\eta/(2k \sin^2(\theta/2))] \exp[-i\eta \ln \sin^2(\theta/2)]$, where k is the relative wavenumber and the Sommerfeld parameter $\eta = Z^2\alpha/\beta$, with βc the relative speed, rises from 10.1 to 16.5 over the range. Let R be the measured differential cross-section divided by $|f(60^\circ)|^2$, the Rutherford value for the projectile alone. How does R behave over the range?

- A** R stays at $1 + \tan^2 30^\circ = 10/9$ at every energy: spin-0 nuclei have no spin states to average over, and the Coulomb phase cancels when each amplitude is squared.
- B** R oscillates between 0 and 4, because the amplitudes of identical bosons always add, so they can interfere completely.
- C** R oscillates between $4/9$ and $16/9$, passing through more than one full cycle as $\eta \ln 3$ changes by about 7 rad.
- D** R oscillates between $10/9$ and $16/9$, because the interference of identical bosons is always constructive, so the cross-section never falls below the sum of the two Rutherford terms.

Answer

3

CORE
COURSE

MULTIPLE CHOICE · ROUTINE · UAQM-03.06 · UAQM-03.08

[1]

A negative kaon, K^- , is a spinless particle of charge $-e$ that can be captured into atomic orbits. Consider a kaon bound to a lead nucleus ($Z = 82$), treated as a point charge, with the strong interaction ignored. Its Klein-Gordon radial equation contains the centrifugal term $\hbar^2 c^2 l(l+1)/r^2$ together with an attractive term $-(Z\alpha\hbar c)^2/r^2$ that comes from squaring the Coulomb energy, so that near the origin the radial function $R(r)$ behaves as r^s , with $s(s+1) = l(l+1) - (Z\alpha)^2$. Take $\alpha = 1/137.04$. Which statement about the kaon's s, p and d orbitals ($l = 0, 1$ and 2) is correct?

- A** Only the s orbitals fail: for $l = 0$, s is complex and the solutions oscillate without limit near the origin, a fall to the centre, while the p and d orbitals have $s \approx 0.88$ and $s \approx 1.93$.
- B** None fails, because $Z\alpha = 0.60$ is below 1; the s orbitals merely acquire a weak singularity, $R \propto r^s$ with $s \approx -0.36$.
- C** Every orbital fails, because the attractive $-(Z\alpha)^2/r^2$ term outweighs the Coulomb term near the origin whatever l is.
- D** Only the s orbitals fail, and the p and d orbitals keep $s = 1$ and $s = 2$ exactly, as in the non-relativistic atom, because $(Z\alpha)^2$ is negligible beside $l(l+1)$.

Answer

4

CORE
COURSE

MULTIPLE CHOICE · ROUTINE · UAQM-05.05 · UAQM-05.06

[1]

In Fermi's theory of beta decay and its generalisations, $n \rightarrow p e^- \bar{\nu}$ arises from contact terms in the Lagrangian density, each the product of a bilinear in the proton and neutron fields and a bilinear in the electron and neutrino fields, with $\bar{\psi} = \psi^\dagger \gamma^0$, $\gamma^5 = i\gamma^0 \gamma^1 \gamma^2 \gamma^3$ and $\sigma^{\mu\nu} = (i/2)[\gamma^\mu, \gamma^\nu]$. Under parity each Dirac field becomes $\gamma^0 \psi(t, -x)$ times an intrinsic phase, and the phases are chosen so that Fermi's vector term $G_V(\bar{\psi}_p \gamma^\mu \psi_n)(\bar{\psi}_e \gamma_\mu \psi_\nu)$ conserves parity. Which further term, with a real constant G , would make the interaction violate parity?

- A** $G(\bar{\psi}_p \psi_n)(\bar{\psi}_e \psi_\nu)$
- B** $G(\bar{\psi}_p \sigma^{\mu\nu} \psi_n)(\bar{\psi}_e \sigma_{\mu\nu} \psi_\nu)$
- C** $G(\bar{\psi}_p \gamma^\mu \gamma^5 \psi_n)(\bar{\psi}_e \gamma_\mu \gamma^5 \psi_\nu)$
- D** $G(\bar{\psi}_p \gamma^\mu \psi_n)(\bar{\psi}_e \gamma_\mu \gamma^5 \psi_\nu)$

Answer

5

CORE
COURSE

MULTIPLE CHOICE · ROUTINE · UAQM-08.02 · UAQM-08.06

[1]

In a uniform static electric field of strength $\mathcal{E}$, the potential energy of an electron changes steadily along the field, so that a positive-energy electron state at one point has the same total energy as a negative-energy state a distance $d = 2mc^2/(e\mathcal{E})$ further along: Sauter's smooth version of the Klein step. In hole theory an electron tunnelling from the filled negative-energy states across this gap leaves a hole behind, so the field creates electron-positron pairs. Take $mc^2 = 0.511$ MeV, the reduced Compton wavelength $\hbar/mc = 3.86 \times 10^{-13}$ m and $e = 1.602 \times 10^{-19}$ C. At about what field strength does pair creation stop being exponentially suppressed?

- A** About $m^2c^3/(e\hbar) \approx 1.3 \times 10^{18}$ V m⁻¹, at which the gap d has shrunk to two reduced Compton wavelengths, so tunnelling across it is no longer suppressed.
- B** About 1.9×10^{16} V m⁻¹, at which the potential energy changes by $2mc^2$ across one Bohr radius, the size of the atoms that would supply the electrons.
- C** Any field at all, because Klein's step needs only a total rise of more than $2mc^2$, which a uniform field supplies over a long enough distance, whatever its gradient.
- D** About 3.6×10^{20} V m⁻¹, at which the potential energy changes by $2mc^2$ across one classical electron radius, 2.82 fm, the length at which classical electrodynamics fails.

Answer

6

CORE
COURSE

MULTIPLE CHOICE · RECALL · UAQM-09.06 · UAQM-09.08 · UAQM-09.09

[1]

A free complex scalar field and a free Dirac field are each quantised in two ways: with commutators and with anticommutators of their mode operators. Two requirements are imposed: a Hamiltonian bounded below on a space of states of positive norm, and local observables that commute at spacelike separation. Which statement is correct?

- A** The Dirac field with commutators keeps a positive energy but fails microcausality, while the scalar field with anticommutators has an energy unbounded below.
- B** The Dirac field with commutators has an energy unbounded below, or states of negative norm if creators and annihilators are relabelled, while the scalar field with anticommutators fails microcausality; only the scalar with commutators and the Dirac field with anticommutators pass both tests.
- C** Both wrong quantisations fail only the positivity requirement, since microcausality holds for any choice because the vacuum amplitude $D(x - y)$ vanishes outside the light cone.
- D** The scalar field with anticommutators is excluded only because it allows at most one quantum in each mode, which contradicts the classical limit of the field.

Answer

7

CORE
COURSE

MULTIPLE CHOICE · ROUTINE · UAQM-10.01 · UAQM-10.03

[1]

Three fermion orbitals are ordered 1, 2, 3, and occupation-number states are defined by $|n_1 n_2 n_3\rangle = (c_1^\dagger)^{n_1} (c_2^\dagger)^{n_2} (c_3^\dagger)^{n_3} |0\rangle$, with $\{c_i, c_j^\dagger\} = \delta_{ij}$ and $\{c_i, c_j\} = 0$. The one-body operator $T = t(c_3^\dagger c_1 + c_1^\dagger c_3)$ moves a fermion between orbitals 1 and 3. What is $T|1 1 0\rangle$?

- A $+t|0 1 1\rangle$
- B 0, because orbital 2 lies between orbitals 1 and 3 and is occupied
- C $-t|1 0 1\rangle$
- D $-t|0 1 1\rangle$

Answer

8

CORE
COURSE

MULTIPLE CHOICE · ROUTINE · UAQM-11.07

[1]

A single mode of the quantised field is prepared first in the number state $|n = 4\rangle$ and then in the coherent state $|\alpha\rangle$ with $|\alpha|^2 = 4$. Its normalised second-order correlation at zero delay is $g^{(2)}(0) = \langle a^\dagger a^\dagger a a \rangle / \langle a^\dagger a \rangle^2$. What are the two values of $g^{(2)}(0)$, number state first?

- A 1 and 1
- B 0.75 and 2
- C 0.75 and 1
- D 0 and 1

Answer

9

CORE
COURSE

MULTIPLE CHOICE · ROUTINE · UAQM-12.08

[1]

A quantum dot emitting at a free-space wavelength $\lambda = 930$ nm sits at the field maximum of a GaAs micropillar cavity of refractive index $n = 3.5$, quality factor $Q = 6000$ and mode volume $V = 1.5(\lambda/n)^3$. Its transition is resonant with the cavity mode and its dipole is parallel to the cavity field. The Purcell factor, the ratio of its emission rate into the cavity mode to its spontaneous emission rate in bulk GaAs, is $F_P = (3/4\pi^2)(\lambda/n)^3(Q/V)$. What is F_P ?

- A 304
- B 1.30×10^4
- C 4.00×10^3
- D It cannot be found without the dot's transition dipole moment, which sets both rates.

Answer

In Hartree-Fock theory the energy per electron of the uniform electron gas, in rydbergs, is $E/N = 2.21/r_s^2 - 0.916/r_s$, where r_s is the radius, in Bohr radii, of the sphere that contains one electron, and $1 \text{ Ry} = 13.61 \text{ eV}$. The conduction electrons of lithium have $r_s = 3.25$. What is E/N at lithium's density, and how does that density compare with the density at which the Hartree-Fock E/N is lowest?

- A $E/N = -0.073 \text{ Ry} (-0.99 \text{ eV})$, and lithium's electron gas is less dense than at the Hartree-Fock minimum.
- B $E/N = -0.282 \text{ Ry} (-3.84 \text{ eV})$, and lithium's electron gas is denser than at the Hartree-Fock minimum.
- C $E/N = +0.209 \text{ Ry} (+2.85 \text{ eV})$, and lithium's electron gas is denser than at the Hartree-Fock minimum.
- D $E/N = -0.073 \text{ Ry} (-0.99 \text{ eV})$, and lithium's electron gas is denser than at the Hartree-Fock minimum.

Answer

A negative muon, a spin-half Dirac particle of charge $q = -e$ and mass m about 207 times the electron's, is captured by a lead nucleus, ^{208}Pb ($Z = 82$), and cascades to the $1s$ orbit of muonic lead. That orbit is so small that the muon spends most of its time inside the nucleus, modelled as a uniformly charged sphere of radius $R = 7.1 \text{ fm}$, where its potential energy is $V(r) = -(Z\alpha\hbar c/R)(3/2 - r^2/2R^2)$. In static potentials ϕ and A its Dirac Hamiltonian is $H = c\alpha \cdot \pi + \beta mc^2 + q\phi$, with $\pi = p - qA$, $p = -i\hbar\nabla$ and $V = q\phi$. In the Dirac representation, writing a stationary state as $e^{-i(mc^2 + W)t/\hbar}$ times the column (ξ, χ) of upper and lower two-component spinors, $H\psi = (mc^2 + W)\psi$ becomes $(W - V)\xi = c\sigma \cdot \pi \chi$ and $(W - V + 2mc^2)\chi = c\sigma \cdot \pi \xi$. Pauli's anomalous-moment term adds to H , in a magnetic field B , the operator $-a(q\hbar/2m)\beta\Sigma \cdot B$, where $\Sigma = \text{diag}(\sigma, \sigma)$. For vector operators a and b that commute with the Pauli matrices, $(\sigma \cdot a)(\sigma \cdot b) = a \cdot b + i\sigma \cdot (a \times b)$, and for any function $f(r)$, $p f - f p = -i\hbar\nabla f$. In a storage-ring measurement of the anomaly, muons of Lorentz factor $\gamma = 29.3$ circulate in a uniform field $B = 1.4513 \text{ T}$, with no electric field acting on them, and the rate of their decay positrons oscillates at the frequency $\omega_a/2\pi = 229.08 \text{ kHz}$ at which the spin turns relative to the momentum. Take $mc^2 = 105.66 \text{ MeV}$, $m = 1.8835 \times 10^{-28} \text{ kg}$, $\hbar c = 197.33 \text{ MeV fm}$, $\alpha = 1/137.036$, $e = 1.602 \times 10^{-19} \text{ C}$ and the muon's lifetime at rest $\tau = 2.197 \mu\text{s}$.

(a) SHOW THAT

[2]

Show that the Dirac equation $i\hbar\partial\psi/\partial t = H\psi$ keeps its form under the gauge transformation $A \rightarrow A + \nabla\Lambda$, $\phi \rightarrow \phi - \partial\Lambda/\partial t$, for any smooth function $\Lambda(r, t)$, provided that $\psi \rightarrow e^{i(q\Lambda/\hbar)}\psi$.

(b) ESTIMATE

[2]

Inside the nucleus V is the potential energy of a three-dimensional harmonic oscillator. Estimate, stating your assumptions, the oscillator quantum $\hbar\omega$, the muon's speed in the $1s$ state as a fraction of c and hence the size of χ relative to ξ , and judge whether an expansion in v/c is trustworthy for muonic lead.

- (c) **DERIVE** [3]
- For a slow muon in a uniform magnetic field B , with $A = \frac{1}{2}B \times r$ and no electric field, eliminate χ to leading order in v/c and derive the Hamiltonian for ξ to first order in B . Hence find the g -factors with which the orbital angular momentum $L = r \times p$ and the spin $S = (\hbar/2)\sigma$ couple to B under minimal coupling alone, and the spin g -factor once Pauli's term is included.
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- (d) **CALCULATE** [2]
- For a slow muon the Pauli Hamiltonian makes the spin precess at $\omega_s = g|q|B/2m$ while the momentum turns at $\omega_c = |q|B/m$, so the spin turns relative to the momentum at $\omega_a = a|q|B/m$; with no electric field the Thomas-BMT equation shows that this holds at any speed. Calculate a for the muon from the storage-ring measurement, and the number of cycles of the positron-rate oscillation in one dilated lifetime $\gamma\tau$.
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- (e) **SHOW THAT** [3]
- The Foldy-Wouthuysen reduction to order $(v/c)^2$ contains the even term $-(1/8m^2c^4)[O, [O, V]]$, where $O = c\alpha \cdot p$ is the odd part of H when $A = 0$. Show that for a static V this term equals $(\hbar^2/8m^2c^2)\nabla^2V + (\hbar/4m^2c^2)\Sigma \cdot (\nabla V \times p)$, and that inside the uniformly charged nucleus the Darwin part is the constant $3Z\alpha(\hbar c)^3/(8(mc^2)^2R^3)$. Evaluate it for muonic lead.
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- (f) **EXPLAIN** [2]
- The $1s$ and $2s$ states of muonic lead are orthogonal four-component spinors. Using your estimate from (b), explain why their upper components ξ_{1s} and ξ_{2s} cannot be eigenfunctions of any Hermitian Hamiltonian at order $(v/c)^2$, so that no two-component Schrödinger equation for ξ can be exact to that order, and what the Foldy-Wouthuysen transformation does instead.
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The Lyman- α X-rays of hydrogen-like uranium, U^{91+} ($Z = 92$), emitted when bare uranium nuclei circulating in a heavy-ion storage ring capture an electron that cascades to the ground state, test the Dirac-Coulomb spectrum where $Z\alpha$ is not small. The two lines are $Ly\alpha 1$, $2p_{3/2} \rightarrow 1s_{1/2}$, and $Ly\alpha 2$, $2p_{1/2} \rightarrow 1s_{1/2}$, and spectroscopy of the stored ions places $Ly\alpha 1$ at 102.17 keV. In a central potential $V(r)$ the radial functions $G(r)$ and $F(r)$ of the upper and lower components satisfy $dG/dr = -(\kappa/r)G + [(E + mc^2 - V)/\hbar c]F$ and $dF/dr = (\kappa/r)F - [(E - mc^2 - V)/\hbar c]G$, where E includes mc^2 , $\kappa = (l - j)(2j + 1)$ and l is the orbital angular momentum of the upper component. For a point nucleus $V = -Z\alpha\hbar c/r$, and the exact energies are $E_{nj} = mc^2[1 + (Z\alpha)^2/(n - |\kappa| + \gamma)^2]^{-1/2}$, with $\gamma = \sqrt{\kappa^2 - (Z\alpha)^2}$. The normalised point-nucleus $1s$ density, both components together, is $|\psi_{1s}(r)|^2 = [(2Z/a_0)^{2\gamma+1}/(4\pi\Gamma(2\gamma + 1))]r^{2\gamma-2}e^{-2Zr/a_0}$, with $\Gamma(2\gamma + 1) = 1.313$ for $Z = 92$, while the Schrödinger $1s$ density is $(Z^3/\pi a_0^3)e^{-2Zr/a_0}$. The uranium nucleus has its surface at about $r = 7.5$ fm and is treated as infinitely heavy. Take $mc^2 = 510.999$ keV, $\alpha = 1/137.036$ and $a_0 = 5.2918 \times 10^{-10}$ m.

(a) STATE

[2]

State which conserved operator takes the place of L^2 in labelling the electron's states, and state κ and the orbital angular momentum l' of the lower component for each of $1s_{1/2}$, $2p_{1/2}$ and $2p_{3/2}$, saying which of their components are s waves, able to reach the nucleus.

(b) DERIVE

[3]

Derive from the radial equations how G and F rise from the origin. For the point nucleus, writing $G \approx ar^\gamma$ and $F \approx br^\gamma$, find γ and b/a , evaluate b/a for $1s_{1/2}$ and for $2p_{1/2}$ at $Z = 92$, and say which component dominates near the nucleus in each. Then find the powers of r with which G and F rise inside a nucleus of finite size, where $V(r)$ tends to a finite $V(0)$.

(c) CALCULATE

[2]

Calculate, for a point nucleus, the energies of $Ly\alpha 1$ and $Ly\alpha 2$ in keV, and the $2p$ fine-structure splitting.

(d) DETERMINE

[2]

Treating the $2p_{3/2}$ level as given correctly by the point-nucleus formula, determine from the measured $Ly\alpha 1$ energy the shift of the $1s$ level that the point-nucleus Dirac theory omits, its sign, and its size as a fraction of the $1s$ binding energy.

- (e) **COMPARE** [2]
Compare the Dirac 1s density at the nuclear surface, $r = 7.5$ fm, with the Schrödinger 1s density there, and say what the comparison implies for the finite-size part of the shift found in (d).

- (f) **PREDICT** [1]
In the point-nucleus Dirac theory $2s_{1/2}$ and $2p_{1/2}$ are exactly degenerate. Predict which of the two the finite size of the nucleus raises more, and so which lies higher.

13 CORE COURSE

STRUCTURED · DEMANDING · UAQM-09.01 · UAQM-09.03 · UAQM-09.04

A free complex scalar field $\phi(x, t)$, with ϕ and $\phi^\dagger$ treated as independent fields, describes spinless particles of mass m and charge q through the Lagrangian density $\mathcal{L} = (1/c^2)(\partial\phi^\dagger/\partial t)(\partial\phi/\partial t) - \nabla\phi^\dagger \cdot \nabla\phi - \kappa^2\phi^\dagger\phi$, where $\kappa = mc/\hbar$. In a box of volume V with periodic boundary conditions the quantised field is $\phi(x, t) = \sum_{\mathbf{k}} N_{\mathbf{k}}[a_{\mathbf{k}} e^{i(\mathbf{k}\cdot\mathbf{x} - \omega_{\mathbf{k}} t)} + b_{\mathbf{k}}^\dagger e^{-i(\mathbf{k}\cdot\mathbf{x} - \omega_{\mathbf{k}} t)}]$, with $\omega_{\mathbf{k}} = c\sqrt{k^2 + \kappa^2}$, $N_{\mathbf{k}} = \sqrt{(\hbar c^2)/(2\omega_{\mathbf{k}}V)}$, $[a_{\mathbf{k}}, a_{\mathbf{k}'}^\dagger] = [b_{\mathbf{k}}, b_{\mathbf{k}'}^\dagger] = \delta_{\mathbf{k}\mathbf{k}'}$ and all other commutators zero. After normal ordering the Hamiltonian is $H = \sum_{\mathbf{k}} \hbar\omega_{\mathbf{k}}(a_{\mathbf{k}}^\dagger a_{\mathbf{k}} + b_{\mathbf{k}}^\dagger b_{\mathbf{k}})$. Take $\hbar c = 197.3$ MeV fm.

- (a) **DERIVE** [3]
Apply the Euler-Lagrange equation for $\phi^\dagger$ to derive the field equation for ϕ , and use it to show that the density $\rho = (iq/\hbar c^2)(\phi^\dagger\partial\phi/\partial t - \phi\partial\phi^\dagger/\partial t)$ and the current $\mathbf{j} = -(iq/\hbar)(\phi^\dagger\nabla\phi - \phi\nabla\phi^\dagger)$ satisfy $\partial\rho/\partial t + \nabla \cdot \mathbf{j} = 0$.

- (b) **SHOW THAT** [3]
By substituting the mode expansion, show that after normal ordering the charge $Q = \int \rho d^3x$ is $q\sum_{\mathbf{k}}(a_{\mathbf{k}}^\dagger a_{\mathbf{k}} - b_{\mathbf{k}}^\dagger b_{\mathbf{k}})$, and hence that $a_{\mathbf{k}}^\dagger$ creates a quantum of charge $+q$ and $b_{\mathbf{k}}^\dagger$ one of charge $-q$, each with energy $\hbar\omega_{\mathbf{k}}$.

- (c) **EXPLAIN** [2]
The field commutator is $[\phi(x), \phi^\dagger(y)] = D(x - y) - D(y - x)$, where $D(x - y) = \langle 0 | \phi(x)\phi^\dagger(y) | 0 \rangle = \sum_{\mathbf{k}} N_{\mathbf{k}}^2 e^{i(\mathbf{k}\cdot(\mathbf{x} - \mathbf{y}) - \omega_{\mathbf{k}}(t_{\mathbf{x}} - t_{\mathbf{y}}))}$. Explain why the commutator vanishes when $x - y$ is spacelike although $D(x - y)$ does not, and what would go wrong if the field contained the $a_{\mathbf{k}}$ terms alone.

(d) **ESTIMATE** [2]

At equal times and separation r , D is proportional to $(1/r)K_1(\kappa r)$, which for $\kappa r \gg 1$ behaves as $r^{-3/2}e^{-\kappa r}$. For a π^+ , with $mc^2 = 139.6$ MeV, estimate the length $1/\kappa$ over which the amplitude extends outside the light cone, and the factor by which D falls between $r = 5$ fm and $r = 10$ fm, stating your assumptions.

(e) **COMPARE** [2]

Compare the density ρ of this question, as an operator of the quantised field, with the same expression read as a probability density in the one-particle Klein-Gordon theory.

Two electrons occupy a molecule of two sites, 1 and 2, each with one orbital, described by the Hubbard Hamiltonian $H = -t \sum_{\sigma} (c_{1\sigma}^\dagger c_{2\sigma} + c_{2\sigma}^\dagger c_{1\sigma}) + U(n_{1\uparrow} n_{1\downarrow} + n_{2\uparrow} n_{2\downarrow})$, with hopping $t = 0.40$ eV and on-site repulsion $U = 3.2$ eV. The operators obey $\{c_{i\sigma}, c_{j\sigma'}^\dagger\} = \delta_{ij} \delta_{\sigma\sigma'}$ and $\{c_{i\sigma}, c_{j\sigma'}\} = 0$. In the sector with $S_z = 0$ a basis is $|D_1\rangle = c_{1\uparrow}^\dagger c_{1\downarrow}^\dagger |0\rangle$ and $|D_2\rangle = c_{2\uparrow}^\dagger c_{2\downarrow}^\dagger |0\rangle$, with both electrons on one site, and $|A\rangle = c_{1\uparrow}^\dagger c_{2\downarrow}^\dagger |0\rangle$ and $|B\rangle = c_{2\uparrow}^\dagger c_{1\downarrow}^\dagger |0\rangle$, with one electron on each.

(a) SHOW THAT

[3]

Show that the hopping term T sends both $|A\rangle$ and $|B\rangle$ to $-t(|D_1\rangle + |D_2\rangle)$, and hence that in the basis $|S\rangle = (|A\rangle + |B\rangle)/\sqrt{2}$, $|D_+\rangle = (|D_1\rangle + |D_2\rangle)/\sqrt{2}$ the Hamiltonian is the matrix $\begin{bmatrix} 0 & -2t \\ -2t & U \end{bmatrix}$, while $(|A\rangle - |B\rangle)/\sqrt{2}$ and $(|D_1\rangle - |D_2\rangle)/\sqrt{2}$ are eigenstates with energies 0 and U .

(b) CALCULATE

[2]

Calculate the ground-state energy and the singlet-triplet splitting, and compare the splitting with the superexchange coupling $4t^2/U$.

(c) DETERMINE

[2]

Determine the probability of finding both electrons on the same site in the ground state.

(d) EVALUATE

[3]

A student describes the ground state by the restricted Hartree-Fock determinant, with both electrons in the bonding orbital, created by $(c_{1\uparrow}^\dagger + c_{2\uparrow}^\dagger)/\sqrt{2}$. Evaluate this description: find its energy and its probability of double occupation, and say what it gets wrong as U/t grows.

(e) EXPLAIN

[2]

Unrestricted Hartree-Fock lets the up-spin and down-spin electrons occupy different orbitals, and its best determinant has energy $-2t^2/U = -0.10$ eV. Explain why it recovers only about half of the exact binding, and what symmetry of H it breaks to do so.

In Bethe's non-relativistic calculation a hydrogen atom in a state $|n\rangle$ is coupled to the transverse vacuum field through $H' = (e/m)A \cdot p$ in the dipole approximation, photon energies being cut off at K . Summing the second-order energy over photon modes and polarisations gives $W_n = -(2\alpha/(3\pi m^2 c^2)) \sum_m |\langle m|p|n\rangle|^2 \int_0^K k dk / (E_m - E_n + k)$, where $k = \hbar\omega$ is the photon energy and the sum runs over all bound and continuum states $|m\rangle$. For a free electron of momentum p the same calculation gives $W_{\text{free}} = -(2\alpha/(3\pi m^2 c^2))p^2 K$. Write $p_{mn} = \langle m|p|n\rangle$. Take $mc^2 = 0.510999$ MeV, $\alpha = 1/137.036$, $1 \text{ Ry} = 13.6057$ eV and $\hbar = 4.1357 \times 10^{-15}$ eV s.

(a) SHOW THAT

[2]

Show that, for K large compared with every $|E_m - E_n|$ that matters, W_n grows linearly with K , and that the coefficient of K is the free-electron result averaged over the state $|n\rangle$.

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(b) EXPLAIN

[2]

Explain why the linear term is removed by mass renormalisation, and why what remains depends on K only through a logarithm.

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(c) SHOW THAT

[3]

The sum rule $\sum_m |p_{mn}|^2 (E_m - E_n) = (\hbar^2/2) \langle n | \nabla^2 V | n \rangle$ holds for $V = -e^2/(4\pi\epsilon_0 r)$. Defining the mean excitation energy K_0 by $\ln K_0 = \sum_m |p_{mn}|^2 (E_m - E_n) \ln |E_m - E_n| / \sum_m |p_{mn}|^2 (E_m - E_n)$, show that $\Delta E_n = (4\alpha^5 mc^2 / (3\pi n^3)) \ln(K/K_0)$ for s states, and that the term in $\ln K$ vanishes in every other state. You may use $|\psi_{ns}(0)|^2 = 1/(\pi n^3 a_0^3)$, $a_0 = \hbar/(\alpha mc)$ and $e^2/(4\pi\epsilon_0) = \alpha \hbar c$.

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(d) CALCULATE

[3]

With the cutoff at $K = mc^2$ and the quoted mean excitation energies $K_0(2s) = 16.64$ Ry and $K_0(1s) = 19.77$ Ry, calculate the shifts of $2s$ and of $1s$ in frequency units, and compare them with the measured $2s_{1/2} - 2p_{1/2}$ splitting of 1057.8 MHz and $1s$ shift of 8.17 GHz.

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(e) EVALUATE

[2]

The non-relativistic calculation fixes the cutoff K only to within a factor of about two. Evaluate whether the agreement found in (d) shows that Bethe's choice $K = mc^2$ is correct.

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16
CORE
COURSE

DATA ANALYSIS · DEMANDING · UAQM-14.02 · UAQM-14.06

[11]

A single InGaAs quantum dot at 4 K is driven resonantly by a narrow-band laser, and its fluorescence is recorded as the laser frequency is scanned across the transition. For each laser power P at the dot, the full width at half maximum $\Delta\nu$ of the fluorescence line, as a frequency, is recorded. A separate time-resolved measurement gives the population relaxation time $T_1 = 0.80$ ns. For a two-level emitter with population relaxation time T_1 and coherence time T_2 , driven at Rabi frequency Ω and detuning Δ (both angular frequencies), the steady state of the optical Bloch equations has the excited-state population $\rho_{ee} = \frac{1}{2}\Omega^2 T_1 T_2 / (1 + \Delta^2 T_2^2 + \Omega^2 T_1 T_2)$, and Ω^2 is proportional to P . Without pure dephasing $T_2 = 2T_1$; in general $1/T_2 = 1/(2T_1) + 1/T_\phi$, where T_ϕ is the pure dephasing time.

Fluorescence linewidth of one quantum dot at six laser powers

Run	Laser power P / nW	Linewidth $\Delta\nu$ / MHz
1	2.0	289
2	5.0	314
3	10.0	361
4	20.0	429
5	40.0	554
6	80.0	732

(a) SHOW THAT

[2]

Show that $\Delta\nu = (1/\pi T_2)\sqrt{1 + \Omega^2 T_1 T_2}$, and hence that $\Delta\nu^2 = \Delta\nu_0^2(1 + P/P_{\text{sat}})$, where $\Delta\nu_0 = 1/(\pi T_2)$ and P_{sat} is the power at which $\Omega^2 T_1 T_2 = 1$.

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(b) DESCRIBE

[2]

Describe how the readings should be plotted to test this model and to extract $\Delta\nu_0$ and P_{sat} , and explain why the narrowest line measured is not itself $\Delta\nu_0$.

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- (c) **DETERMINE** [3]
Determine the gradient and intercept of your graph, and hence $\Delta\nu_0$ and P_{sat} .

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- (d) **EVALUATE** [3]
Evaluate whether this emitter's line is lifetime-limited, finding T_2 and, if it is needed, the pure dephasing time T_ϕ .

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- (e) **PREDICT** [1]
Predict the rate at which the dot scatters photons when it is driven on resonance at $P = 40 \text{ nW}$.

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17
CORE
COURSE

FREE RESPONSE · EXTENDED DERIVATION · DISCRIMINATING · UAQM-11.03 · UAQM-11.05 · UAQM-12.01 · UAQM-12.02
· UAQM-12.03

[15]

In a cubic box of volume V with periodic boundary conditions, the transverse vector potential in Coulomb gauge is, in the Heisenberg picture, $A(\mathbf{r}, t) = \sum_{\mathbf{k}, \lambda} \sqrt{\hbar/(2\epsilon_0\omega_{\mathbf{k}}V)} [a_{\mathbf{k}\lambda}(t) \boldsymbol{\varepsilon}_{\mathbf{k}\lambda} e^{i(\mathbf{k}\cdot\mathbf{r} - \omega_{\mathbf{k}}t)} + a_{\mathbf{k}\lambda}^\dagger(t) \boldsymbol{\varepsilon}_{\mathbf{k}\lambda}^* e^{-i(\mathbf{k}\cdot\mathbf{r} - \omega_{\mathbf{k}}t)}]$, with $\omega_{\mathbf{k}} = ck$, two unit polarisation vectors $\boldsymbol{\varepsilon}_{\mathbf{k}\lambda}$ perpendicular to $\mathbf{k}$ for each $\mathbf{k}$, and $[a_{\mathbf{k}\lambda}, a_{\mathbf{k}'\lambda'}^\dagger] = \delta_{\mathbf{k}\mathbf{k}'} \delta_{\lambda\lambda'}$. A one-electron atom or ion, with an infinitely heavy nucleus at the origin, has an excited state $|b\rangle$ and a lower state $|a\rangle$ separated by $\hbar\omega_0$. It couples to the field through $H' = (e/m)A(0) \cdot \mathbf{p}$, the dipole approximation, where $-e$ and m are the electron's charge and mass, and $\langle a|\mathbf{p}|b\rangle = -im\omega_0\langle a|\mathbf{r}|b\rangle$. For a hydrogen-like ion of nuclear charge Ze , $|\langle 1s|r|2p, m\rangle|^2 = (2^{15}/3^{10})(a_0/Z)^2$ for each m , and the 2p-1s energy difference is $(3/4)Z^2 \times 13.606 \text{ eV}$. Take $\hbar = 1.055 \times 10^{-34} \text{ J s}$, $e = 1.602 \times 10^{-19} \text{ C}$, $\epsilon_0 = 8.854 \times 10^{-12} \text{ F m}^{-1}$, $c = 2.998 \times 10^8 \text{ m s}^{-1}$ and $a_0 = 5.292 \times 10^{-11} \text{ m}$.

- (a) **DERIVE** [2]
Derive the transverse electric field operator from A , and show that in the vacuum each mode contributes $\hbar\omega_{\mathbf{k}}/(2\epsilon_0V)$ to $\langle E^2 \rangle$, so that its mean electric energy is half its zero-point energy.

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- (b) **SHOW THAT** [2]
Show that the matrix element for emission of a photon into a mode $(\mathbf{k}, \lambda)$ already holding n photons is $\langle a; n+1|H'|b; n\rangle = (e/m)\sqrt{\hbar/(2\epsilon_0\omega_{\mathbf{k}}V)} \sqrt{n+1} \boldsymbol{\varepsilon}_{\mathbf{k}\lambda}^* \cdot \langle a|\mathbf{p}|b\rangle$, and explain why this makes an excited atom in the vacuum emit, though an atom in a classical field of zero amplitude never does.

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(c) **DERIVE** [4]

Using Fermi's golden rule, and summing over all modes, directions and both polarisations, derive $A = \omega_0^3 e^2 |\langle a | r | b \rangle|^2 / (3\pi\epsilon_0 \hbar c^3)$ for spontaneous emission from $|b\rangle$ to $|a\rangle$.

(d) **CALCULATE** [3]

Calculate A , the lifetime and the natural linewidth $\Gamma/2\pi$ of the 2p state of the hydrogen-like helium ion He^+ ($Z = 2$).

(e) **EXPLAIN** [2]

The atom now sits in thermal radiation at temperature T , whose modes near ω_0 hold $\bar{n}$ photons on average. Explain how the $\sqrt{n}$ and $\sqrt{n+1}$ factors of the field operators lead to Planck's distribution, rather than assuming it as Einstein did.

(f) **JUSTIFY** [2]

Justify the dipole approximation, and the use of the golden rule leading to exponential decay at the rate A , for the He^+ 2p state.

18
CORE
COURSE

FREE RESPONSE · MODEL, SOLVE AND CHECK THE LIMITS · DISCRIMINATING · UAQM-15.07 · UAQM-15.08 · UAQM-15.09

[16]

A uniform gas of N spinless bosons of mass m in a box of volume V , with periodic boundary conditions, interacts through a short-range potential represented at low energy by the contact coupling $g = 4\pi\hbar^2 a_s/m$, where a_s is the s-wave scattering length. In second quantisation $H = \sum_k \epsilon_k a_k^\dagger a_k + (g/2V) \sum_{(k,k',q)} a_{(k+q)}^\dagger a_{(k'-q)}^\dagger a_{(k')} a_k$, with $\epsilon_k = \hbar^2 k^2/2m$. Bogoliubov's approximation replaces a_0 and $a_0^\dagger$ by $\sqrt{N_0}$, where N_0 is the number of bosons in the condensate, and keeps the terms of H up to second order in the operators a_k with $k \neq 0$, the sums over such k being written Σ' . Write $n = N/V$. Take $\hbar = 1.055 \times 10^{-34}$ J s, $1 \text{ u} = 1.661 \times 10^{-27}$ kg and $k_B = 1.381 \times 10^{-23}$ J K⁻¹.

- (a) **SHOW THAT** [3]
 Show that, to this order and with N_0 eliminated in favour of N , $H \approx gN^2/(2V) + \sum[(\epsilon_k + gn)a_k^\dagger a_k + (gn/2)(a_k^\dagger a_{-k}^\dagger + a_k a_{-k})]$.
- (b) **DERIVE** [4]
 Writing $a_k = u_k b_k - v_k b_{-k}^\dagger$ with u_k and v_k real, derive the condition on u_k and v_k that keeps $[b_k, b_k^\dagger] = 1$, the choice that removes the terms $b_k b_{-k}$ and $b_k^\dagger b_{-k}^\dagger$, and the excitation energy $E_k = \sqrt{\epsilon_k(\epsilon_k + 2gn)}$.
- (c) **SKETCH** [2]
 Sketch E_k against k , with ϵ_k on the same axes, marking the behaviour at small and at large k and the scale $k \approx 1/\xi$, where $\xi = \hbar/\sqrt{2mgn}$, at which it changes.
- (d) **CALCULATE** [3]
 For a condensate of ^{87}Rb ($m = 87 \text{ u}$, $a_s = 5.3 \text{ nm}$) of density $n = 2.0 \times 10^{20} \text{ m}^{-3}$, calculate gn/k_B in nanokelvin, the speed of sound c , the healing length ξ and na_s^3 .
- (e) **DETERMINE** [2]
 Determine $\langle a_k^\dagger a_k \rangle$ for $k \neq 0$ in the ground state, the vacuum of every b_k , and hence, given that the sum over k gives a depletion $(N - N_0)/N = (8/(3\sqrt{\pi}))\sqrt{na_s^3}$, the fraction of the atoms of (d) that lie outside the condensate at zero temperature.
- (f) **PREDICT** [2]
 A tightly focused repulsive laser beam is dragged through the condensate of (d) at 1.5 mm s^{-1} . Predict, using Landau's criterion, whether it heats the gas, and whether an obstacle moving at the same speed through an ideal Bose gas would.

University Advanced Quantum Mechanics · 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 · ROUTINE · UAQM-01.06 · UAQM-01.07 **[1]**

CORE
COURSE

A metallic grain a few nanometres across holds an odd number N of conduction electrons. Its shape is irregular, its impurities are random, and strong spin-orbit scattering mixes spin with orbital motion, so that no spatial symmetry and no component of the total spin is conserved. No magnetic field is applied, so every term in the grain's Hamiltonian H is even under time reversal, and for N spin-half particles the time-reversal operator satisfies $\Theta^2 = (-1)^N$. Which statement about the energy levels of the grain is correct?

KEY B Every level is at least twofold degenerate: for an eigenstate $|\psi\rangle$, $\Theta|\psi\rangle$ has the same energy, and $\Theta^2 = -1$ makes it orthogonal to $|\psi\rangle$.

B is correct. Because H is even under time reversal, $\Theta H = H \Theta$, so $\Theta|\psi\rangle$ is an eigenstate with the same energy as $|\psi\rangle$. Antiunitarity, $\langle \Theta a | \Theta b \rangle = \langle b | a \rangle$, applied with $a = \Theta\psi$ and $b = \psi$ gives $\langle \psi | \Theta\psi \rangle = \langle \Theta^2\psi | \Theta\psi \rangle = -\langle \psi | \Theta\psi \rangle$ when $\Theta^2 = -1$, so $\langle \psi | \Theta\psi \rangle = 0$ and the two states are distinct: every level is a Kramers doublet, whatever the shape, the disorder or the strength of the spin-orbit scattering. A is tempting because a system with no spatial symmetry is expected to have no degeneracy at all, which is right for an even number of electrons; it forgets that time reversal is itself a symmetry, and for odd N it forces the pairing. C pictures the doublets as spin-up and spin-down copies of one orbital, which they are only without spin-orbit coupling; Kramers' theorem pairs $|\psi\rangle$ with $\Theta|\psi\rangle$, which need not be eigenstates of any spin component, so the degeneracy survives spin-orbit scattering of any strength, though a magnetic field would split each pair, with a g -factor that the scattering reduces. D treats the many-electron levels as if they were built from single-electron pairs; with $N + 1$ electrons $\Theta^2 = +1$, $\Theta|\psi\rangle$ can be a multiple of $|\psi\rangle$, nothing forces the levels to pair, and a grain with an even number of electrons generically has non-degenerate levels.

U1

2 MULTIPLE CHOICE · DEMANDING · UAQM-02.05 · UAQM-02.08 **[1]**

CORE
COURSE

The elastic scattering of ^{16}O by ^{16}O is followed at a fixed centre-of-mass angle $\theta = 60^\circ$ while the centre-of-mass energy is stepped down from 8.0 MeV to 3.0 MeV, below the Coulomb barrier of about 10 MeV; at this angle the nuclei never come closer than about 17 fm, so only the Coulomb interaction acts. ^{16}O nuclei are identical spin-0 bosons. The Coulomb amplitude the pair would have if the nuclei were distinguishable is, up to a phase that does not depend on θ , $f(\theta) = -[\eta/(2k \sin^2(\theta/2))] \exp[-i\eta \ln \sin^2(\theta/2)]$, where k is the relative wavenumber and the Sommerfeld parameter $\eta = Z^2\alpha/\beta$, with βc the relative speed, rises from 10.1 to 16.5 over the range. Let R be the measured differential cross-section divided by $|f(60^\circ)|^2$, the Rutherford value for the projectile alone. How does R behave over the range?

KEY C R oscillates between 4/9 and 16/9, passing through more than one full cycle as $\eta \ln 3$ changes by about 7 rad.

For identical spin-0 bosons the amplitude is $f(\theta) + f(\pi - \theta)$. At $\theta = 60^\circ$, $|f(120^\circ)|/|f(60^\circ)| = \sin^2 30^\circ / \cos^2 30^\circ = \tan^2 30^\circ = 1/3$, and the relative phase of the two amplitudes is $\eta \ln[\cos^2(\theta/2)/\sin^2(\theta/2)] = \eta \ln 3$. So $R = |1 + (1/3)e^{i(\eta \ln 3)}|^2 = 1 + 1/9 + (2/3)\cos(\eta \ln 3)$. As η rises from 10.1 to 16.5 the phase $\eta \ln 3$ runs from 11.1 rad to 18.1 rad, more than 2π , so R swings through its whole range, from $(1 - 1/3)^2 = 4/9$ to $(1 + 1/3)^2 = 16/9$: these are Mott oscillations (C). A keeps $|f(\theta)|^2 + |f(\pi - \theta)|^2$ and drops the cross term, as if the nuclei were distinguishable; the Coulomb phase does cancel in each squared amplitude, but not in the cross term, which is where exchange shows up. B would need the two amplitudes to have equal size, which happens only at 90° , and even there the relative phase $\eta \ln 1$ vanishes, so R is fixed at 4 rather than oscillating; at 60° the exchanged amplitude is a third of the direct one and the cancellation can never be complete. D confuses symmetrisation with constructive interference: bosons add amplitudes, not intensities, and when the relative phase is near π the two amplitudes partly cancel, taking R below the incoherent sum 10/9.

U2

A negative kaon, K^- , is a spinless particle of charge $-e$ that can be captured into atomic orbits. Consider a kaon bound to a lead nucleus ($Z = 82$), treated as a point charge, with the strong interaction ignored. Its Klein-Gordon radial equation contains the centrifugal term $\hbar^2 c^2 l(l+1)/r^2$ together with an attractive term $-(Z\alpha\hbar c)^2/r^2$ that comes from squaring the Coulomb energy, so that near the origin the radial function $R(r)$ behaves as r^s , with $s(s+1) = l(l+1) - (Z\alpha)^2$. Take $\alpha = 1/137.04$. Which statement about the kaon's s, p and d orbitals ($l = 0, 1$ and 2) is correct?

KEY A Only the s orbitals fail: for $l = 0$, s is complex and the solutions oscillate without limit near the origin, a fall to the centre, while the p and d orbitals have $s \approx 0.88$ and $s \approx 1.93$.

Solving $s(s+1) = l(l+1) - (Z\alpha)^2$ gives $s = -\frac{1}{2} + \sqrt{(l + \frac{1}{2})^2 - (Z\alpha)^2}$, which is real only while $Z\alpha < l + \frac{1}{2}$. With $Z\alpha = 82/137.04 = 0.598$, $(Z\alpha)^2 = 0.358$ exceeds $\frac{1}{4}$, so for the s waves $s = -\frac{1}{2} \pm 0.329i$: R oscillates as $r^{-1/2} \cos(0.329 \ln r)$ infinitely often near the origin, the point-nucleus problem has no lowest level, and the particle falls to the centre (A). For $l = 1$, $s = -\frac{1}{2} + \sqrt{2.25 - 0.358} = 0.876$, and for $l = 2$, $s = -\frac{1}{2} + \sqrt{6.25 - 0.358} = 1.927$, both real. B borrows the Dirac condition $Z\alpha < |\kappa| = 1$ and the small- $Z\alpha$ result $s \approx -(Z\alpha)^2$, which holds only for $Z\alpha \ll \frac{1}{2}$; for the Klein-Gordon equation the threshold is $Z\alpha = l + \frac{1}{2}$, which lead's s waves have already passed. C forgets that the centrifugal term has the same $1/r^2$ form: what matters is the net coefficient $(l + \frac{1}{2})^2 - (Z\alpha)^2$ in the indicial equation, which stays positive for $l \geq 1$ until $Z\alpha$ reaches 1.5. D picks the failing orbitals correctly but treats $(Z\alpha)^2$ as negligible; at $Z\alpha = 0.6$ it lowers the p-wave exponent by 12%, from 1 to 0.88.

U2

In Fermi's theory of beta decay and its generalisations, $n \rightarrow p e^- \bar{\nu}$ arises from contact terms in the Lagrangian density, each the product of a bilinear in the proton and neutron fields and a bilinear in the electron and neutrino fields, with $\bar{\psi} = \psi^\dagger \gamma^0$, $\gamma^5 = i\gamma^0 \gamma^1 \gamma^2 \gamma^3$ and $\sigma^{\mu\nu} = (i/2)[\gamma^\mu, \gamma^\nu]$. Under parity each Dirac field becomes $\gamma^0 \psi(t, -x)$ times an intrinsic phase, and the phases are chosen so that Fermi's vector term $G_V(\bar{\psi}_p \gamma^\mu \psi_n)(\bar{\psi}_e \gamma_\mu \psi_\nu)$ conserves parity. Which further term, with a real constant G , would make the interaction violate parity?

KEY D $G(\bar{\psi}_p \gamma^\mu \psi_n)(\bar{\psi}_e \gamma_\mu \gamma^5 \psi_\nu)$

With the phases fixed so that the vector term is even, every term carries the same overall phase factor, so each term's parity is set by its bilinears. Under parity a bilinear $\bar{\psi}_1 \Gamma \psi_2$ becomes $\bar{\psi}_1 \gamma^0 \Gamma \gamma^0 \psi_2$ evaluated at $-x$. For $\Gamma = 1$ it is unchanged, a scalar. For $\Gamma = \gamma^\mu$ the time component keeps its sign and the space components reverse, a polar vector. For $\Gamma = \gamma^\mu \gamma^5$, $\gamma^0 \gamma^\mu \gamma^5 \gamma^0 = -\gamma^\mu \gamma^5$, so the time component reverses and the space components do not, an axial vector. For $\Gamma = \sigma^{\mu\nu}$ the components σ^{0i} reverse and σ^{ij} do not, so a contraction of two tensors is even. D contracts a polar vector with an axial vector, which changes sign under parity, so adding it to the vector term leaves no choice of phases that makes both even: this cross term is how the $V - A$ weak interaction violates parity (D). A is tempting to a candidate who suspects a coupling without γ^μ , but $\bar{\psi}\psi$ is a true scalar and a product of two scalars is even. B is tempting because $\sigma^{\mu\nu}$ mixes components of opposite parity, but each component is contracted with one of the same kind, so the product is even. C is tempting because γ^5 marks a pseudo-quantity, but there are two axial vectors, and their two sign changes cancel.

U1

In a uniform static electric field of strength $\mathcal{E}$, the potential energy of an electron changes steadily along the field, so that a positive-energy electron state at one point has the same total energy as a negative-energy state a distance $d = 2mc^2/(e\mathcal{E})$ further along: Sauter's smooth version of the Klein step. In hole theory an electron tunnelling from the filled negative-energy states across this gap leaves a hole behind, so the field creates electron-positron pairs. Take $mc^2 = 0.511$ MeV, the reduced Compton wavelength $\hbar/mc = 3.86 \times 10^{-13}$ m and $e = 1.602 \times 10^{-19}$ C. At about what field strength does pair creation stop being exponentially suppressed?

KEY A About $m^2c^3/(e\hbar) \approx 1.3 \times 10^{18}$ V m $^{-1}$, at which the gap d has shrunk to two reduced Compton wavelengths, so tunnelling across it is no longer suppressed.

Tunnelling through a forbidden gap is exponentially suppressed unless the gap is no wider than the decay length of the wavefunction inside it, which for an electron between the two continua is of order $\hbar/mc$. Setting $d = 2mc^2/(e\mathcal{E})$ equal to $2\hbar/mc$ gives $\mathcal{E} = mc^2/(e \times \hbar/mc) = m^2c^3/(e\hbar) = 0.511 \times 10^6$ V/3.86 $\times 10^{-13}$ m = 1.3×10^{18} V m $^{-1}$, the critical field; below it the pair-creation rate carries the factor $\exp(-\pi m^2c^3/(e\hbar\mathcal{E}))$ (A). C applies Klein's sharp-step result to a smooth field. An abrupt step higher than $2mc^2$ does transmit freely, but only because it is sharper than $\hbar/mc$; spreading the same rise over a macroscopic distance makes the gap wide and the transmission vanishingly small, which is why laboratory fields do not break down the vacuum. B and D choose the wrong length. The Bohr radius has nothing to do with the vacuum, whose electrons are the negative-energy sea everywhere, and the field it gives is about 70 times too weak. The classical electron radius is α times the reduced Compton wavelength, so it gives a field about 270 times too strong.

U1

A free complex scalar field and a free Dirac field are each quantised in two ways: with commutators and with anticommutators of their mode operators. Two requirements are imposed: a Hamiltonian bounded below on a space of states of positive norm, and local observables that commute at spacelike separation. Which statement is correct?

KEY B The Dirac field with commutators has an energy unbounded below, or states of negative norm if creators and annihilators are relabelled, while the scalar field with anticommutators fails microcausality; only the scalar with commutators and the Dirac field with anticommutators pass both tests.

B is correct, and the two failures are different in kind. Quantised canonically with commutators, the Dirac field has mode operators with $[b, b^\dagger] = [d, d^\dagger] = 1$, where d multiplies the negative-frequency modes, and $H = \sum E_p(b^\dagger b - d^\dagger d)$: every quantum that $d^\dagger$ creates lowers the energy, without limit. Making $d^\dagger$ the annihilation operator instead, to cure this, turns its commutator with its adjoint into -1 and gives states of negative norm. The canonical commutator of the Dirac field is nevertheless causal, so A puts the Dirac field's failure in the wrong place, and the positive energy it claims is exactly what commutators cannot deliver on states of positive norm. For the scalar field the failure is of the other kind: anticommutators replace the commutator $D(x - y) - D(y - x)$ by the anticommutator $D(x - y) + D(y - x)$, which does not vanish at spacelike separation, and local observables built from the field then fail to commute there, so measurements outside each other's light cones would interfere. C repeats the commonest misconception of the unit: the propagation amplitude $D(x - y)$ does not vanish outside the light cone, falling only as $e^{-(mcr/\hbar)}$; only the commutator, in which the antiparticle term cancels it, vanishes. D offers a heuristic rather than the argument: the limit on occupation is a consequence of anticommutators, not the reason they are excluded, and the decisive failure is causality.

U1

7

CORE
COURSE

MULTIPLE CHOICE · ROUTINE · UAQM-10.01 · UAQM-10.03

[1]

Three fermion orbitals are ordered 1, 2, 3, and occupation-number states are defined by $|n_1 n_2 n_3\rangle = (c_1^\dagger)^{n_1} (c_2^\dagger)^{n_2} (c_3^\dagger)^{n_3} |0\rangle$, with $\{c_i, c_j^\dagger\} = \delta_{ij}$ and $\{c_i, c_j\} = 0$. The one-body operator $T = t(c_3^\dagger c_1 + c_1^\dagger c_3)$ moves a fermion between orbitals 1 and 3. What is $T|1 1 0\rangle$?

KEY **D** $-t|0 1 1\rangle$

The term $c_1^\dagger c_3$ gives zero because orbital 3 is empty. In the other term, c_1 acting on $c_1^\dagger c_2^\dagger |0\rangle$ gives $c_2^\dagger |0\rangle$, and $c_3^\dagger$ must then be moved past $c_2^\dagger$ to reach its standard place on the right of the product: $c_3^\dagger c_2^\dagger |0\rangle = -c_2^\dagger c_3^\dagger |0\rangle = -|0 1 1\rangle$. So $T|1 1 0\rangle = -t|0 1 1\rangle$ (D). The sign is -1 raised to the number of occupied orbitals between the two that the fermion moves between, and it is physical: on a ring or a lattice it decides whether a hopping process lowers or raises the energy. A is the answer of a candidate who moves the electron but not the operator, which is what a product wavefunction without antisymmetry would give. B treats the occupied orbital as an obstacle; the hop is between orbitals, not along a line, and orbital 2 contributes only a sign. C moves the wrong fermion: $c_3^\dagger c_1$ empties orbital 1, so the final state must have $n_1 = 0$.

U2

8

CORE
COURSE

MULTIPLE CHOICE · ROUTINE · UAQM-11.07

[1]

A single mode of the quantised field is prepared first in the number state $|n = 4\rangle$ and then in the coherent state $|\alpha\rangle$ with $|\alpha|^2 = 4$. Its normalised second-order correlation at zero delay is $g^{(2)}(0) = \langle a^\dagger a^\dagger a a \rangle / \langle a^\dagger a \rangle^2$. What are the two values of $g^{(2)}(0)$, number state first?

KEY **C** **0.75 and 1**

For a number state $a^\dagger a^\dagger a a |n\rangle = n(n-1)|n\rangle$, so $g^{(2)}(0) = n(n-1)/n^2 = 1 - 1/n = 0.75$. For a coherent state $a|\alpha\rangle = \alpha|\alpha\rangle$, so $\langle a^\dagger a^\dagger a a \rangle = |\alpha|^4 = \langle a^\dagger a \rangle^2$ and $g^{(2)}(0) = 1$ whatever $|\alpha|$ is (C). The number state's value below 1 is impossible for any classical field, for which $g^{(2)}(0) = \langle I^2 \rangle / \langle I \rangle^2$ is at least 1 by the Cauchy-Schwarz inequality: it records that once one photon has been detected only three remain. A supposes that $g^{(2)}(0)$ depends only on the mean photon number, which the two states share. B gives the coherent state the value 2 of thermal light, whose photon-number fluctuations are larger than Poissonian. D reasons that a number state has no fluctuations in photon number and so no correlation; its variance is indeed zero, but $g^{(2)}(0) = 1 + (\text{Var } n - \langle n \rangle) / \langle n \rangle^2$, which is $1 - 1/n$, not 0.

U3

9

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MULTIPLE CHOICE · ROUTINE · UAQM-12.08

[1]

A quantum dot emitting at a free-space wavelength $\lambda = 930$ nm sits at the field maximum of a GaAs micropillar cavity of refractive index $n = 3.5$, quality factor $Q = 6000$ and mode volume $V = 1.5(\lambda/n)^3$. Its transition is resonant with the cavity mode and its dipole is parallel to the cavity field. The Purcell factor, the ratio of its emission rate into the cavity mode to its spontaneous emission rate in bulk GaAs, is $F_P = (3/4\pi^2)(\lambda/n)^3(Q/V)$. What is F_P ?

KEY **A** **304**

With $V = 1.5(\lambda/n)^3$ the factor $(\lambda/n)^3/V$ is $1/1.5$, so $F_P = 3 \times 6000 / (4\pi^2 \times 1.5) = 304$ (A): the dot emits into the single cavity mode about 300 times faster than into the continuum of modes of bulk GaAs. B uses the free-space λ^3 against a mode volume measured in units of $(\lambda/n)^3$, which inflates the result by $n^3 = 42.9$; the wavelength that matters is the one in the medium, because the bulk rate it is compared with is the rate inside GaAs. C omits the factor $3/4\pi^2$, which comes from comparing one mode, of linewidth ω/Q , with the density of modes summed over all directions and both polarisations, as in the A coefficient. D overlooks that the dipole moment enters both rates as $|d|^2$ and cancels from their ratio: the Purcell factor belongs to the cavity, and the emitter has only to sit at the field maximum, aligned and on resonance.

U3

In Hartree-Fock theory the energy per electron of the uniform electron gas, in rydbergs, is $E/N = 2.21/r_s^2 - 0.916/r_s$, where r_s is the radius, in Bohr radii, of the sphere that contains one electron, and $1 \text{ Ry} = 13.61 \text{ eV}$. The conduction electrons of lithium have $r_s = 3.25$. What is E/N at lithium's density, and how does that density compare with the density at which the Hartree-Fock E/N is lowest?

KEY D $E/N = -0.073 \text{ Ry} (-0.99 \text{ eV})$, and lithium's electron gas is denser than at the Hartree-Fock minimum.

At $r_s = 3.25$ the kinetic term is $2.21/10.56 = +0.209 \text{ Ry}$ and the exchange term is $-0.916/3.25 = -0.282 \text{ Ry}$, so $E/N = -0.073 \text{ Ry}$, or -0.99 eV . Setting $d(E/N)/dr_s = -4.42/r_s^3 + 0.916/r_s^2 = 0$ puts the Hartree-Fock minimum at $r_s = 4.42/0.916 = 4.83$. Lithium's r_s is smaller, and the electron density, $3/(4\pi r_s^3 a_0^3)$, rises as r_s falls, so lithium's electron gas is denser than the Hartree-Fock optimum (D): in this approximation, and on its own, it would push outward on the positive background that holds it. A has the right energy but reads a larger r_s as a higher density, forgetting that r_s is the radius of the volume each electron occupies. B keeps only the exchange term, forgetting the kinetic energy that opposes it. C keeps only the kinetic energy, which is the whole story only for electrons that do not interact. What actually binds lithium also involves the ions, which jellium smears into a uniform background, and correlation, quoted rather than derived in the course.

U3

A negative muon, a spin-half Dirac particle of charge $q = -e$ and mass m about 207 times the electron's, is captured by a lead nucleus, ^{208}Pb ($Z = 82$), and cascades to the $1s$ orbit of muonic lead. That orbit is so small that the muon spends most of its time inside the nucleus, modelled as a uniformly charged sphere of radius $R = 7.1 \text{ fm}$, where its potential energy is $V(r) = -(Z\alpha\hbar c/R)(3/2 - r^2/2R^2)$. In static potentials ϕ and A its Dirac Hamiltonian is $H = c\alpha \cdot \pi + \beta mc^2 + q\phi$, with $\pi = p - qA$, $p = -i\hbar\nabla$ and $V = q\phi$. In the Dirac representation, writing a stationary state as $e^{-i(mc^2 + W)t/\hbar}$ times the column (ξ, χ) of upper and lower two-component spinors, $H\psi = (mc^2 + W)\psi$ becomes $(W - V)\xi = c\sigma \cdot \pi \chi$ and $(W - V + 2mc^2)\chi = c\sigma \cdot \pi \xi$. Pauli's anomalous-moment term adds to H , in a magnetic field B , the operator $-a(q\hbar/2m)\beta\Sigma \cdot B$, where $\Sigma = \text{diag}(\sigma, \sigma)$. For vector operators a and b that commute with the Pauli matrices, $(\sigma \cdot a)(\sigma \cdot b) = a \cdot b + i\sigma \cdot (a \times b)$, and for any function $f(r)$, $pf - fp = -i\hbar\nabla f$. In a storage-ring measurement of the anomaly, muons of Lorentz factor $\gamma = 29.3$ circulate in a uniform field $B = 1.4513 \text{ T}$, with no electric field acting on them, and the rate of their decay positrons oscillates at the frequency $\omega_a/2\pi = 229.08 \text{ kHz}$ at which the spin turns relative to the momentum. Take $mc^2 = 105.66 \text{ MeV}$, $m = 1.8835 \times 10^{-28} \text{ kg}$, $\hbar c = 197.33 \text{ MeV fm}$, $\alpha = 1/137.036$, $e = 1.602 \times 10^{-19} \text{ C}$ and the muon's lifetime at rest $\tau = 2.197 \mu\text{s}$.

(a) SHOW THAT · U2

Show that the Dirac equation $i\hbar\partial\psi/\partial t = H\psi$ keeps its form under the gauge transformation $A \rightarrow A + \nabla\Lambda$, $\phi \rightarrow \phi - \partial\Lambda/\partial t$, for any smooth function $\Lambda(r, t)$, provided that $\psi \rightarrow e^{i(q\Lambda/\hbar)}\psi$.

- 1 $p(e^{i(q\Lambda/\hbar)}\psi) = e^{i(q\Lambda/\hbar)}(p + q\nabla\Lambda)\psi$, so $(p - qA)\psi' = e^{i(q\Lambda/\hbar)}(p - qA)\psi$: the kinetic momentum acting on ψ' is the phase times π acting on ψ , and $c\alpha \cdot \pi$ and βmc^2 pass through the phase unchanged
- 2 $i\hbar\partial\psi'/\partial t = e^{i(q\Lambda/\hbar)}(i\hbar\partial\psi/\partial t - q(\partial\Lambda/\partial t)\psi)$, and the extra term $-q(\partial\Lambda/\partial t)\psi'$ is exactly the change $q\phi' - q\phi = -q\partial\Lambda/\partial t$ in the potential energy, so ψ' obeys the same equation with the new potentials

Candidates who use a constant phase, or the wrong sign in the exponent, cannot cancel both the gradient and the time-derivative terms. The point of minimal coupling is that p and the energy enter only as $p - qA$ and $i\hbar\partial/\partial t - q\phi$, so a local phase on ψ is absorbed by the potentials.

(b) ESTIMATE · U4**[2]**

Inside the nucleus V is the potential energy of a three-dimensional harmonic oscillator. Estimate, stating your assumptions, the oscillator quantum $\hbar\omega$, the muon's speed in the $1s$ state as a fraction of c and hence the size of χ relative to ξ , and judge whether an expansion in v/c is trustworthy for muonic lead.

- 1 assuming the $1s$ muon lies mostly inside the nucleus, $V = V(0) + \frac{1}{2}kr^2$ with $k = Z\alpha\hbar c/R^3$, so $\hbar\omega = \hbar c\sqrt{(Z\alpha\hbar c/(mc^2R^3))} = 197.33 \text{ MeV fm} \times \sqrt{(0.5984 \times 197.33 \text{ MeV fm}/(105.66 \text{ MeV} \times 357.9 \text{ fm}^3))} \approx 11.0 \text{ MeV}$, and the oscillator length $\sqrt{(\hbar/m\omega)} \approx 5.8 \text{ fm}$, less than $R = 7.1 \text{ fm}$, supports the assumption
- 2 with $\langle T \rangle = \frac{3}{4}\hbar\omega \approx 8.3 \text{ MeV}$, $v^2/c^2 \approx 2\langle T \rangle/mc^2 \approx 0.16$ and $v/c \approx 0.4$; the lower equation gives $\chi \approx (\sigma \cdot p/2mc)\xi$, so $|\chi|/|\xi| \approx v/2c \approx 0.2$ and χ carries about 4% of the probability: the expansion converges, but its order- $(v/c)^2$ terms are corrections of order 15%, not the parts in 10^5 of hydrogen

Candidates who carry hydrogen's $v/c \approx \alpha$ across to muonic lead miss the point. The muon's speed is set by the nuclear charge it sits inside, not by the mass ratio, and at $v/c \approx 0.4$ the relativistic corrections are large though still perturbative.

(c) DERIVE · U2**[3]**

For a slow muon in a uniform magnetic field B , with $A = \frac{1}{2}B \times r$ and no electric field, eliminate χ to leading order in v/c and derive the Hamiltonian for ξ to first order in B . Hence find the g -factors with which the orbital angular momentum $L = r \times p$ and the spin $S = (\hbar/2)\sigma$ couple to B under minimal coupling alone, and the spin g -factor once Pauli's term is included.

- 1 with $V = 0$ and W neglected beside $2mc^2$, the lower equation gives $\chi \approx (\sigma \cdot \pi/2mc)\xi$, so $W\xi = (\sigma \cdot \pi)^2\xi/2m$; $(\sigma \cdot \pi)^2 = \pi^2 + i\sigma \cdot (\pi \times \pi)$, and because the components of π do not commute, $\pi \times \pi = -q(p \times A + A \times p) = iq\hbar\nabla \times A = iq\hbar B$, so $(\sigma \cdot \pi)^2 = \pi^2 - q\hbar\sigma \cdot B$
- 2 with $A = \frac{1}{2}B \times r$, $\nabla \cdot A = 0$, so $p \cdot A = A \cdot p$ and $\pi^2 = p^2 - 2qA \cdot p + q^2A^2$, where $2A \cdot p = (B \times r) \cdot p = B \cdot L$; to first order in B , $H = p^2/2m - (q/2m)L \cdot B - (q/m)S \cdot B$: an orbital moment $(q/2m)L$, with $g_L = 1$, and a spin moment $(q/m)S = g(q/2m)S$, with $g = 2$
- 3 the upper block of $\beta\Sigma \cdot B$ is $\sigma \cdot B$, so Pauli's term adds $-a(q\hbar/2m)\sigma \cdot B = -a(q/m)S \cdot B$, making the spin term $-(1+a)(q/m)S \cdot B$ and $g = 2(1+a)$ while leaving the orbital term alone; a is a parameter the Dirac equation itself does not fix

Candidates who write $\pi \times \pi = 0$, as for ordinary vectors, lose the spin term entirely: the components of π do not commute in a magnetic field, and that is the whole origin of $g = 2$. Those who drop $p \cdot A$ halve the orbital term. Setting the two terms side by side shows the factor of two between spin and orbit that (d) exploits, and that the anomaly enters only through Pauli's term.

(d) CALCULATE · U3**[2]**

For a slow muon the Pauli Hamiltonian makes the spin precess at $\omega_s = g|q|B/2m$ while the momentum turns at $\omega_c = |q|B/m$, so the spin turns relative to the momentum at $\omega_a = a|q|B/m$; with no electric field the Thomas-BMT equation shows that this holds at any speed. Calculate a for the muon from the storage-ring measurement, and the number of cycles of the positron-rate oscillation in one dilated lifetime $\gamma\tau$.

- 1 $a = \omega_a m/(eB) = 2\pi \times 229.08 \times 10^3 \text{ s}^{-1} \times 1.8835 \times 10^{-28} \text{ kg}/(1.602 \times 10^{-19} \text{ C} \times 1.4513 \text{ T}) = 1.166 \times 10^{-3}$
- 2 $\gamma\tau = 29.3 \times 2.197 \mu\text{s} = 64.4 \mu\text{s}$, so the positron rate completes $229.08 \text{ kHz} \times 64.4 \mu\text{s} \approx 14.7$ cycles per dilated lifetime, enough to fit the frequency directly rather than measuring ω_s and ω_c separately

Candidates who divide by γm rather than m come out a factor 29 too large. The anomalous precession involves the rest mass, which is why a measurement on fast muons gives a directly, while time dilation lets many cycles be counted.

(e) SHOW THAT · U2

[3]

The Foldy-Wouthuysen reduction to order $(v/c)^2$ contains the even term $-(1/8m^2c^4)[O, [O, V]]$, where $O = c\alpha \cdot p$ is the odd part of H when $A = 0$. Show that for a static V this term equals $(\hbar^2/8m^2c^2)\nabla^2V + (\hbar/4m^2c^2)\Sigma \cdot (\nabla V \times p)$, and that inside the uniformly charged nucleus the Darwin part is the constant $3Z\alpha(\hbar c)^3/(8(mc^2)^2R^3)$. Evaluate it for muonic lead.

- 1 $[O, V] = c\alpha_j[p_j, V] = -i\hbar c\alpha \cdot \nabla V$, so $[O, [O, V]] = -i\hbar c^2\Sigma_{jk}[\alpha_j p_j, \alpha_k \partial_k V]$; using $p_j \partial_k V = (\partial_k V)p_j - i\hbar \partial_j \partial_k V$ this is $-i\hbar c^2\Sigma_{jk}[(\alpha_j \alpha_k - \alpha_k \alpha_j)(\partial_k V)p_j - i\hbar \alpha_j \alpha_k \partial_j \partial_k V]$
- 2 with $\alpha_j \alpha_k = \delta_{jk} + i\epsilon_{jkl}\Sigma_l$ the symmetric part gives $-\hbar^2 c^2 \nabla^2 V$ and the antisymmetric part $-2\hbar c^2 \Sigma \cdot (\nabla V \times p)$, so $-(1/8m^2c^4)[O, [O, V]] = (\hbar^2/8m^2c^2)\nabla^2V + (\hbar/4m^2c^2)\Sigma \cdot (\nabla V \times p)$
- 3 inside the sphere $dV/dr = Z\alpha\hbar c/R^3$, so $\nabla^2V = (1/r^2)d(r^2dV/dr)/dr = 3Z\alpha\hbar c/R^3$ and the Darwin term is $3Z\alpha(\hbar c)^3/(8(mc^2)^2R^3) = 3 \times 0.5984 \times (197.33 \text{ MeV fm})^3/(8 \times (105.66 \text{ MeV})^2 \times 357.9 \text{ fm}^3) \approx 0.43 \text{ MeV}$, a uniform upward shift wherever the muon is inside the nucleus

Candidates who carry over the hydrogen result, a delta function at the origin, miss that ∇^2V is proportional to the charge density producing V . For a point nucleus the Darwin term is a contact term; a muon inside a uniform nucleus feels it everywhere as a constant.

(f) EXPLAIN · U1

[2]

The $1s$ and $2s$ states of muonic lead are orthogonal four-component spinors. Using your estimate from (b), explain why their upper components ξ_{1s} and ξ_{2s} cannot be eigenfunctions of any Hermitian Hamiltonian at order $(v/c)^2$, so that no two-component Schrödinger equation for ξ can be exact to that order, and what the Foldy-Wouthuysen transformation does instead.

- 1 orthonormality belongs to the whole spinor, $\int(\xi_{1s}^\dagger \xi_{2s} + \chi_{1s}^\dagger \chi_{2s})d^3r = 0$, and with $\chi \approx (\sigma \cdot p/2mc)\xi$ this gives $\int \xi_{1s}^\dagger \xi_{2s} d^3r \approx -\langle \xi_{1s} | p^2 | \xi_{2s} \rangle / (4m^2c^2)$, which is not zero, while $\int \xi_{1s}^\dagger \xi_{1s} d^3r \approx 1 - \langle p^2 \rangle / (4m^2c^2) \approx 0.96$; eigenfunctions of a Hermitian operator belonging to different eigenvalues are orthogonal, so no such operator has the ξ as its eigenfunctions, and expanding $1/(W - V + 2mc^2)$ one step further gives instead an operator that depends on the energy W
- 2 the Foldy-Wouthuysen transformation is unitary, so it keeps the spinors orthonormal while removing the odd operators order by order; the upper components of the transformed spinors, $\Phi \approx [1 + p^2/(8m^2c^2)]\xi$ to this order, are orthonormal two-component functions obeying one energy-independent Hermitian Hamiltonian, which contains the Darwin and spin-orbit terms of (e)

Candidates who treat the upper components as non-relativistic wavefunctions have forgotten that orthonormality belongs to the whole spinor; renormalising each ξ separately repairs the norms but not the overlaps. With 4% of the $1s$ probability in χ , as in muonic lead, the defect is as large as the order- $(v/c)^2$ terms being sought.

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[12]

The Lyman- α X-rays of hydrogen-like uranium, U^{91+} ($Z = 92$), emitted when bare uranium nuclei circulating in a heavy-ion storage ring capture an electron that cascades to the ground state, test the Dirac-Coulomb spectrum where $Z\alpha$ is not small. The two lines are $Ly\alpha 1$, $2p_{3/2} \rightarrow 1s_{1/2}$, and $Ly\alpha 2$, $2p_{1/2} \rightarrow 1s_{1/2}$, and spectroscopy of the stored ions places $Ly\alpha 1$ at 102.17 keV. In a central potential $V(r)$ the radial functions $G(r)$ and $F(r)$ of the upper and lower components satisfy $dG/dr = -(\kappa/r)G + [(E + mc^2 - V)/\hbar c]F$ and $dF/dr = (\kappa/r)F - [(E - mc^2 - V)/\hbar c]G$, where E includes mc^2 , $\kappa = (l - j)(2j + 1)$ and l is the orbital angular momentum of the upper component. For a point nucleus $V = -Z\alpha\hbar c/r$, and the exact energies are $E_{nj} = mc^2[1 + (Z\alpha)^2/(n - |\kappa| + \gamma)^2]^{-1/2}$, with $\gamma = \sqrt{\kappa^2 - (Z\alpha)^2}$. The normalised point-nucleus $1s$ density, both components together, is $|\psi_{1s}(r)|^2 = [(2Z/a_0)^{2\gamma+1}/(4\pi\Gamma(2\gamma + 1))]r^{2\gamma-2}e^{-(2Zr/a_0)}$, with $\Gamma(2\gamma + 1) = 1.313$ for $Z = 92$, while the Schrödinger $1s$ density is $(Z^3/\pi a_0^3)e^{-(2Zr/a_0)}$. The uranium nucleus has its surface at about $r = 7.5 \text{ fm}$ and is treated as infinitely heavy. Take $mc^2 = 510.999 \text{ keV}$, $\alpha = 1/137.036$ and $a_0 = 5.2918 \times 10^{-4} \text{ fm}$.

(a) STATE · U1

[2]

State which conserved operator takes the place of L^2 in labelling the electron's states, and state κ and the orbital angular momentum l' of the lower component for each of $1s_{1/2}$, $2p_{1/2}$ and $2p_{3/2}$, saying which of their components are s waves, able to reach the nucleus.

- 1 L does not commute with H , because $\alpha \cdot p$ couples an upper component of orbital angular momentum l to a lower one of $l' = 2j - l$; together with J^2 , J_z and parity, $K = \beta(\Sigma \cdot L + \hbar)$ commutes with H , and its eigenvalue $-\kappa\hbar$ labels the state, $|\kappa| = j + \frac{1}{2}$ giving j and the sign of κ telling whether the upper component has $l = j - \frac{1}{2}$ ($\kappa < 0$) or $l = j + \frac{1}{2}$ ($\kappa > 0$)
- 2 $\kappa = -1$ for $1s_{1/2}$, $+1$ for $2p_{1/2}$ and -2 for $2p_{3/2}$, with $l' = 1, 0$ and 2 : the s waves are the upper component of $1s_{1/2}$ and the lower component of $2p_{1/2}$, so both reach the nucleus, while $2p_{3/2}$, with $l = 1$ and $l' = 2$, has none

Candidates who treat $2p_{1/2}$ as a pure p state miss that its lower component is an s wave, which is what makes a $p_{1/2}$ level, unlike $p_{3/2}$, sensitive to the nucleus of a heavy ion. Only the upper component has orbital angular momentum l ; the state as a whole is labelled by κ .

(b) DERIVE · U2

[3]

Derive from the radial equations how G and F rise from the origin. For the point nucleus, writing $G \approx ar^\gamma$ and $F \approx br^\gamma$, find γ and b/a , evaluate b/a for $1s_{1/2}$ and for $2p_{1/2}$ at $Z = 92$, and say which component dominates near the nucleus in each. Then find the powers of r with which G and F rise inside a nucleus of finite size, where $V(r)$ tends to a finite $V(0)$.

- 1 for the point nucleus the Coulomb term is as singular as κ/r and dominates $E \pm mc^2$, and the $r^{\gamma-1}$ terms give $(\gamma + \kappa)a = Z\alpha b$ and $(\gamma - \kappa)b = -Z\alpha a$, which have a nonzero solution only if $\gamma^2 = \kappa^2 - (Z\alpha)^2$; the positive root $\gamma = \sqrt{\kappa^2 - (Z\alpha)^2}$ keeps the density normalisable, and $b/a = (\gamma + \kappa)/(Z\alpha)$
- 2 at $Z = 92$, $Z\alpha = 0.6714$ and $\gamma = \sqrt{1 - 0.4507} = 0.7411$ for $|\kappa| = 1$, so $b/a = (0.7411 + 1)/0.6714 = +2.59$ for $2p_{1/2}$, the s-wave lower component outweighing the upper one near the nucleus, and $b/a = (0.7411 - 1)/0.6714 = -0.386$ for $1s_{1/2}$, the upper component dominating; both components share the non-integer power, so G/r and F/r diverge weakly, as $r^{\gamma-1} = r^{-0.26}$
- 3 inside a finite nucleus V stays finite, so near the origin only the κ/r terms are singular: for $\kappa < 0$, $G \propto r^{-(\kappa)} = r^{(l+1)}$ and $F \propto r^{-(l+2)} = r^{(l'+1)}$, and for $\kappa > 0$, $F \propto r^\kappa = r^{(l'+1)}$ and $G \propto r^{(\kappa+1)} = r^{(l+1)}$; the integer powers of the non-relativistic problem return, each component with its own orbital angular momentum, and the singularity of the point nucleus is removed

Candidates who drop the Coulomb term against κ/r near a point nucleus recover the integer powers $r^{(l+1)}$ and $r^{(l'+1)}$, which hold only inside a finite nucleus. For the point nucleus the two terms are of the same order, both components share the non-integer power γ , and for $2p_{1/2}$ the small component is not small near the origin.

(c) CALCULATE · U3

[2]

Calculate, for a point nucleus, the energies of $Ly\alpha_1$ and $Ly\alpha_2$ in keV, and the 2p fine-structure splitting.

- 1 $E_{1s} = \gamma mc^2 = 0.74113 \times 510.999 \text{ keV} = 378.72 \text{ keV}$; for $2p_{1/2}$, $n - |\kappa| + \gamma = 1.7411$ and $E = 510.999 \text{ keV}/\sqrt{1 + 0.4507/3.0315} = 476.78 \text{ keV}$; for $2p_{3/2}$, $\gamma = \sqrt{4 - 0.4507} = 1.8840$ and $E = 510.999 \text{ keV}/\sqrt{1 + 0.4507/3.5493} = 481.35 \text{ keV}$
- 2 $Ly\alpha_1 = 481.35 \text{ keV} - 378.72 \text{ keV} = 102.63 \text{ keV}$ and $Ly\alpha_2 = 476.78 \text{ keV} - 378.72 \text{ keV} = 98.06 \text{ keV}$, a fine-structure splitting of 4.57 keV, where the non-relativistic theory gives one line at $(3/8)(Z\alpha)^2 mc^2 = 86.4 \text{ keV}$

Candidates who use the Bohr formula find a single line at 86.4 keV, 16% low, with no splitting. At $Z\alpha = 0.67$ the exact formula is needed, and the differences of large energies must be taken to five figures.

(d) DETERMINE · U3

[2]

Treating the $2p_{3/2}$ level as given correctly by the point-nucleus formula, determine from the measured $\text{Ly}\alpha 1$ energy the shift of the $1s$ level that the point-nucleus Dirac theory omits, its sign, and its size as a fraction of the $1s$ binding energy.

- 1 the measured line lies $102.63 \text{ keV} - 102.17 \text{ keV} = 0.46 \text{ keV}$ below the point-nucleus value, so with $2p_{3/2}$ fixed the $1s$ level lies about 0.46 keV higher, less bound, than the point-nucleus Dirac prediction
- 2 the $1s$ binding energy is $mc^2 - E_{1s} = 510.999 \text{ keV} - 378.72 \text{ keV} = 132.28 \text{ keV}$, so the shift is $0.46/132.28 = 0.35\%$ of it, the combined effect of the nucleus's finite size and of the radiative corrections of quantum electrodynamics, which together raise the s level

Candidates who give the shift the wrong sign, or put it down to experimental error, miss what the line measures. The $2p_{3/2}$ level barely overlaps the nucleus, so $\text{Ly}\alpha 1$ isolates the ground-state shift and tests quantum electrodynamics where $Z\alpha$ is close to 1.

(e) COMPARE · U3

[2]

Compare the Dirac $1s$ density at the nuclear surface, $r = 7.5 \text{ fm}$, with the Schrödinger $1s$ density there, and say what the comparison implies for the finite-size part of the shift found in (d).

- 1 the exponentials cancel and the ratio is $[2/\Gamma(2\gamma + 1)](2Zr/a_0)^{(2\gamma-2)}$; with $2Zr/a_0 = 2 \times 92 \times 7.5 \text{ fm}/(5.2918 \times 10^4 \text{ fm}) = 0.0261$ and $2\gamma - 2 = -0.518$ it is $(2/1.313) \times 0.0261^{(-0.518)} \approx 10$
- 2 the weak singularity $r^{(2\gamma-2)}$ puts about ten times more of the Dirac electron's density inside the nucleus than the Schrödinger estimate, so the finite-size shift is about ten times what a non-relativistic calculation gives and makes up a substantial part of the 0.46 keV

Candidates who take the density at the nucleus from the Schrödinger formula, as is fine for hydrogen, underestimate the overlap with the nucleus tenfold. The factor $r^{(2\gamma-2)}$ is harmless to the normalisation but not to anything that samples the nuclear volume.

(f) PREDICT · U1

[1]

In the point-nucleus Dirac theory $2s_{1/2}$ and $2p_{1/2}$ are exactly degenerate. Predict which of the two the finite size of the nucleus raises more, and so which lies higher.

- 1 $2s_{1/2}$, whose s wave is the large upper component, overlaps the nucleus far more than $2p_{1/2}$, whose s wave is the lower component that is small over most of the orbit, so $2s_{1/2}$ is raised more and lies above $2p_{1/2}$, in the same direction as the radiative Lamb shift

Candidates who reason from (b), where the lower component of $2p_{1/2}$ dominates near the origin, may predict the reverse. The ratio b/a fixes the shape near the origin, but the normalisation over the whole orbit, where the upper component dominates, makes the $2p_{1/2}$ density at the nucleus much smaller than that of $2s_{1/2}$.

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[12]

A free complex scalar field $\phi(x, t)$, with ϕ and $\phi^\dagger$ treated as independent fields, describes spinless particles of mass m and charge q through the Lagrangian density $\mathcal{L} = (1/c^2)(\partial\phi^\dagger/\partial t)(\partial\phi/\partial t) - \nabla\phi^\dagger \cdot \nabla\phi - \kappa^2\phi^\dagger\phi$, where $\kappa = mc/\hbar$. In a box of volume V with periodic boundary conditions the quantised field is $\phi(x, t) = \sum_{\mathbf{k}} N_{\mathbf{k}} [a_{\mathbf{k}} e^{i(\mathbf{k}\cdot\mathbf{x} - \omega_{\mathbf{k}} t)} + b_{\mathbf{k}}^\dagger e^{-i(\mathbf{k}\cdot\mathbf{x} - \omega_{\mathbf{k}} t)}]$, with $\omega_{\mathbf{k}} = c\sqrt{k^2 + \kappa^2}$, $N_{\mathbf{k}} = \sqrt{(\hbar c^2/(2\omega_{\mathbf{k}}V))}$, $[a_{\mathbf{k}}, a_{\mathbf{k}'}^\dagger] = [b_{\mathbf{k}}, b_{\mathbf{k}'}^\dagger] = \delta_{\mathbf{k}\mathbf{k}'}$ and all other commutators zero. After normal ordering the Hamiltonian is $H = \sum_{\mathbf{k}} \hbar\omega_{\mathbf{k}}(a_{\mathbf{k}}^\dagger a_{\mathbf{k}} + b_{\mathbf{k}}^\dagger b_{\mathbf{k}})$. Take $\hbar c = 197.3 \text{ MeV fm}$.

(a) DERIVE · U2

[3]

Apply the Euler-Lagrange equation for $\phi^\dagger$ to derive the field equation for ϕ , and use it to show that the density $\rho = (iq/\hbar c^2)(\phi^\dagger \partial \phi / \partial t - \phi \partial \phi^\dagger / \partial t)$ and the current $j = -(iq/\hbar)(\phi^\dagger \nabla \phi - \phi \nabla \phi^\dagger)$ satisfy $\partial \rho / \partial t + \nabla \cdot j = 0$.

- 1 $\partial \mathcal{L} / \partial (\partial_t \phi^\dagger) = (1/c^2) \partial_t \phi$, $\partial \mathcal{L} / \partial (\nabla \phi^\dagger) = -\nabla \phi$ and $\partial \mathcal{L} / \partial \phi^\dagger = -\kappa^2 \phi$, so $\partial_t [\partial \mathcal{L} / \partial (\partial_t \phi^\dagger)] + \nabla \cdot [\partial \mathcal{L} / \partial (\nabla \phi^\dagger)] - \partial \mathcal{L} / \partial \phi^\dagger = 0$ gives $(1/c^2) \partial^2 \phi / \partial t^2 - \nabla^2 \phi + \kappa^2 \phi = 0$, the Klein-Gordon equation, with its conjugate for $\phi^\dagger$
- 2 $\partial \rho / \partial t = (iq/\hbar c^2)(\phi^\dagger \partial^2 \phi - \phi \partial^2 \phi^\dagger)$, the products of first time derivatives cancelling, and likewise $\nabla \cdot j = -(iq/\hbar)(\phi^\dagger \nabla^2 \phi - \phi \nabla^2 \phi^\dagger)$
- 3 substituting $\partial^2 \phi = c^2(\nabla^2 \phi - \kappa^2 \phi)$ and its conjugate, the κ^2 terms cancel and $\partial \rho / \partial t = (iq/\hbar)(\phi^\dagger \nabla^2 \phi - \phi \nabla^2 \phi^\dagger) = -\nabla \cdot j$: the current is conserved, the Noether current of the symmetry $\phi \rightarrow e^{(-i\theta)} \phi$

Candidates who treat ϕ and $\phi^\dagger$ as one real field lose the conserved charge altogether, since a real field has no phase to rotate. Varying with respect to ϕ instead gives the equation for $\phi^\dagger$, which is equally valid once conjugated.

(b) SHOW THAT · U2

[3]

By substituting the mode expansion, show that after normal ordering the charge $Q = \int \rho d^3x$ is $q \sum_k (a_{k\dagger} a_k - b_k b_{k\dagger})$, and hence that $a_{k\dagger}$ creates a quantum of charge $+q$ and $b_{k\dagger}$ one of charge $-q$, each with energy $\hbar \omega_k$.

- 1 $\int e^{i(k-k') \cdot x} d^3x = V \delta_{kk'}$ pairs each operator with one of the same mode or of the opposite mode, and the terms in $a_k b_{-k} e^{(-2i\omega_k t)}$ and in $a_{k\dagger} b_{-k\dagger} e^{(2i\omega_k t)}$ enter $\phi^\dagger \partial_t \phi$ and $\phi \partial_t \phi^\dagger$ with the same coefficient and cancel, so Q is independent of time
- 2 each mode then contributes $(iq/\hbar c^2)(-i\omega_k) N_k V (a_{k\dagger} a_k + a_k a_{k\dagger} - b_k b_{k\dagger} - b_{k\dagger} b_k) = (q/2)(a_{k\dagger} a_k + a_k a_{k\dagger} - b_k b_{k\dagger} - b_{k\dagger} b_k)$, since $\omega_k N_k V / \hbar c^2 = 1/2$; normal ordering gives $Q = q \sum_k (a_{k\dagger} a_k - b_k b_{k\dagger})$
- 3 $[Q, a_{k\dagger}] = q a_{k\dagger}$ and $[Q, b_{k\dagger}] = -q b_{k\dagger}$, so $a_{k\dagger}|0\rangle$ has charge $+q$ and $b_{k\dagger}|0\rangle$ charge $-q$, while $[H, a_{k\dagger}] = \hbar \omega_k a_{k\dagger}$ and $[H, b_{k\dagger}] = \hbar \omega_k b_{k\dagger}$ give both the energy $\hbar \omega_k$: the antiparticle has the opposite charge and a positive energy

Candidates who keep only the a-terms find a charge of one sign and miss the antiparticles; those who expect b-quanta to have negative energy have confused the sign of the charge with the sign of the energy, which H fixes as positive.

(c) EXPLAIN · U1

[2]

The field commutator is $[\phi(x), \phi^\dagger(y)] = D(x-y) - D(y-x)$, where $D(x-y) = \langle 0 | \phi(x) \phi^\dagger(y) | 0 \rangle = \sum_k N_k e^{i(k \cdot (x-y) - \omega_k(t_x - t_y))}$. Explain why the commutator vanishes when $x-y$ is spacelike although $D(x-y)$ does not, and what would go wrong if the field contained the a_k terms alone.

- 1 for spacelike $x-y$, D depends only on the invariant interval (at equal times it is even in $x-y$, by $k \rightarrow -k$), and a proper Lorentz transformation can carry a spacelike $x-y$ into $-(x-y)$; so $D(x-y) = D(y-x)$ and the commutator vanishes, although each term is nonzero
- 2 the second term comes from the b-operators: the amplitude for an antiparticle to travel from x to y cancels that for a particle to travel from y to x ; with the a-terms alone, $[\phi(x), \phi^\dagger(y)] = D(x-y)$, nonzero at spacelike separation, so a measurement at one point could affect another outside its light cone: a relativistic charged field needs its antiparticle

The error this part catches is the belief that nothing propagates outside the light cone. The amplitude does; causality is a property of the commutator, and it is the antiparticle term that secures it.

(d) ESTIMATE · U4 [2]

At equal times and separation r , D is proportional to $(1/r)K_1(kr)$, which for $kr \gg 1$ behaves as $r^{-3/2}e^{-kr}$. For a π^+ , with $mc^2 = 139.6$ MeV, estimate the length $1/k$ over which the amplitude extends outside the light cone, and the factor by which D falls between $r = 5$ fm and $r = 10$ fm, stating your assumptions.

- 1 $1/k = \hbar c/mc^2 = 197.3 \text{ MeV fm}/139.6 \text{ MeV} = 1.41 \text{ fm}$, the pion's reduced Compton wavelength
- 2 assuming the asymptotic form already holds at $kr = 5/1.41 = 3.5$, $D(10 \text{ fm})/D(5 \text{ fm}) \approx (1/2)^{3/2} e^{-5/1.41} = 0.354 \times 0.029 = 0.010$ (the Bessel functions themselves give 0.0098): a hundredfold fall, but never zero

Candidates who keep only the exponential find 0.029, three times too large, since the $r^{-3/2}$ is not negligible over a factor of two in r . That $kr = 3.5$ is only moderately large is an assumption to state, not to hide.

(e) COMPARE · U1 [2]

Compare the density ρ of this question, as an operator of the quantised field, with the same expression read as a probability density in the one-particle Klein-Gordon theory.

- 1 in the one-particle theory the same bilinear (without the factor q) is negative on negative-frequency solutions and can be given either sign by the initial data, so it cannot be a probability density, and the negative-energy solutions have no consistent meaning
- 2 in the field theory it is the charge density: its integral has eigenvalues $q(N_a - N_b)$, negative values counting antiparticles, which have positive energy and states of positive norm; the indefinite sign becomes the two signs of charge, not of probability

The comparison must say what changes and why. Candidates who say the sign problem simply disappears miss that it is reinterpreted: the same indefinite quantity is now a charge, for which both signs are physical.

14
CORE
COURSE

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[12]

Two electrons occupy a molecule of two sites, 1 and 2, each with one orbital, described by the Hubbard Hamiltonian $H = -t \sum_{\sigma} (c_{1\sigma}^\dagger c_{2\sigma} + c_{2\sigma}^\dagger c_{1\sigma}) + U(n_{1\uparrow} n_{1\downarrow} + n_{2\uparrow} n_{2\downarrow})$, with hopping $t = 0.40$ eV and on-site repulsion $U = 3.2$ eV. The operators obey $\{c_{i\sigma}, c_{j\sigma'}^\dagger\} = \delta_{ij} \delta_{\sigma\sigma'}$ and $\{c_{i\sigma}, c_{j\sigma'}\} = 0$. In the sector with $S_z = 0$ a basis is $|D_1\rangle = c_{1\uparrow}^\dagger c_{1\downarrow}^\dagger |0\rangle$ and $|D_2\rangle = c_{2\uparrow}^\dagger c_{2\downarrow}^\dagger |0\rangle$, with both electrons on one site, and $|A\rangle = c_{1\uparrow}^\dagger c_{2\downarrow}^\dagger |0\rangle$ and $|B\rangle = c_{2\uparrow}^\dagger c_{1\downarrow}^\dagger |0\rangle$, with one electron on each.

(a) SHOW THAT · U2 [3]

Show that the hopping term T sends both $|A\rangle$ and $|B\rangle$ to $-t(|D_1\rangle + |D_2\rangle)$, and hence that in the basis $|S\rangle = (|A\rangle + |B\rangle)/\sqrt{2}$, $|D_+\rangle = (|D_1\rangle + |D_2\rangle)/\sqrt{2}$ the Hamiltonian is the matrix $[[0, -2t], [-2t, U]]$, while $(|A\rangle - |B\rangle)/\sqrt{2}$ and $(|D_1\rangle - |D_2\rangle)/\sqrt{2}$ are eigenstates with energies 0 and U .

- 1 on $|A\rangle$ only $c_{2\uparrow}^\dagger c_{1\uparrow}$ and $c_{1\downarrow}^\dagger c_{2\downarrow}$ act: $c_{2\uparrow}^\dagger c_{1\uparrow} c_{1\uparrow}^\dagger c_{2\downarrow}^\dagger |0\rangle = c_{2\uparrow}^\dagger c_{2\downarrow}^\dagger |0\rangle = |D_2\rangle$, and $c_{1\downarrow}^\dagger c_{2\downarrow} c_{1\uparrow}^\dagger c_{2\downarrow}^\dagger |0\rangle = -c_{1\downarrow}^\dagger c_{1\uparrow}^\dagger |0\rangle = +|D_1\rangle$, two anticommutation signs cancelling; likewise $c_{1\uparrow}^\dagger c_{2\uparrow} |B\rangle = |D_1\rangle$ and $c_{2\downarrow}^\dagger c_{1\downarrow} |B\rangle = |D_2\rangle$, so $T|A\rangle = T|B\rangle = -t(|D_1\rangle + |D_2\rangle)$
- 2 the U term acts only on $|D_1\rangle$ and $|D_2\rangle$, each with eigenvalue U , and $|A\rangle$, $|B\rangle$ have energy 0; by Hermiticity $T|D_1\rangle = T|D_2\rangle = -t(|A\rangle + |B\rangle)$, so T annihilates $(|A\rangle - |B\rangle)/\sqrt{2}$ and $(|D_1\rangle - |D_2\rangle)/\sqrt{2}$, which are eigenstates with energies 0 and U
- 3 $\langle S|T|D_+\rangle = \frac{1}{2}(\langle A| + \langle B|)(-2t)(|A\rangle + |B\rangle) = -2t$, so on $\{|S\rangle, |D_+\rangle\}$ $H = [[0, -2t], [-2t, U]]$; $|S\rangle = (c_{1\uparrow}^\dagger c_{2\downarrow}^\dagger - c_{1\downarrow}^\dagger c_{2\uparrow}^\dagger)|0\rangle/\sqrt{2}$ is the spin singlet and $(|A\rangle - |B\rangle)/\sqrt{2}$ the triplet with $m = 0$

Every sign here comes from moving one operator past another. A candidate who drops them can find $T|B\rangle = -t(|D_1\rangle - |D_2\rangle)$, couple the triplet to the doubly occupied states, and obtain a ground state of the wrong spin.

(b) CALCULATE · U3 [2]

Calculate the ground-state energy and the singlet-triplet splitting, and compare the splitting with the superexchange coupling $4t^2/U$.

- 1 $E_0 = [U - \sqrt{U^2 + 16t^2}]/2 = [3.2 - \sqrt{(10.24 + 2.56)}]/2 \text{ eV} = (3.2 - 3.578)/2 \text{ eV} = -0.189 \text{ eV}$, a spin singlet
- 2 the triplet lies at 0, so the splitting is 0.189 eV, against $4t^2/U = 4(0.40)^2/3.2 \text{ eV} = 0.200 \text{ eV}$, 6% high because $t/U = 0.125$ is not very small; the coupling is antiferromagnetic

Candidates who quote $4t^2/U$ as the splitting have used the large- U limit without checking t/U . The exact 2×2 result is available, and the superexchange formula should be judged against it.

(c) DETERMINE · U3 [2]

Determine the probability of finding both electrons on the same site in the ground state.

- 1 the first row of $(H - E_0)$ acting on the amplitudes s of $|S\rangle$ and d of $|D_+\rangle$ gives $-2td = E_0s$, so $d/s = -E_0/2t = 0.189/0.80 = 0.236$
- 2 $P = d^2/(s^2 + d^2) = 0.0557/1.0557 = 0.053$, about 5%, against 50% for two electrons that ignore each other

Normalising is the step most often missed: 0.236 is a ratio of amplitudes, and the probability is $d^2/(1 + d^2)$, not 0.236 or 0.236^2 .

(d) EVALUATE · U1 [3]

A student describes the ground state by the restricted Hartree-Fock determinant, with both electrons in the bonding orbital, created by $(c_1\sigma\uparrow + c_2\sigma\downarrow)/\sqrt{2}$. Evaluate this description: find its energy and its probability of double occupation, and say what it gets wrong as U/t grows.

- 1 the determinant is $\frac{1}{2}(c_1\uparrow\uparrow + c_2\uparrow\downarrow)(c_1\downarrow\uparrow + c_2\downarrow\downarrow)|0\rangle = (|S\rangle + |D_+\rangle)/\sqrt{2}$, with energy $\frac{1}{2}(0 + U) - 2t = U/2 - 2t = +0.80 \text{ eV}$, 0.99 eV above the exact -0.19 eV : the correlation energy, -0.99 eV , is about five times the magnitude of the exact energy itself
- 2 its probability of double occupation is 50% whatever U is, against the exact 5%: one determinant of delocalised orbitals cannot keep the two electrons apart
- 3 as U/t grows the restricted energy rises as $U/2$ while the exact energy tends to $-4t^2/U$, approaching zero from below: restricted Hartree-Fock fails worst exactly where the spins localise and couple antiferromagnetically, the dissociation problem of H_2

The expected answer, that the restricted determinant is a reasonable first approximation, is what this part tests. Its energy is positive here although the exact ground state is bound, and its error grows without limit with U .

(e) EXPLAIN · U1 [2]

Unrestricted Hartree-Fock lets the up-spin and down-spin electrons occupy different orbitals, and its best determinant has energy $-2t^2/U = -0.10 \text{ eV}$. Explain why it recovers only about half of the exact binding, and what symmetry of H it breaks to do so.

- 1 for $U \gg t$ the unrestricted determinant approaches $|A\rangle = (|S\rangle + |T_0\rangle)/\sqrt{2}$, with $|T_0\rangle = (|A\rangle - |B\rangle)/\sqrt{2}$: an equal mixture of the singlet, near $-4t^2/U$, and the triplet, at 0, so its energy is about their average, $-2t^2/U$
- 2 to localise the spins it breaks the spin-rotation symmetry, since the determinant is not an eigenstate of S^2 , and the symmetry exchanging the sites; the singlet $(|A\rangle + |B\rangle)/\sqrt{2}$, which the exact ground state $0.973|S\rangle + 0.230|D_+\rangle$ approaches as U/t grows, is a sum of two determinants, which no single determinant can represent

Candidates who take the lower unrestricted energy as proof of a better state should notice that it has no definite total spin. Broken symmetry buys energy at the price of a state that is not an eigenstate of S^2 .

In Bethe's non-relativistic calculation a hydrogen atom in a state $|n\rangle$ is coupled to the transverse vacuum field through $H' = (e/m)A \cdot p$ in the dipole approximation, photon energies being cut off at K . Summing the second-order energy over photon modes and polarisations gives $W_n = -(2\alpha/(3\pi m^2 c^2)) \sum_m |\langle m|p|n\rangle|^2 \int_0^K k dk / (E_m - E_n + k)$, where $k = \hbar\omega$ is the photon energy and the sum runs over all bound and continuum states $|m\rangle$. For a free electron of momentum p the same calculation gives $W_{\text{free}} = -(2\alpha/(3\pi m^2 c^2)) p^2 K$. Write $p_{mn} = \langle m|p|n\rangle$. Take $mc^2 = 0.510999$ MeV, $\alpha = 1/137.036$, $1 \text{ Ry} = 13.6057$ eV and $\hbar = 4.1357 \times 10^{-15}$ eV s.

(a) SHOW THAT · U2

[2]

Show that, for K large compared with every $|E_m - E_n|$ that matters, W_n grows linearly with K , and that the coefficient of K is the free-electron result averaged over the state $|n\rangle$.

- 1 with $\Delta = E_m - E_n$, $\int_0^K k dk / (\Delta + k) = K - \Delta \ln|(\Delta + K)/\Delta| \approx K - \Delta \ln(K/|\Delta|)$ for $K \gg |\Delta|$, so $W_n = -(2\alpha/3\pi m^2 c^2) [K \sum_m |p_{mn}|^2 - \sum_m |p_{mn}|^2 \Delta \ln(K/|\Delta|)]$
- 2 by closure $\sum_m |p_{mn}|^2 = \langle n|p^2|n\rangle$, so the linear term is $-(2\alpha K/3\pi m^2 c^2) \langle n|p^2|n\rangle = \langle n|W_{\text{free}}|n\rangle$: the bound electron's self-energy diverges exactly as a free electron's with the same momentum distribution

Candidates who try to evaluate the sum over states before separating the divergence get lost in the continuum. Closure does the sum in one line, and shows that the divergence knows nothing about the binding.

(b) EXPLAIN · U1

[2]

Explain why the linear term is removed by mass renormalisation, and why what remains depends on K only through a logarithm.

- 1 $W_{\text{free}} = -(2\alpha K/3\pi m^2 c^2) p^2$ changes the coefficient of p^2 : $p^2/2m_0 + W_{\text{free}} = p^2/2(m_0 + \delta m)$ with $\delta m = 4\alpha K/(3\pi c^2)$, an electromagnetic mass; the measured mass already contains it, so writing H with the observed mass subtracts W_{free} and removes the linear term from every state (the A^2 term, the same for every state in the dipole approximation, drops out of all intervals)
- 2 what remains, $\Delta E_n = (2\alpha/3\pi m^2 c^2) \sum_m |p_{mn}|^2 (E_m - E_n) \ln(K/|E_m - E_n|)$, exists only because the electron is bound, vanishing for a free one, and keeps K only in a logarithm, because photons much more energetic than the binding cannot tell a bound electron from a free one

The subtraction is not an arbitrary deletion of an infinity: the same divergent operator appears for the free electron, where it is observable only as part of the mass. A candidate who cannot say what is subtracted, and why it is the same for every state, has not explained it.

(c) SHOW THAT · U2

[3]

The sum rule $\sum_m |p_{mn}|^2 (E_m - E_n) = (\hbar^2/2) \langle n|\nabla^2 V|n\rangle$ holds for $V = -e^2/(4\pi\epsilon_0 r)$. Defining the mean excitation energy K_0 by $\ln K_0 = \sum_m |p_{mn}|^2 (E_m - E_n) \ln|E_m - E_n| / \sum_m |p_{mn}|^2 (E_m - E_n)$, show that $\Delta E_n = (4\alpha^5 mc^2/(3\pi n^3)) \ln(K/K_0)$ for s states, and that the term in $\ln K$ vanishes in every other state. You may use $|\psi_{ns}(0)|^2 = 1/(\pi n^3 a_0^3)$, $a_0 = \hbar/(\alpha mc)$ and $e^2/(4\pi\epsilon_0) = \alpha \hbar c$.

- 1 $\nabla^2(1/r) = -4\pi\delta^3(r)$ gives $\nabla^2 V = (e^2/\epsilon_0)\delta^3(r) = 4\pi\alpha\hbar c \delta^3(r)$, so the sum rule gives $2\pi\alpha\hbar^3 c |\psi_n(0)|^2$, which vanishes unless $l = 0$: the term in $\ln K$ acts on s states only
- 2 with the definition of K_0 , $\Delta E_n = (2\alpha/3\pi m^2 c^2) \times 2\pi\alpha\hbar^3 c |\psi_n(0)|^2 \times \ln(K/K_0) = (4\alpha^2\hbar^3/3m^2 c) |\psi_n(0)|^2 \ln(K/K_0)$
- 3 with $|\psi_{ns}(0)|^2 = 1/(\pi n^3 a_0^3) = \alpha^3 m^3 c^3/(\pi n^3 \hbar^3)$, $\Delta E_n = (4\alpha^5 mc^2/(3\pi n^3)) \ln(K/K_0)$: of order $\alpha^5 mc^2/n^3$ times a large logarithm

The sum rule is the step that turns an intractable sum over states into a contact term. Candidates who miss the delta function in $\nabla^2(1/r)$ find zero, and those who forget that $\psi(0) = 0$ for $l \geq 1$ cannot explain why $2p_{1/2}$ stays put.

(d) CALCULATE · U3

[3]

With the cutoff at $K = mc^2$ and the quoted mean excitation energies $K_0(2s) = 16.64$ Ry and $K_0(1s) = 19.77$ Ry, calculate the shifts of 2s and of 1s in frequency units, and compare them with the measured $2s_{1/2}-2p_{1/2}$ splitting of 1057.8 MHz and 1s shift of 8.17 GHz.

- 1 for $n = 2$, $4\alpha^5 mc^2 / (3\pi \times 8) = 5.610 \times 10^{-7}$ eV, which is 135.6 MHz
- 2 $\ln(mc^2/K_0) = \ln(510999 \text{ eV}/226.4 \text{ eV}) = 7.722$, so the 2s shift is $135.6 \text{ MHz} \times 7.722 = 1047 \text{ MHz}$, 1% below the measured 1057.8 MHz, $2p_{1/2}$ receiving no logarithmic shift
- 3 for 1s the prefactor is $8 \times 135.6 \text{ MHz} = 1085 \text{ MHz}$ and $\ln(510999 \text{ eV}/269.0 \text{ eV}) = 7.549$, giving 8.19 GHz against the measured 8.17 GHz

Leaving K_0 in rydbergs while mc^2 is in electronvolts gives a logarithm near 10.3 and a 2s shift a third too large. The 1s shift is less than eight times the 2s shift because its mean excitation energy is higher.

(e) EVALUATE · U4

[2]

The non-relativistic calculation fixes the cutoff K only to within a factor of about two. Evaluate whether the agreement found in (d) shows that Bethe's choice $K = mc^2$ is correct.

- 1 a factor of two in K changes the 2s shift by $135.6 \text{ MHz} \times \ln 2 = 94 \text{ MHz}$, about 9%, and the 1s shift by 0.75 GHz; agreement at the 1% level is therefore much closer than the method can guarantee, and is partly fortunate
- 2 what the calculation does establish is robust against the cutoff: a shift of order $\alpha^5 mc^2 / n^3$ times a logarithm, confined to s states, with a 1s to 2s ratio of 7.8 rather than 8; removing the cutoff needs the covariant QED calculation, which also adds vacuum polarisation and the anomalous moment, each worth tens of MHz

A good evaluation sizes the uncertainty before admiring the agreement. Candidates who conclude that the non-relativistic theory is accurate to 1% have mistaken a fortunate cutoff for a precise one.

16 CORE COURSE

DATA ANALYSIS · DEMANDING · UAQM-14.02 · UAQM-14.06

[11]

A single InGaAs quantum dot at 4 K is driven resonantly by a narrow-band laser, and its fluorescence is recorded as the laser frequency is scanned across the transition. For each laser power P at the dot, the full width at half maximum $\Delta\nu$ of the fluorescence line, as a frequency, is recorded. A separate time-resolved measurement gives the population relaxation time $T_1 = 0.80$ ns. For a two-level emitter with population relaxation time T_1 and coherence time T_2 , driven at Rabi frequency Ω and detuning Δ (both angular frequencies), the steady state of the optical Bloch equations has the excited-state population $\rho_{ee} = \frac{1}{2} \Omega^2 T_1 T_2 / (1 + \Delta^2 T_2^2 + \Omega^2 T_1 T_2)$, and Ω^2 is proportional to P . Without pure dephasing $T_2 = 2T_1$; in general $1/T_2 = 1/(2T_1) + 1/T_\phi$, where T_ϕ is the pure dephasing time.

(a) SHOW THAT · U2

[2]

Show that $\Delta\nu = (1/\pi T_2) \sqrt{1 + \Omega^2 T_1 T_2}$, and hence that $\Delta\nu^2 = \Delta\nu_0^2 (1 + P/P_{\text{sat}})$, where $\Delta\nu_0 = 1/(\pi T_2)$ and P_{sat} is the power at which $\Omega^2 T_1 T_2 = 1$.

- 1 ρ_{ee} is a Lorentzian in Δ that falls to half its peak value when $\Delta^2 T_2^2 = 1 + \Omega^2 T_1 T_2$, so its full width in angular frequency is $(2/T_2) \sqrt{1 + \Omega^2 T_1 T_2}$
- 2 dividing by 2π , $\Delta\nu = (1/\pi T_2) \sqrt{1 + \Omega^2 T_1 T_2}$; with $\Omega^2 T_1 T_2 = P/P_{\text{sat}}$ this gives $\Delta\nu^2 = \Delta\nu_0^2 (1 + P/P_{\text{sat}})$, linear in P

Candidates who take the half-width for the full width, or forget the 2π between angular and ordinary frequency, carry a factor of 2 or 2π into T_2 .

- (b) DESCRIBE · U4 [2]
- Describe how the readings should be plotted to test this model and to extract $\Delta\nu_0$ and P_{sat} , and explain why the narrowest line measured is not itself $\Delta\nu_0$.
- 1 plot $\Delta\nu^2$ against P : the model predicts a straight line whose intercept at $P = 0$ is $\Delta\nu_0^2$ and whose gradient is $\Delta\nu_0^2/P_{\text{sat}}$, so $P_{\text{sat}} = \text{intercept}/\text{gradient}$; a plot of $\Delta\nu$ against P curves and cannot be extrapolated reliably
 - 2 even the lowest power, 2.0 nW, is about a sixth of P_{sat} , so the 289 MHz line is already power-broadened by about 8%; the zero-power width has to be found by extrapolation
- Taking the narrowest line as the unbroadened one is the error this part catches: it gives $T_2 = 1.10$ ns and a dephasing time that is too short.*
- (c) DETERMINE · U4 [3]
- Determine the gradient and intercept of your graph, and hence $\Delta\nu_0$ and P_{sat} .
- 1 $\Delta\nu^2 = 0.835, 0.986, 1.303, 1.840, 3.069$ and $5.358 \times 10^5 \text{ MHz}^2$, which lie on a straight line to within 2%
 - 2 gradient = $5.8 \times 10^3 \text{ MHz}^2 \text{ nW}^{-1}$ (accept 5.7 to $6.0 \times 10^3 \text{ MHz}^2 \text{ nW}^{-1}$) and intercept = $7.1 \times 10^4 \text{ MHz}^2$ (accept 6.9 to $7.3 \times 10^4 \text{ MHz}^2$)
 - 3 $\Delta\nu_0 = \sqrt{\text{intercept}} = 266 \text{ MHz}$ (accept 263 to 270 MHz) and $P_{\text{sat}} = \text{intercept}/\text{gradient} = 12 \text{ nW}$ (accept 11.5 to 12.8 nW)
- A line forced through the origin, or fitted to $\Delta\nu$ rather than $\Delta\nu^2$, gives no meaningful intercept. The intercept is in MHz^2 , so $\Delta\nu_0$ is its square root; candidates who forget the root report a width of $7 \times 10^4 \text{ MHz}$.*
- (d) EVALUATE · U4 [3]
- Evaluate whether this emitter's line is lifetime-limited, finding T_2 and, if it is needed, the pure dephasing time T_ϕ .
- 1 $T_2 = 1/(\pi\Delta\nu_0) = 1/(\pi \times 266 \times 10^6 \text{ Hz}) = 1.20 \text{ ns}$ (accept 1.18 to 1.21 ns)
 - 2 a lifetime-limited line would have $T_2 = 2T_1 = 1.60 \text{ ns}$ and $\Delta\nu_0 = 1/(2\pi T_1) = 199 \text{ MHz}$; the measured 266 MHz is a third wider, so the line is not lifetime-limited
 - 3 $1/T_\phi = 1/T_2 - 1/(2T_1) = (0.836 - 0.625) \text{ ns}^{-1} = 0.211 \text{ ns}^{-1}$, so $T_\phi = 4.7 \text{ ns}$ (accept 4.5 to 5.0 ns): pure dephasing, from phonons or fluctuating charges near the dot, which a measurement of T_1 cannot see
- Candidates who compare T_2 with T_1 rather than with $2T_1$ conclude that coherence outlasts population and that something has gone wrong. The bound is $T_2 \leq 2T_1$, and the shortfall from it measures the pure dephasing.*
- (e) PREDICT · U3 [1]
- Predict the rate at which the dot scatters photons when it is driven on resonance at $P = 40 \text{ nW}$.
- 1 with $P/P_{\text{sat}} = 40/12 = 3.3$, $\rho_{ee} = \frac{1}{2} \times 3.3/4.3 = 0.38$, and the scattering rate $\rho_{ee}/T_1 = 0.38/(0.80 \text{ ns}) = 4.8 \times 10^8 \text{ s}^{-1}$, about 77% of the saturated maximum $1/(2T_1) = 6.3 \times 10^8 \text{ s}^{-1}$
- The rate is ρ_{ee}/T_1 , not ρ_{ee}/T_2 : only the decay of population emits photons, and however hard the dot is driven the rate cannot exceed $1/(2T_1)$.*

17 CORE COURSE

FREE RESPONSE · EXTENDED DERIVATION · DISCRIMINATING · UAQM-11.03 · UAQM-11.05 · UAQM-12.01 · UAQM-12.02 · UAQM-12.03

[15]

In a cubic box of volume V with periodic boundary conditions, the transverse vector potential in Coulomb gauge is, in the Heisenberg picture, $A(\mathbf{r}, t) = \sum_{\mathbf{k}, \lambda} \sqrt{\hbar/(2\epsilon_0\omega_{\mathbf{k}}V)} [a_{\mathbf{k}\lambda}(\mathbf{k}) \epsilon_{\mathbf{k}\lambda} e^{i(\mathbf{k}\cdot\mathbf{r} - \omega_{\mathbf{k}}t)} + a_{\mathbf{k}\lambda}^\dagger \epsilon_{\mathbf{k}\lambda}^* e^{-i(\mathbf{k}\cdot\mathbf{r} - \omega_{\mathbf{k}}t)}]$, with $\omega_{\mathbf{k}} = ck$, two unit polarisation vectors $\epsilon_{\mathbf{k}\lambda}$ perpendicular to $\mathbf{k}$ for each $\mathbf{k}$, and $[a_{\mathbf{k}\lambda}, a_{\mathbf{k}'\lambda'}^\dagger] = \delta_{\mathbf{k}\mathbf{k}'} \delta_{\lambda\lambda'}$. A one-electron atom or ion, with an infinitely heavy nucleus at the origin, has an excited state $|b\rangle$ and a lower state $|a\rangle$ separated by $\hbar\omega_0$. It couples to the field through $H' = (e/m)A(0) \cdot \mathbf{p}$, the dipole approximation, where $-e$ and m are the electron's charge and mass, and $\langle a|\mathbf{p}|b\rangle = -im\omega_0\langle a|\mathbf{r}|b\rangle$. For a hydrogen-like ion of nuclear charge Ze , $|\langle 1s|\mathbf{r}|2p, m\rangle|^2 = (2^{15}/3^{10})(a_0/Z)^2$ for each m , and the 2p-1s energy difference is $(3/4)Z^2 \times 13.606 \text{ eV}$. Take $\hbar = 1.055 \times 10^{-34} \text{ J s}$, $e = 1.602 \times 10^{-19} \text{ C}$, $\epsilon_0 = 8.854 \times 10^{-12} \text{ F m}^{-1}$, $c = 2.998 \times 10^8 \text{ m s}^{-1}$ and $a_0 = 5.292 \times 10^{-11} \text{ m}$.

(a) DERIVE · U2

[2]

Derive the transverse electric field operator from A , and show that in the vacuum each mode contributes $\hbar\omega_k/(2\epsilon_0V)$ to $\langle E^2 \rangle$, so that its mean electric energy is half its zero-point energy.

- 1 in Coulomb gauge the transverse field is $E = -\partial A/\partial t = \sum_{\mathbf{k}, \lambda} i\sqrt{\hbar\omega_k/(2\epsilon_0V)} [a_{\mathbf{k}\lambda}\epsilon_{\mathbf{k}\lambda}e^{i(\mathbf{k}\cdot\mathbf{r} - \omega_k t)} - a_{\mathbf{k}\lambda}^\dagger\epsilon_{\mathbf{k}\lambda}^*e^{-i(\mathbf{k}\cdot\mathbf{r} - \omega_k t)}]$
- 2 in $\langle 0|E^2|0 \rangle$ only the product $a a^\dagger$ of each mode survives, with $\langle 0|a a^\dagger|0 \rangle = 1$ and $|\epsilon|^2 = 1$, so each mode contributes $\hbar\omega_k/(2\epsilon_0V)$; its electric energy $(\epsilon_0/2)\langle E^2 \rangle V = \hbar\omega_k/4$ is half the zero-point energy $\hbar\omega_k/2$, the magnetic field carrying the other half

Candidates who lose the relative minus sign between the a and $a^\dagger$ terms write a field that is not Hermitian and find $\langle E^2 \rangle$ negative, which should stop them at once. The factor $-i\omega_k$ from the time derivative is what turns the normalisation of A into $\sqrt{\hbar\omega_k/2\epsilon_0V}$.

(b) SHOW THAT · U2

[2]

Show that the matrix element for emission of a photon into a mode $(\mathbf{k}, \lambda)$ already holding n photons is $\langle a; n+1|H'|b; n \rangle = (e/m)\sqrt{\hbar/(2\epsilon_0\omega_kV)}\sqrt{n+1}\epsilon_{\mathbf{k}\lambda}^* \cdot \langle a|p|b \rangle$, and explain why this makes an excited atom in the vacuum emit, though an atom in a classical field of zero amplitude never does.

- 1 only the $a^\dagger$ term of A raises the photon number, and $a^\dagger|n \rangle = \sqrt{n+1}|n+1 \rangle$ gives the stated element, with atomic factor $\epsilon_{\mathbf{k}\lambda}^* \cdot \langle a|p|b \rangle$
- 2 for $n=0$ the factor is $\sqrt{1}$, not zero: the 1 in $n+1$ has no classical counterpart, since a classical field of zero amplitude gives $H' = 0$ and leaves $|b \rangle$ stationary; stimulated emission, proportional to n , and spontaneous emission, the 1, come from the same matrix element

The error this part catches is to say that the atom decays because a classical random field shakes it. The rate is set by the $\sqrt{n+1}$ of the creation operator; a classical noise field with the same $\langle E^2 \rangle$ would drive absorption as often as emission.

(c) DERIVE · U2

[4]

Using Fermi's golden rule, and summing over all modes, directions and both polarisations, derive $A = \omega_0^3 e^2 |\langle a|r|b \rangle|^2 / (3\pi\epsilon_0\hbar c^3)$ for spontaneous emission from $|b \rangle$ to $|a \rangle$.

- 1 $\Gamma = (2\pi/\hbar)\sum_{\mathbf{k}, \lambda} |M_{\mathbf{k}\lambda}|^2 \delta(\hbar\omega_k - \hbar\omega_0)$, with $|M_{\mathbf{k}\lambda}|^2 = (e^2/m^2)(\hbar/(2\epsilon_0\omega_kV))m^2\omega_0^2 |\epsilon_{\mathbf{k}\lambda}^* \cdot r_{ab}|^2$ for $n=0$, using $p_{ab} = -im\omega_0 r_{ab}$
- 2 the mode sum becomes an integral, $\sum_{\mathbf{k}} \rightarrow (V/(2\pi)^3) \int k^2 dk d\Omega = (V/(8\pi^3 c^3)) \int \omega^2 d\omega d\Omega$, in which V cancels the $1/V$ of $|M|^2$, and $\delta(\hbar\omega - \hbar\omega_0) = \delta(\omega - \omega_0)/\hbar$ sets $\omega = \omega_0$
- 3 the two polarisations perpendicular to $\mathbf{k}$ give $\sum_{\lambda} |\epsilon_{\mathbf{k}\lambda}^* \cdot r_{ab}|^2 = |r_{ab}|^2 - |\hat{\mathbf{k}} \cdot r_{ab}|^2$, and since $|\hat{\mathbf{k}} \cdot r_{ab}|^2$ averages to $|r_{ab}|^2/3$ over directions, the angular integral is $4\pi |r_{ab}|^2 - (4\pi/3)|r_{ab}|^2 = (8\pi/3)|r_{ab}|^2$ (for a real r_{ab} this is $\int |r_{ab}|^2 \sin^2\Theta d\Omega$, Θ the angle between $\mathbf{k}$ and r_{ab})
- 4 $\Gamma = (2\pi/\hbar)(e^2\hbar\omega_0/2\epsilon_0)|r_{ab}|^2(\omega_0^2/(8\pi^3 c^3\hbar))(8\pi/3) = \omega_0^3 e^2 |r_{ab}|^2 / (3\pi\epsilon_0\hbar c^3) = A$, obtained from the quantised field without any appeal to Planck's law

The polarisation sum is where marks are lost. Candidates who take $\sum_{\lambda} |\epsilon_{\mathbf{k}\lambda} \cdot r|^2 = |r|^2$, forgetting that a photon cannot be polarised along its own direction, are out by a factor of 3/2.

(d) CALCULATE · U3

[3]

Calculate A , the lifetime and the natural linewidth $\Gamma/2\pi$ of the 2p state of the hydrogen-like helium ion He^+ ($Z=2$).

- 1 $\hbar\omega_0 = (3/4)(4)(13.606 \text{ eV}) = 40.82 \text{ eV}$, so $\omega_0 = (40.82 \times 1.602 \times 10^{-19} \text{ J})/(1.055 \times 10^{-34} \text{ J s}) = 6.198 \times 10^{16} \text{ rad s}^{-1}$ (a wavelength of 30.4 nm), and $|r_{ab}|^2 = 0.5549 \times (2.646 \times 10^{-11} \text{ m})^2 = 3.885 \times 10^{-22} \text{ m}^2$
- 2 $A = (6.198 \times 10^{16} \text{ s}^{-1})^3 (1.602 \times 10^{-19} \text{ C})^2 (3.885 \times 10^{-22} \text{ m}^2) / [3\pi(8.854 \times 10^{-12} \text{ F m}^{-1})(1.055 \times 10^{-34} \text{ J s})(2.998 \times 10^8 \text{ m s}^{-1})^3] = 1.00 \times 10^{10} \text{ s}^{-1}$
- 3 $\tau = 1/A = 100 \text{ ps}$ and $\Gamma/2\pi = A/2\pi = 1.59 \text{ GHz}$; A scales as Z^4 , ω_0^3 growing as Z^6 and $|r_{ab}|^2$ falling as Z^{-2} , so it is sixteen times hydrogen's $6.26 \times 10^8 \text{ s}^{-1}$

Candidates who scale ω_0 but not the matrix element obtain a Z^6 law and a rate four times too large. Hydrogen's 1.6 ns lifetime divided by sixteen is the check.

(e) EXPLAIN · U1

[2]

The atom now sits in thermal radiation at temperature T , whose modes near ω_0 hold $\bar{n}$ photons on average. Explain how the $\sqrt{n}$ and $\sqrt{n+1}$ factors of the field operators lead to Planck's distribution, rather than assuming it as Einstein did.

- 1 because $|\langle n+1|a^\dagger|n\rangle|^2 = n+1$ and $|\langle n-1|a|n\rangle|^2 = n$, the emission rate from $|b\rangle$ is $A(\bar{n}+1)$, stimulated plus spontaneous, and the absorption rate from $|a\rangle$ is $A\bar{n}$ for non-degenerate levels: the B coefficients and A come from the same matrix element
- 2 in equilibrium $N_b A(\bar{n}+1) = N_a A\bar{n}$ with $N_b/N_a = e^{-(\hbar\omega_0/k_B T)}$, the Boltzmann factor being the one thermal input, so $\bar{n} = 1/(e^{(\hbar\omega_0/k_B T)} - 1)$: Planck's distribution is an output of the quantised field, and Einstein's relations follow with it

Candidates who reproduce Einstein's argument, using Planck's law to fix A , have run the logic backwards. Here A is already known from (c), and the thermal photon distribution is what the balance delivers.

(f) JUSTIFY · U4

[2]

Justify the dipole approximation, and the use of the golden rule leading to exponential decay at the rate A , for the $\text{He}^+ 2p$ state.

- 1 the dipole approximation needs $ka \ll 1$ across the ion: $k = \omega_0/c = 2.07 \times 10^8 \text{ m}^{-1}$ and the orbit size $a_0/Z = 2.65 \times 10^{-11} \text{ m}$ give $ka = 5.5 \times 10^{-3}$, so $e^{i\mathbf{k}\cdot\mathbf{r}} \approx 1$ to better than 1%
- 2 the golden rule and the Markov step need a weak coupling and a mode density smooth across the line: $\Gamma/\omega_0 = (1.00 \times 10^{10} \text{ s}^{-1})/(6.20 \times 10^{16} \text{ s}^{-1}) = 1.6 \times 10^{-7}$, so the free-space modes are flat over many linewidths and the decay is exponential, with departures only at times of order $1/\omega_0$ and at very long times, both negligible

A justification must put numbers to its small parameters. 'The ion is small' earns nothing until ka is evaluated, and 'the coupling is weak' nothing until Γ is set beside ω_0 .

18
CORE
COURSE

FREE RESPONSE · MODEL, SOLVE AND CHECK THE LIMITS · DISCRIMINATING · UAQM-15.07 · UAQM-15.08 · UAQM-15.09

[16]

A uniform gas of N spinless bosons of mass m in a box of volume V , with periodic boundary conditions, interacts through a short-range potential represented at low energy by the contact coupling $g = 4\pi\hbar^2 a_s/m$, where a_s is the s -wave scattering length. In second quantisation $H = \sum_{\mathbf{k}} \epsilon_{\mathbf{k}} a_{\mathbf{k}}^\dagger a_{\mathbf{k}} + (g/2V) \sum_{\mathbf{k}, \mathbf{k}', \mathbf{q}} a_{\mathbf{k}+\mathbf{q}}^\dagger a_{\mathbf{k}'-\mathbf{q}}^\dagger a_{\mathbf{k}'} a_{\mathbf{k}}$, with $\epsilon_{\mathbf{k}} = \hbar^2 k^2/2m$. Bogoliubov's approximation replaces a_0 and $a_0^\dagger$ by $\sqrt{N_0}$, where N_0 is the number of bosons in the condensate, and keeps the terms of H up to second order in the operators $a_{\mathbf{k}}$ with $\mathbf{k} \neq 0$, the sums over such $\mathbf{k}$ being written Σ' . Write $n = N/V$. Take $\hbar = 1.055 \times 10^{-34} \text{ J s}$, $1 \text{ u} = 1.661 \times 10^{-27} \text{ kg}$ and $k_B = 1.381 \times 10^{-23} \text{ J K}^{-1}$.

(a) SHOW THAT · U2

[3]

Show that, to this order and with N_0 eliminated in favour of N , $H \approx gN^2/(2V) + \Sigma'[(\epsilon_{\mathbf{k}} + gn)a_{\mathbf{k}}^\dagger a_{\mathbf{k}} + (gn/2)(a_{\mathbf{k}}^\dagger a_{-\mathbf{k}}^\dagger + a_{\mathbf{k}} a_{-\mathbf{k}})]$.

- 1 the term with all four momenta zero gives $(g/2V)N_0^2$; terms with one nonzero momentum vanish by momentum conservation, and those with three or four are dropped as of higher order
- 2 with two nonzero momenta, the four ways of placing one condensate operator among the creators and one among the annihilators each give $N_0 a_{\mathbf{k}}^\dagger a_{\mathbf{k}}$, and $a_{\mathbf{q}}^\dagger a_{-\mathbf{q}}^\dagger a_0 a_0$ and $a_0^\dagger a_0^\dagger a_{-\mathbf{q}} a_{\mathbf{q}}$ give $N_0(a_{\mathbf{q}}^\dagger a_{-\mathbf{q}}^\dagger + a_{\mathbf{q}} a_{-\mathbf{q}})$, so the interaction is $(g/2V)[N_0^2 + 4N_0 \Sigma' a_{\mathbf{k}}^\dagger a_{\mathbf{k}} + N_0 \Sigma'(a_{\mathbf{k}}^\dagger a_{-\mathbf{k}}^\dagger + a_{\mathbf{k}} a_{-\mathbf{k}})]$
- 3 with $N_0 = N - \Sigma' a_{\mathbf{k}}^\dagger a_{\mathbf{k}}$, $N_0^2 \approx N^2 - 2N \Sigma' a_{\mathbf{k}}^\dagger a_{\mathbf{k}}$ cancels half of the $4N_0$ term, leaving $gN/V = gn$ for each particle outside the condensate; elsewhere N_0 may be replaced by N to this order, which gives the stated H

Candidates who replace N_0 by N before counting obtain $2gn$ instead of gn on the diagonal, and with it a spectrum with a gap at $k = 0$. The depletion hidden in N_0^2 is what makes the phonon gapless.

(b) DERIVE · U2 [4]

Writing $a_k = u_k b_k - v_k b_{-k}^\dagger$ with u_k and v_k real, derive the condition on u_k and v_k that keeps $[b_k, b_k^\dagger] = 1$, the choice that removes the terms $b_k b_{-k}$ and $b_k^\dagger b_{-k}^\dagger$, and the excitation energy $E_k = \sqrt{\epsilon_k(\epsilon_k + 2gn)}$.

- 1 $[a_k, a_k^\dagger] = u_k^2[b_k, b_k^\dagger] - v_k^2[b_{-k}, b_{-k}^\dagger] = u_k^2 - v_k^2$ must equal 1, so $u_k = \cosh \theta_k$ and $v_k = \sinh \theta_k$: a hyperbolic rotation rather than an ordinary one
- 2 for the pair $k, -k$, with $X_k = \epsilon_k + gn$ and $Y = gn$, $H_k = X_k(a_k^\dagger a_k + a_{-k}^\dagger a_{-k}) + Y(a_k^\dagger a_{-k}^\dagger + a_k a_{-k})$; after substitution the coefficient of $b_k b_{-k} + b_k^\dagger b_{-k}^\dagger$ is $-2X_k u_k v_k + Y(u_k^2 + v_k^2) = -X_k \sinh 2\theta_k + Y \cosh 2\theta_k$
- 3 setting it to zero gives $\tanh 2\theta_k = gn/(\epsilon_k + gn)$, which has a solution for every $k \neq 0$ because gn is less than $\epsilon_k + gn$
- 4 the coefficient of $b_k^\dagger b_k + b_{-k}^\dagger b_{-k}$ is $X_k \cosh 2\theta_k - Y \sinh 2\theta_k = \sqrt{(X_k^2 - Y^2)}$, so $H = \text{constant} + \sum E_k b_k^\dagger b_k$ with $E_k = \sqrt{(\epsilon_k + gn)^2 - (gn)^2} = \sqrt{\epsilon_k(\epsilon_k + 2gn)}$

Candidates who take $u^2 + v^2 = 1$, by analogy with a rotation, destroy the boson commutator. For bosons the transformation is hyperbolic, and that is what lets u_k and v_k both grow without bound as k approaches zero.

(c) SKETCH · U1 [2]

Sketch E_k against k , with ϵ_k on the same axes, marking the behaviour at small and at large k and the scale $k \approx 1/\xi$, where $\xi = \hbar/\sqrt{2mgn}$, at which it changes.

- 1 both curves start at the origin, E_k rising linearly with slope $\hbar c$, where $c = \sqrt{gn/m}$, a phonon branch, while ϵ_k starts as a parabola of zero slope; both curves are labelled and E_k lies above ϵ_k everywhere
- 2 the change from linear to quadratic is marked near $k \approx 1/\xi$, where $\epsilon_k \approx gn$, and at large k E_k approaches from below the parabola $\epsilon_k + gn$, a free particle displaced upward by the mean field gn

A sketch with a gap at $k = 0$ shows the error described in (a). The two features to show are the linear start, which makes the gas a superfluid, and the offset gn at large k .

(d) CALCULATE · U3 [3]

For a condensate of ^{87}Rb ($m = 87 \text{ u}$, $a_s = 5.3 \text{ nm}$) of density $n = 2.0 \times 10^{20} \text{ m}^{-3}$, calculate gn/k_B in nanokelvin, the speed of sound c , the healing length ξ and $n a_s^3$.

- 1 $m = 87 \times 1.661 \times 10^{-27} \text{ kg} = 1.445 \times 10^{-25} \text{ kg}$ and $g = 4\pi\hbar^2 a_s/m = 4\pi(1.055 \times 10^{-34} \text{ J s})^2(5.3 \times 10^{-9} \text{ m})/(1.445 \times 10^{-25} \text{ kg}) = 5.13 \times 10^{-51} \text{ J m}^3$, so $gn = 1.03 \times 10^{-30} \text{ J}$ and $gn/k_B = 74 \text{ nK}$
- 2 $c = \sqrt{gn/m} = \sqrt{(1.03 \times 10^{-30} \text{ J})/(1.445 \times 10^{-25} \text{ kg})} = 2.66 \times 10^{-3} \text{ m s}^{-1}$ and $\xi = \hbar/\sqrt{2mgn} = 1.9 \times 10^{-7} \text{ m}$, about $0.19 \mu\text{m}$
- 3 $n a_s^3 = 2.0 \times 10^{20} \text{ m}^{-3} \times (5.3 \times 10^{-9} \text{ m})^3 = 3.0 \times 10^{-5} \ll 1$, so the gas is dilute and Bogoliubov's quadratic theory, an expansion in $\sqrt{n a_s^3}$, is well justified

Using h for $\hbar$ in g is out by $4\pi^2$, and leaving the mass in atomic mass units gives nonsense. The diluteness check belongs to the answer: without it the numbers have no claim to be right.

(e) DETERMINE · U3 [2]

Determine $\langle a_k^\dagger a_k \rangle$ for $k \neq 0$ in the ground state, the vacuum of every b_k , and hence, given that the sum over k gives a depletion $(N - N_0)/N = (8/(3\sqrt{\pi}))\sqrt{n a_s^3}$, the fraction of the atoms of (d) that lie outside the condensate at zero temperature.

- 1 $a_k = u_k b_k - v_k b_{-k}^\dagger$ gives $\langle a_k^\dagger a_k \rangle = v_k^2 \langle b_{-k} b_{-k}^\dagger \rangle = v_k^2 = \frac{1}{2}[(\epsilon_k + gn)/E_k - 1]$, nonzero for every k : the pair term of the interaction holds atoms out of the condensate in pairs of opposite momentum even at $T = 0$
- 2 $(N - N_0)/N = 1.505 \times \sqrt{(3.0 \times 10^{-5})} = 8.2 \times 10^{-3}$: less than 1% of the atoms are outside the condensate, consistent with keeping H to quadratic order

Candidates who take the ground state to be the vacuum of the a_k conclude that every atom is in the condensate. The quasiparticle vacuum is not the particle vacuum: it contains correlated pairs.

A tightly focused repulsive laser beam is dragged through the condensate of (d) at 1.5 mm s^{-1} . Predict, using Landau's criterion, whether it heats the gas, and whether an obstacle moving at the same speed through an ideal Bose gas would.

- 1 an obstacle moving at v can create an excitation of momentum p only if $E(p) - p \cdot v \leq 0$, which needs $v \geq E(p)/p$ for some p ; for the Bogoliubov spectrum $E/p = \sqrt{c^2 + (p/2m)^2}$ is least as $p \rightarrow 0$, so the critical speed is $c = 2.66 \text{ mm s}^{-1}$, and at 1.5 mm s^{-1} no excitation can be made: the flow is frictionless and the gas is not heated (vortex nucleation, beyond this theory, is neglected)
- 2 for the ideal gas $E = p^2/2m$, so $E/p = p/2m$ can be made as small as desired and the critical speed is zero: the obstacle creates excitations at any speed and heats the gas, so superfluidity comes from the interaction, which turns the low-energy spectrum into phonons

Candidates who argue that a condensate flows without friction simply because its atoms share one state miss the point of Landau's criterion. The ideal condensate shares that property and is not a superfluid.

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 26 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 45 MARKS · 39%	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 · 24%

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

16 MARKS · 14%

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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