

ADVANCED QUANTUM PHYSICS

Michaelmas 2008

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EXAMPLES SHEET

Before starting, you should make sure that you have done and understood the examples given in the *Quantum Physics course from last year*.

The examples marked with an asterisk are probably harder, and are the ones to omit if your time is very short, or if you are finding the course difficult. Examples based on past tripos questions are indicated and some numerical and algebraic answers are given at the end of the sheet.

Many of the questions begin with a routine piece of bookwork. This is the kind of thing you will have to do in the exam. You are strongly encouraged to do these parts and get feedback in supervisions.

In several of the examples, you need to use the wavefunctions for the hydrogen atom, which are given here:

$$\begin{aligned}\psi_{1s} &= \left(\frac{1}{\pi a_0^3}\right)^{\frac{1}{2}} \exp(-r/a_0) \\ \psi_{2s} &= \left(\frac{1}{8\pi a_0^3}\right)^{\frac{1}{2}} (1-r/2a_0) \exp(-r/2a_0) \\ \psi_{2p_0} &= \left(\frac{1}{32\pi a_0^5}\right)^{\frac{1}{2}} r \exp(-r/2a_0) \cos \theta \\ \psi_{2p_{\pm 1}} &= \left(\frac{1}{64\pi a_0^5}\right)^{\frac{1}{2}} r \exp(-r/2a_0) \sin \theta e^{\pm i\phi}\end{aligned}$$

where $a_0 = 4\pi\epsilon_0\hbar^2/me^2$. For a Hydrogen-like single electron atom with nuclear charge Z , a_0 is replaced by a_0/Z . In a number of the problems you will find the following standard integrals useful:

$$\begin{aligned}\int_0^\infty x^n e^{-ax} dx &= \frac{n!}{a^{n+1}} \quad (a > 0; n \geq 0) \\ \int_{-\infty}^\infty x^{2n} e^{-ax^2} dx &= \frac{1 \cdot 3 \cdot 5 \cdots (2n-1)}{(2a)^n} \sqrt{\frac{\pi}{a}} \\ \int_0^\infty x^{2n+1} e^{-ax^2} dx &= \frac{n!}{2 \cdot a^{n+1}}\end{aligned}$$

The Pauli spin matrices are:

$$\hat{\sigma}_x = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}, \hat{\sigma}_y = \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}, \hat{\sigma}_z = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$$

1 Eigenvectors, eigenvalues and time development

The Hamiltonian \hat{H} has two normalized eigenstates $|\psi_1\rangle$ and $|\psi_2\rangle$ which correspond to different eigenvalues E_1 and E_2 .

- (a) Show that $|\psi_1\rangle$ and $|\psi_2\rangle$ are orthogonal.
- (b) For an observable \hat{A} where $\hat{A}|\psi_1\rangle = |\psi_2\rangle$ and $\hat{A}|\psi_2\rangle = |\psi_1\rangle$ calculate the eigenvalues and eigenvectors (which are combinations of $|\psi_1\rangle$ and $|\psi_2\rangle$).
- (c) Assuming that at $t=0$ the system is in the state $|\psi(t=0)\rangle = \frac{1}{\sqrt{2}}[|\psi_1\rangle - |\psi_2\rangle]$, find the state of the system $|\psi(t)\rangle$ at time t and show that the probability of the system returning to its initial state is given by: $P = \cos^2((E_1 - E_2)t / 2\hbar)$.

2 Harmonic Oscillator: Ladder operators

The potential energy of a one-dimensional harmonic oscillator of mass m and angular frequency ω can be written as

$$V(x) = \frac{m\omega^2 x^2}{2}$$

Using the raising and lowering operators,

$$\hat{a}^\dagger = \frac{1}{\sqrt{2m\hbar\omega}}(-i\hat{p} + m\omega\hat{x}) \quad \hat{a} = \frac{1}{\sqrt{2m\hbar\omega}}(i\hat{p} + m\omega\hat{x})$$

Show that:

- (a) The expectation values of the position and momentum are zero for energy eigenstate $|\psi_n\rangle$.
- (b) The expectation values of the potential and kinetic energies are each equal to $\frac{1}{2}(n + \frac{1}{2})\hbar\omega$ where n is the quantum number of the state $|\psi_n\rangle$.
- (c) The uncertainties Δx and Δp in position and momentum are related by $\Delta x \Delta p = (n + \frac{1}{2})\hbar$.

$$[You\ may\ assume\ that\ \hat{a}^\dagger|\psi_n\rangle = \sqrt{n+1}|\psi_{n+1}\rangle\ \text{and}\ \hat{a}|\psi_n\rangle = \sqrt{n}|\psi_{n-1}\rangle.]$$

3 Spin

Using the Pauli matrices, $\hat{\sigma}_x, \hat{\sigma}_y, \hat{\sigma}_z$, for a spin- $\frac{1}{2}$ particle, write down the operator corresponding to a component of spin along the axis (θ, ϕ) in spherical polar coordinates. Show that the eigenvalues of spin in this direction are $\pm \frac{1}{2}\hbar$ (as expected), and deduce the corresponding wavefunctions. Hence, infer the wavefunctions for particles whose spins are aligned along the $+x$, $-x$, $+y$ and $-y$ directions.

[You can conveniently find the relevant spin operator by taking the dot product of the vector $(\hat{\sigma}_x, \hat{\sigma}_y, \hat{\sigma}_z)$ with a unit vector in the desired direction.]

4 Angular momentum

a) Consider the addition of two angular momenta, $\ell_1=1$ and $\ell_2=2$. The state $|L=3, M=3\rangle$, where L and M are the total angular momentum quantum numbers, can be written down as

$$|\ell_1=1, m_1=1; \ell_2=2, m_2=2\rangle.$$

Use ladder operators to construct explicitly the state $|L=3, M=2\rangle$ and then orthogonality to construct the state $|L=2, M=2\rangle$ in terms of the $|\ell_1, m_1; \ell_2, m_2\rangle$ states.

b) Consider two identical spin- $\frac{1}{2}$ fermions, and let $\chi_+(i)$ represent the state of particle i with spin up, and $\chi_-(i)$ the state with spin down. Find the four possible states of the system which have definite exchange symmetry along with the corresponding total quantum numbers S and M .

At a given moment, the system is in a state

$$\psi = \sqrt{\frac{2}{3}}\chi_+(1)\chi_-(2) + \sqrt{\frac{1}{3}}\chi_-(1)\chi_+(2).$$

What is the probability of a measurement of the total spin giving the result $S=1$?

5 Matrix Methods

Show that for a system with orbital angular momentum $\ell=1$, and using basis states $|\phi_1\rangle=|Y_{11}\rangle$, $|\phi_2\rangle=|Y_{10}\rangle$ and $|\phi_3\rangle=|Y_{1-1}\rangle$, the angular momentum operators may be represented by the matrices

$$\hat{L}_x = \frac{\hbar}{\sqrt{2}} \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}, \quad \hat{L}_y = \frac{i\hbar}{\sqrt{2}} \begin{pmatrix} 0 & -1 & 0 \\ 1 & 0 & -1 \\ 0 & 1 & 0 \end{pmatrix}, \quad \hat{L}_z = \hbar \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}.$$

A rotating body has the Hamiltonian

$$\hat{H} = \frac{\hat{L}_x^2}{2I_x} + \frac{\hat{L}_y^2}{2I_y} + \frac{\hat{L}_z^2}{2I_z}$$

Find the energy levels and corresponding eigenstates when $\ell=1$.

6 Identical particles

Discuss the special considerations which apply to systems of indistinguishable particles in quantum mechanics, giving examples where they lead to observable consequences.

Two non-interacting particles of mass m move in one dimension, their positions given by x_1 and x_2 . The potential is

$$V(x) = 0 \quad (0 < x < L) \\ = \infty \quad \text{otherwise}$$

Show that the energy of the system is of the form:

$$E = (n_1^2 + n_2^2)\epsilon$$

where n_1 and n_2 are integers and find an expression for ε .

Consider the state with $E = 5\varepsilon$ for each of the following three cases:

- (a) spin-zero particles
- (b) spin- $\frac{1}{2}$ particles in a singlet spin state
- (c) spin- $\frac{1}{2}$ particles in a triplet spin state

In each case, what is the symmetry of the spin and spatial parts of the wavefunction? Hence write down the spatial wavefunction, and sketch the probability density $|\psi(x_1, x_2)|^2$ in the (x_1, x_2) plane.

Describe qualitatively how the energies of these states would change if the particles carried electric charge and hence interacted with each other (an example of the exchange interaction).

7 Variational Method

Give an account of the variational method for estimating the ground state energy of a quantum mechanical system. Explain how the method may also be applied to excited states.

Use a trial wavefunction of the form:

$$\psi(x) = A(a^2 - x^2) \quad (-a < x < a)$$

$$= 0 \quad \text{otherwise}$$

to place an upper bound on the ground state energy of the one-dimensional harmonic oscillator with potential

$$V(x) = \frac{1}{2}m\omega^2 x^2$$

where m is the mass of the particle and ω the oscillator frequency. Compare your answer with the exact result, and comment.

8 Variational Method

By taking a trial wavefunction proportional to $\exp(-\beta r)$ where β is a variational parameter, obtain an upper limit on the ground state energy of the H atom in terms of atomic constants. Comment on your result. *[Ignore the motion of the proton.]*

9 Variational Method*

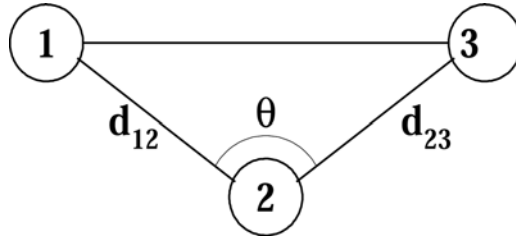
a) E_1 and E_2 are the ground state energies of a particle moving in attractive potentials $V_1(\mathbf{r})$ and $V_2(\mathbf{r})$. Use the principles of the variational method to show that $E_1 \leq E_2$ if $V_1(\mathbf{r}) \leq V_2(\mathbf{r})$. *[use the wavefunction of a particle moving in $V_2(\mathbf{r})$ as a trial wavefunction for potential $V_1(\mathbf{r})$.]*

b) Consider a particle moving in a one-dimensional attractive potential $V(x)$, i.e. a potential such that $V(x) \leq 0$, for all x and $V(x) \rightarrow 0$, as $|x| \rightarrow \infty$. Use the variational principle with trial function $A \exp(-\lambda x^2)$ to show that the upper bound on the ground state energy is negative, and hence that for any such potential at least one bound state must exist.

10 Molecular bonding (Tripos 1998)

Explain what is meant by the Born-Oppenheimer approximation and discuss how molecular wavefunctions can be formed within this approximation by using the Linear Combination of Atomic Orbitals (LCAO).

The H_3^+ ion exists as an isosceles triangle (distance $d_{12}=d_{23}$) as shown, with $60^\circ \leq \theta \leq 180^\circ$.



Treat this ion in the LCAO approximation by introducing as a basis the $1s$ wavefunctions $|\psi_i\rangle$ for the i^{th} atom. Show that the electron energy levels are solutions of the determinantal equation

$$\begin{vmatrix} \alpha - E & \beta & \gamma\beta \\ \beta & \alpha - E & \beta \\ \gamma\beta & \beta & \alpha - E \end{vmatrix} = 0$$

where we assume $\alpha = \langle \psi_1 | \hat{H} | \psi_1 \rangle = \langle \psi_2 | \hat{H} | \psi_2 \rangle = \langle \psi_3 | \hat{H} | \psi_3 \rangle$, $\beta = \langle \psi_1 | \hat{H} | \psi_2 \rangle = \langle \psi_2 | \hat{H} | \psi_3 \rangle < 0$ and $\beta\gamma = \langle \psi_1 | \hat{H} | \psi_3 \rangle$ and \hat{H} is the Hamiltonian for the ion. In this case, ignore the overlap integrals, so $\langle \psi_i | \psi_j \rangle = \delta_{ij}$. By solving the determinantal equation[§] show that one energy level has the value $E = \alpha - \gamma\beta$ and find expressions for the other two. Sketch the energy levels in the range $0 \leq \gamma \leq 1$ and explain why the ground state must be a spin singlet.

[§][rearrange the cubic in $E - \alpha$ so that you can take out a factor of $E - \alpha + \gamma\beta$].

11 Molecular bonding*

In the pure valence bonding approximation, the electronic ground-state wave function of the H_2 molecule is

$$\psi^{VB} = C[\psi_a(\mathbf{r}_1)\psi_b(\mathbf{r}_2) + \psi_b(\mathbf{r}_1)\psi_a(\mathbf{r}_2)]$$

where ψ_a and ψ_b are the ground-state wave functions of the two hydrogen atoms.

- Express the normalization constant C in terms of the overlap integral $S = \int \psi_a \psi_b d^3\mathbf{r}$.
- Express ψ^{VB} in terms of the molecular orbitals $\sigma_g(1)\sigma_g(2)$ and $\sigma_u^*(1)\sigma_u^*(2)$ defined in the lectures.
- Hence find a second molecular state, ψ_\perp which is orthogonal to ψ^{VB} and interpret it in terms of covalent and ionic components.
- Use the result $S = (1 + \rho + \rho^2/3)e^{-\rho}$ with $\rho = R/a_0 \approx 1.6$ to estimate the configuration mixing (i.e. the relative contributions of VB and IB) in ψ_\perp .

12 Perturbation Theory

Describe how perturbation theory can be used to obtain approximate values for the energy of a non-degenerate state when exact solution of the Schrödinger equation is not possible.

An anharmonic one-dimensional oscillator for a particle of mass m has potential

$$V(x) = \frac{1}{2}m\omega^2x^2 + \lambda x^4$$

where λ is small. Use perturbation theory, treating λx^4 as a perturbation, to determine the ground state energy to first order in λ .

[The ground state wavefunction for the harmonic oscillator with $V(x) = \frac{1}{2}m\omega^2x^2$ is $(m\omega/\pi\hbar)^{1/4} \exp(-m\omega x^2/2\hbar)$.]

13 Perturbation Theory

The fact that the proton is not a point charge influences the energy levels of the Hydrogen atom. This problem may be treated (for simplicity) by regarding the proton as a uniformly charged hollow spherical shell of radius $b = 5 \times 10^{-16}$ m. Show that the change in the electrostatic potential energy corresponds to introducing a perturbation

$$\frac{e^2}{4\pi\epsilon_0} \left(\frac{1}{r} - \frac{1}{b} \right) ; r < b$$

into the normal Schrödinger equation for the Hydrogen atom. Use first order perturbation theory to estimate the energy shifts of the hydrogen 2s and 2p states. Comment on your results. Explain why measurement of such energy shifts is not a good way of studying the proton charge distribution.

[You can, and should, simplify the integrals considerably by noting that the size of the nucleus \ll the Bohr radius, i.e. $b \ll a_0$.]

14 Perturbation Theory*

This example shows how perturbation theory may be used to estimate the polarizability of the H atom in its ground state (the induced dipole moment in an applied electric field \mathcal{E} is $\alpha\epsilon_0\mathcal{E}$ where α is the polarizability).

Show that the energy shift in the ground state $|0\rangle$ is (to second order in \mathcal{E}):

$$e^2\mathcal{E}^2 \sum_{k \neq 0} \frac{|\langle k|z|0\rangle|^2}{E_0 - E_k}$$

and hence

$$\alpha = \frac{2e^2}{\epsilon_0} \sum_{k \neq 0} \frac{|\langle k|z|0\rangle|^2}{E_k - E_0}$$

where E_k is the unperturbed energy of state $|k\rangle$.

Show that the same result may be obtained by considering the perturbed wavefunction to first order in \mathcal{E} and evaluating the expectation value of the electric dipole moment.

Evaluation of α is tedious, but a useful upper bound may be obtained as follows: note that $E_k \geq E_1$ where E_1 is the energy of the first excited state, and that

$$\sum_{k \neq 0} \langle 0|z|k\rangle \langle k|z|0\rangle = \sum_k \langle 0|z|k\rangle \langle k|z|0\rangle - \langle 0|z|0\rangle^2 = \langle 0|z^2|0\rangle - 0$$

Evaluate the matrix element $\langle 0|z^2|0\rangle$ and thus obtain

$$\alpha \leq \frac{64\pi a_0^3}{3}$$

Compare this with the experimental value of $\alpha = 8.5 \cdot 10^{-30} \text{ m}^3$.

15 Degenerate Perturbation Theory

A particle of mass m is constrained to move in the $x - y$ plane so that the Hamiltonian is:

$$\hat{H} = \frac{1}{2m} (\hat{p}_x^2 + \hat{p}_y^2) + \frac{m\omega^2}{2} (\hat{x}^2 + \hat{y}^2) + \lambda \hat{x}\hat{y}$$

(a) Using raising and lowering operators show that for $\lambda = 0$ the (unperturbed) energy eigenvalues can be described by the equation $E_{n_x, n_y} = (n_x + n_y + 1)\hbar\omega$.

(b) For the ground state and first two excited states describe the eigenstates for the system in terms of the eigenstates for a 1D harmonic oscillator, $|n_x\rangle$ and $|n_y\rangle$. Note the degeneracies for each of these energy levels.

(c) In the case when $\lambda \neq 0$, use degenerate perturbation theory to determine the energy splitting for the lowest degenerate states as well as the first order corrections to the wavefunctions for these states.

[The following equations may prove useful:

$$\hat{a}^\dagger = \frac{1}{\sqrt{2m\hbar\omega}}(-i\hat{p} + m\omega\hat{x}), \quad \hat{a} = \frac{1}{\sqrt{2m\hbar\omega}}(i\hat{p} + m\omega\hat{x}), \quad \hat{a}|n\rangle = \sqrt{n}|n-1\rangle, \quad \hat{a}^\dagger|n\rangle = \sqrt{n+1}|n+1\rangle]$$

16 Magnetic fields; time dependence; precession

A beam of hydrogen molecules is moving in the y -direction. An x Stern-Gerlach apparatus is used as a filter which rejects para- H_2 (resultant nuclear spin zero) and passes ortho- H_2 (resultant nuclear spin one) with spin component $+\hbar$ in the x direction. A magnetic field B in the z direction acts over 20 mm of path between two such filters in series, and it is found that no molecules of kinetic energy 0.025 eV emerge when $B = 1.8(n + \frac{1}{2}) \times 10^{-3} \text{ T}$, where n is an integer. Explain this phenomenon and deduce a value for the magnetic moment of the proton.

[The \hat{S}_x operator and eigenstates in the basis of \hat{S}_z eigenstates are:

$$\hat{S}_x = \frac{\hbar}{\sqrt{2}} \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix} \text{ with eigenstates: } \begin{matrix} m_x = 1 & m_x = 0 & m_x = -1 \\ \frac{1}{2} \begin{pmatrix} 1 \\ \sqrt{2} \\ 1 \end{pmatrix} & \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 0 \\ -1 \end{pmatrix} & \frac{1}{2} \begin{pmatrix} 1 \\ -\sqrt{2} \\ 1 \end{pmatrix} \end{matrix}$$

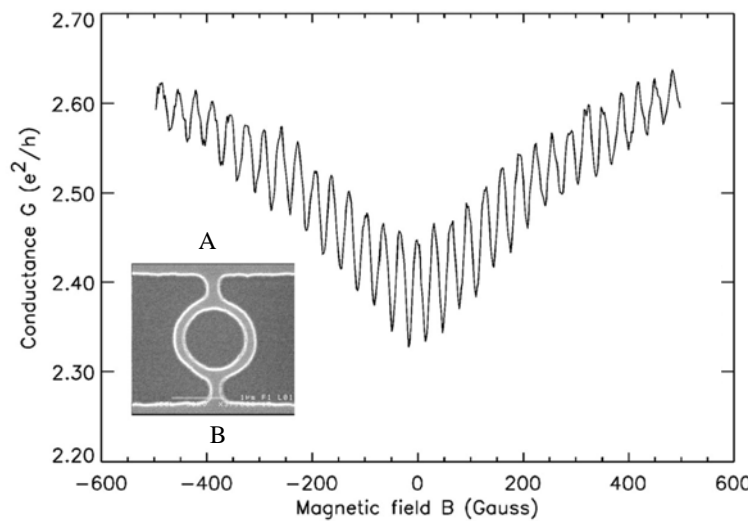
[Continued overleaf]

Write the wavefunction corresponding to spin $+\hbar$ in the x direction using as a basis the \hat{S}_z eigenstates. Then write the time dependence of this wavefunction in presence of the uniform field B , and find the fraction of the $S_x = +\hbar$ state in this wavefunction at a later time. You can also obtain the same result from a classical precession argument.]

17 Magnetic fields; the Aharonov Bohm effect

A ring shaped semiconductor device is fabricated from a high mobility two-dimensional electron gas (see picture below; the lighter grey is the conducting region). The ring is cooled in a cryostat to 0.3K. A voltage is applied across the ring, between point A and point B and the current flow is measured as a function of magnetic field perpendicular to the plane of the ring. Explain why the oscillations in conductance occur, account for their periodicity and obtain a value for the inside diameter of the ring.

(note that 1 Tesla = 10^4 Gauss)



(S Pedersen et al Phys Rev B 61,5457-5460 (2000))

18 Relativistic quantum mechanics

Prove the identity $(\boldsymbol{\sigma} \cdot \mathbf{a})(\boldsymbol{\sigma} \cdot \mathbf{b}) = \mathbf{a} \cdot \mathbf{b} + i\boldsymbol{\sigma} \cdot (\mathbf{a} \times \mathbf{b})$ for the Pauli spin matrices $\boldsymbol{\sigma} = (\sigma_x, \sigma_y, \sigma_z)$ where \mathbf{a} and \mathbf{b} are vector operators.

Using this identity show that the Dirac equation possesses both negative and positive energy plane wave solutions and explain what these solutions represent.

19 Relativistic quantum mechanics

Write an essay on relativistic quantum mechanics. Your answer should include a discussion of electron spin, the spin orbit interaction and the existence of antiparticles.

20 Magnetic fields*

Explain why a magnetic field B in the z -direction acting on an electron in an atom may be treated as the perturbation

$$\frac{eB}{2m_e}(\hat{L}_z + 2\hat{S}_z) + \frac{e^2 B^2}{8m_e}(x^2 + y^2) .$$

Find the corresponding energy change to second order in B in terms of atomic quantum numbers, expectation values and matrix elements. Separate the terms corresponding to *normal paramagnetism*, *diamagnetism* and (by a process of elimination) *Van Vleck paramagnetism*.

21 Magnetic fields; Landau Levels

A spinless particle of charge q is confined to the x - y plane. It is subjected to a magnetic field $\mathbf{B} = (0, 0, B)$. Using the *Landau gauge* $\mathbf{A} = (0, Bx, 0)$ show that the eigenvalue equation can be written;

$$\frac{-\hbar^2}{2m} \left(\frac{\partial^2}{\partial x^2} + \left(\frac{\partial}{\partial y} - i \frac{qB}{\hbar} x \right)^2 \right) \Psi(x, y) = E \Psi(x, y)$$

Show that this equation has a solution of the form $\Psi(x, y) = e^{iky} u(x - a)$ and find an expression for k in terms of a . Explain the nature of the function $u(x - a)$ and why the corresponding energy eigenvalues are given by the equation

$$E = \left(n + \frac{1}{2} \right) \frac{\hbar q B}{m} \quad n = 0, 1, 2, \dots$$

The particles are confined to an area of length X in the x -direction and Y in the y -direction. By imposing periodic boundary conditions in the y -direction find an expression for the maximum number of states per unit area in a full Landau level.

[remember that $0 \leq a \leq X$]

Try to reconcile the solution with that described in lectures where the potential $\mathbf{A} = \frac{1}{2}(-By, Bx, 0)$ was used.

22 Magnetic fields; Hyperfine interaction *

The magnetic part of the Hamiltonian for a hydrogen atom in the 1s state, in the presence of a constant magnetic field B along the z axis, may be written in the form

$$H = B(\mu_e \sigma_{ze} + \mu_p \sigma_{zp}) + W \vec{\sigma}_e \cdot \vec{\sigma}_p,$$

where the subscripts e and p refer to the electron and proton, the vector components of $\vec{\sigma}$ are the Pauli spin operators, μ is the magnetic dipole moment, and W is a constant.

(a) Explain the physical origin of each term in the Hamiltonian.

(b) Using as a basis the states $|\uparrow_e \uparrow_p\rangle, |\uparrow_e \downarrow_p\rangle, |\downarrow_e \uparrow_p\rangle, |\downarrow_e \downarrow_p\rangle$ and neglecting the small term in μ_p , show that H may be represented by the matrix

$$\begin{pmatrix} b+W & 0 & 0 & 0 \\ 0 & b-W & 2W & 0 \\ 0 & 2W & -b-W & 0 \\ 0 & 0 & 0 & -b+W \end{pmatrix} \quad \text{where } b = \mu_p B.$$

(c) Determine the energy levels and sketch them as functions of B , labelling them with as much information as possible about the angular momenta of the states.

23 Transitions: Two state system (Tripos 1999)

A spin $-\frac{1}{2}$ particle has gyromagnetic ratio γ , so that its magnetic moment is given by $\hat{\boldsymbol{\mu}} = \gamma \hat{\mathbf{S}}$ where $\hat{\mathbf{S}}$ is the spin operator. Show that the equation of motion for the spin state $|\psi(t)\rangle$ of such a particle in a magnetic field \mathbf{B} is

$$-\frac{1}{2}\gamma\mathbf{B}\cdot\hat{\boldsymbol{\sigma}}|\psi(t)\rangle = i\frac{d}{dt}|\psi(t)\rangle,$$

where $\hat{\boldsymbol{\sigma}}$ is a vector with the Pauli matrices $\hat{\sigma}_i$ as components.

If \mathbf{B} is a constant field in the z-direction with magnitude B_0 , and

$$|\psi(0)\rangle = \cos(\theta/2)|\uparrow\rangle + \sin(\theta/2)|\downarrow\rangle$$

Show that at time t

$$|\psi(t)\rangle = \cos(\theta/2)\exp(i\omega_0 t/2)|\uparrow\rangle + \sin(\theta/2)\exp(-i\omega_0 t/2)|\downarrow\rangle$$

where $\omega_0 = \gamma B_0$, and find the expectation values of the components of the magnetic moment $\hat{\boldsymbol{\mu}}$ at time t.

Using the general relation
$$\frac{d}{dt}\langle\hat{A}\rangle = \frac{i}{\hbar}\langle[\hat{H}, \hat{A}]\rangle$$

For the time evolution of the expectation value of an operator \hat{A} , show that for an arbitrarily-varying magnetic field $\mathbf{B}(t)$ the magnetic moment operator satisfies

$$\frac{d}{dt}\langle\hat{\mathbf{S}}\rangle = \langle\hat{\boldsymbol{\mu}}\rangle \times \mathbf{B}(t)$$

and demonstrate explicitly that the expectation values found above for the constant field satisfy this relation. Interpret your results physically.

24 Write brief notes on the following:

- a) The measurement of the magnetic moment of a particle
- b) The discovery of the positron
- c) Landau levels

25 Time Dependence

A system is, at $t=0$, in an energy eigenstate ψ_0 when a weak perturbation $\hat{H}'(t)$ is applied. Show that the probability of finding the system in state ψ_n at time t is given approximately by $|c_n|^2$ where

$$c_n(t) = \frac{1}{i\hbar} \int_0^t dt' \exp(i(E_n - E_0)t'/\hbar) \langle\psi_n | H'(t') | \psi_0 \rangle.$$

An electric field $\mathcal{E}_z = 0$ for $t < 0$, $\mathcal{E}_z = \mathcal{E}_0 \exp(-t/\tau)$ for $t > 0$, is applied to a hydrogen atom, initially in its ground state. Find the first order probability that, after a long time, the atom is in (i) the 2s state, and (ii) one of the 2p states (which one?).

26 Time Dependence* (Tripos 2001)

Use the equation derived for $c_n(t)$ in the previous question to answer the following problem:

A one-dimensional harmonic oscillator with Hamiltonian: $\hat{H}_0 = \frac{\hat{p}_x^2}{2m} + \frac{m\omega^2 x^2}{2}$, initially in the ground state, is subjected to a perturbation:

$$\hat{H}'(t) = \begin{cases} 0 & \text{for } t < 0 \text{ and } t > T \\ \lambda x \left(1 - \frac{t}{T}\right) & \text{for } 0 \leq t \leq T \end{cases}$$

Find, to first order in λ , the probability that the oscillator is in the first excited state at time $t > T$.

Verify that for $\omega T \gg 1$ this probability approaches the value of $|\langle \psi_1 | \psi'_0 \rangle|^2$ where $|\psi'_0\rangle$ is the ground state for the Hamiltonian $\hat{H}_0 + \lambda x$.

[The ground state and first excited state of a harmonic oscillator have wavefunctions:

$$\psi_0(x) = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} \exp\left(-\frac{m\omega}{2\hbar}x^2\right), \quad \psi_1(x) = \left(\frac{2m\omega}{\hbar}\right)^{1/2} x \psi_0(x)]$$

27 The Fermi golden rule (Tripos 2004)

A system is described by a Hamiltonian \hat{H}_0 which has eigenstates $|\psi_n\rangle$ with energies E_n . At time $t = 0$, when the system is in the state $|\psi_1\rangle$, a perturbation $V(\mathbf{r})\exp(-i\omega t)$ is applied to the system. Show that, to first order in V , the state of the system for $t \geq 0$ can be written as

$$|\psi(t)\rangle = |\psi_1\rangle \exp(-i\omega_1 t) - \sum_{n \neq 1} \frac{1}{\hbar} \langle \psi_n | \hat{V} | \psi_1 \rangle \frac{\exp(i(\omega_n - \omega - \omega_1)t) - 1}{\omega_n - \omega - \omega_1} |\psi_n\rangle \exp(-i\omega_n t)$$

where $\hbar\omega_n = E_n$.

How does the probability of occupying state $|\psi_n\rangle$ with $n \neq 1$ vary with time when

(i) $E_n = E_1 + \hbar\omega$ and (ii) $E_n \neq E_1 + \hbar\omega$?

Calculate the transition rates in each of these cases.

From the expression for $|\psi(t)\rangle$ derive the Fermi golden rule for the transition rate:

$$T = \frac{2\pi}{\hbar} |\langle \psi_n | \hat{V} | \psi_1 \rangle|^2 g(E_k)$$

where $g(E_k)$ is the density of states per unit energy at energy $E_k = E_1 + \hbar\omega$.

State the assumptions you need to obtain this result and comment on the validity of these assumptions.

$$[\text{you may use the result } \int_{-\infty}^{\infty} \left(\frac{\sin x}{x}\right)^2 dx = \pi]$$

28 Scattering

Show that the Born approximation yields the following expression for the elastic scattering of a particle of mass m and momentum $\hbar k$ from a spherically symmetric potential $V(r)$:

$$\frac{d\sigma}{d\Omega} = \left(\frac{2m}{\hbar^2 K} \right)^2 \left| \int_0^\infty V(r) r \sin(Kr) dr \right|^2,$$

where $K = 2k \sin \frac{1}{2}\theta$ and θ is the angle through which the particle is scattered.

Obtain the differential cross-section for scattering from a potential given by

$$\begin{aligned} V(r) &= -V_0 & r \leq a \\ V(r) &= 0 & r > a \end{aligned}$$

and verify that the scattering is isotropic when the energy of the incident particle or the size of the scatterer is sufficiently low, so that $Ka \ll 1$. Obtain an expression for the total cross-section in this limit.

29 Spontaneous emission

Use the formula for the Einstein A -coefficient derived in lectures to calculate the lifetime of the 2p state of atomic Hydrogen. [You will need the matrix elements you computed in Q 25.]

Without detailed evaluation of the matrix element, explain why the 3s level of Hydrogen has a lifetime roughly 100 times longer than the 2p level.

Why is the lifetime of the 2s level very much longer (a factor $\sim 10^8$) than the lifetime of the 2p level?

30 Spontaneous emission*

Discuss the connection between matrix elements and selection rules.

In the course of a spontaneous emission, the state of a hydrogen atom is in a mixture of the (n, l, m) states $(2, 1, 1)$ and $(1, 0, 0)$. Show that the components of the atomic dipole moment, $\langle d_x \rangle = e \langle x \rangle$, $\langle d_y \rangle = e \langle y \rangle$, oscillate in quadrature at the frequency of the photon emitted in the transition. Comment on the form of the emitted radiation. Show that the magnitude of the dipole moment is of order ea_0 .

The rate of emission of power for a classical rotating electric dipole d is $W = \omega^4 d^2 / 3\pi\epsilon_0 c^3$. Show that this is consistent with the rate of spontaneous radiation derived in lectures.

31 Coherent states*

Show that the coherent states $|\alpha\rangle$ of an electromagnetic mode can be written in terms of the set of orthonormal number states $|n\rangle$ in the following way:

$$|\alpha\rangle = e^{-|\alpha|^2/2} \sum_{n=0}^{\infty} \frac{\alpha^n}{\sqrt{n!}} |n\rangle$$

Show that the coherent states are not orthogonal to one another and find the probability $p(n)$ of having n photons in the state. Sketch the probability distribution corresponding to a range of different values of $\langle n \rangle$.

32 Lasers (Tripos 2005)

Explain what is meant by the Einstein coefficients, B_{12} , B_{21} and A_{21} for radiative transitions between an upper level (2) and a lower level (1) in an atom.

Given that the energy density per unit ω of black-body radiation is

$$u(\omega) = \frac{\hbar\omega^3}{\pi^2 c^3} \frac{1}{\exp(\hbar\omega/k_B T) - 1}$$

show that the Einstein coefficients satisfy the following equations

$$g_1 B_{12} = g_2 B_{21}, \quad g_2 A_{21} = g_1 B_{12} \frac{\hbar\omega_{12}^3}{\pi^2 c^3}$$

where g_1 and g_2 are the degeneracies of levels 1 and 2 and the difference in energy between the levels is $\hbar\omega_{12}$.

An atom has three levels with energies $E_2 > E_1 > E_0$. Levels 2 and 1 have degeneracies g_2 and g_1 respectively. Spontaneous and stimulated transitions can take place between level 2 and level 1 with coefficients A_{21} , B_{21} and B_{12} . Spontaneous transitions also take place between levels 1 and 0 with coefficient A_{10} . A quantity of these atoms is subjected to a background radiation density $u(\omega)$ and is also optically pumped from level 0 to level 2 at a rate R per atom.

Write down rate equations for the numbers of atoms per unit volume, N_1 and N_2 , in levels 1 and 2.

Show that in equilibrium

$$\frac{N_2}{N_1} = \frac{A_{10} + \frac{g_2}{g_1} B_{21} u(\omega_{12})}{A_{21} + B_{21} u(\omega_{12})}$$

and find an expression for $\Delta N = N_2 - \frac{g_2}{g_1} N_1$.

Comment on the effect of (a) the spontaneous emission coefficients and (b) the level degeneracy, on the use of this atomic system for a laser.

33 Light

Write an essay on the quantum picture of light. Your essay should include references to the magnetic vector potential, creation and annihilation operators, the vacuum state and number states. Describe how these ideas relate to spontaneous and stimulated transitions.

34 Spectroscopic Terms

Determine the possible $^{2s+1}L_J$ values for each of the following configurations: $(2s)(3p)$, $(2p)^2$, $(3d)^2$, $(3d)^{10}$, $(3d)^9$.

Use Hund's rules to determine the angular momentum quantum numbers of the ground state of Sm, which has electronic configuration $(4f)^6$.

35 Single electron spectra

The following three groups of lines, whose frequencies are given in units of 10^{15} Hz, are observed in the emission spectrum of atomic sodium:

(i) Doublets with decreasing doublet splitting:

0.50899	0.90782	1.05086	1.11848
0.50847	0.90765	1.05079	1.11845

(ii) Doublets with constant doublet splitting:

0.26340	0.48713	0.58225	0.63142
0.26288	0.48662	0.58174	0.63090

(iii) Triplets, with two lines sometimes unresolved:

0.36635	0.52756	0.60207	0.64267
0.365833	0.52704	0.60165	0.64215
0.365831			

Make an index of these transitions, i.e. identify them with specific states of the sodium atom. You may find it helpful to answer the following questions. What are the appropriate quantum numbers for the outer electron in Sodium? Which energy levels are split by the spin-orbit interaction? How (qualitatively) does the spin-orbit coupling depend on n ? Which transitions are allowed by selection rules?

Draw an energy level diagram, taking the (3s) state as the zero of energy, and answer the following questions:

- (a) What is the energy difference between the (5p) $J = \frac{3}{2}$ and $J = \frac{1}{2}$ states in Sodium?
- (b) Estimate the first ionization energy of Sodium.
- (c) What are the relative importances of the ℓ -dependence of the electron-electron energy, and the j -dependence of the spin-orbit energy in the $n = 3$ and $n = 6$ shells?

[See lecture notes for an energy level diagram]

36 Atomic Spectra (Tripos 1997)

What are the selection rules for electric dipole transitions in atomic spectra, and what additional rules apply if the atom is accurately described by LS coupling?

The absorption spectrum of Helium shows one series of single lines, the two of lowest wavelength occurring at 58.4 nm and 53.7 nm. If the sample is excited by an electrical discharge, two new prominent single absorption lines are observed, at 2058 nm and 501.6 nm, and two prominent multiplet absorptions at 1083 nm and 389 nm. In emission, in addition to all the above wavelengths, single emission lines are seen at 728 and 668 nm, and multiplets at 707 and 588 nm.

Write the term symbol for the ground state (1s)² of Helium, and for all the excited states of the

form $(1s)^1 (nl)^1$ with $n = 2, 3$. Draw a diagram of the energy levels, and mark on it the spectral transitions described above, giving your reasoning.

Describe qualitatively how the spectra would be modified in the series of increasing atomic number Be, Mg, Ca, each of which has electron configuration $(ns)^2$. Why does Ca display two absorption transitions, at 647 nm and 423 nm, from the ground state to the first excited state: $(4s)^2 \rightarrow (4s)^1 (4p)^1$, and why is each a single line?

[See lecture notes for an energy level diagram]

37 Write brief notes on the following

- The quantum cascade laser
- The Lamb shift
- Quantum jumps

38 Zeeman effect (Tripos 2004)

Explain why, in the L - S (Russell-Saunders) coupling scheme, the good quantum numbers for the electronic configuration of an atom are L , S , J and m_j .

A magnetic field B in the z -direction is applied to an atom described by the L - S coupling scheme so that, to first order in B , the energies of the states change by:

$$\Delta E_{L,S,J,m_j} = \left\langle \phi_{L,S,J,m_j} \left| \frac{Be}{2m_e} (\hat{L}_z + 2\hat{S}_z) \right| \phi_{L,S,J,m_j} \right\rangle.$$

Explain why the state $|\phi_{L=2,S=1,J=3,m_j=3}\rangle$ can be written as

$$|\phi_{L=2,S=1,J=3,m_j=3}\rangle = |\psi_{L=2,m_L=2}\rangle |\chi_{S=1,m_S=1}\rangle$$

where $|\psi_{L,m_L}\rangle$ are orbital angular momentum eigenstates and $|\chi_{S,m_S}\rangle$ are spin angular momentum eigenstates.

Calculate the change in energy of the state with quantum numbers $L = 2, S = 1, J = 3, m_j = 3$ on application of the magnetic field.

Show that your result is consistent with the following formula for the Landé g -factor

$$g = \frac{3}{2} - \frac{L(L+1) - S(S+1)}{2J(J+1)}$$

Calculate the change in energy of the state with quantum numbers $L = 2, S = 1, J = 3, m_j = 2$ and that of the state with quantum numbers $L = 2, S = 1, J = 2, m_j = 2$. Show that these are also consistent with the formula for the Landé g -factor.

[The raising and lowering operators for orbital angular momentum are defined as follows:

$$\hat{L}_\pm |\psi_{L,m_L}\rangle = \hbar \sqrt{L(L+1) - m_L(m_L \pm 1)} |\psi_{L,m_L \pm 1}\rangle$$

and similarly for \hat{J}_\pm and \hat{S}_\pm .]

39 Zeeman Effect

For an atom characterised by LS coupling, and subject to a weak uniform magnetic field, derive the Landé g -factor

$$g = \frac{3J(J+1) - L(L+1) + S(S+1)}{2J(J+1)}.$$

In a Zeeman experiment, the ${}^3S_1 \rightarrow {}^3P_1$ emission of an ensemble of such atoms is observed in the presence of a weak magnetic field B . Describe the resulting Zeeman structure of the atomic levels, and indicate which transitions amongst the split levels are allowed in an electric dipole transition. Sketch the form of the line spectrum seen in some general direction before and after the field is applied. Label, in units of $\mu_B B$ where μ_B is the Bohr magneton, the positions of the components relative to the energy of the unperturbed transition.

If the emission is viewed perpendicular to the direction of the magnetic field, how many lines will be observed and what polarization states will they have?

In a second experiment, a circularly polarised beam of white light, incident along a direction parallel to the magnetic field, is used to excite the ${}^3P_1 \rightarrow {}^3S_1$ absorption. Explain why only two absorption lines are observed. How many lines can subsequently be seen along the same direction when the atoms decay by emission back to the 3P_1 state, and what are their polarizations?

40 Write brief notes on the following

- a) Qubits and quantum gates
- b) Teleportation of quantum states
- c) Quantum cryptography

ANSWERS

1(b) $a = \pm 1, |\psi_{\pm}\rangle = \frac{1}{\sqrt{2}} [|\psi_1\rangle \pm |\psi_2\rangle]$

(c) $|\psi(t)\rangle = \frac{1}{\sqrt{2}} [|\psi_1\rangle e^{-iE_1t/\hbar} - |\psi_2\rangle e^{-iE_2t/\hbar}]$

3 Spin operator $\frac{1}{2}\hbar \begin{pmatrix} \cos\theta & \sin\theta e^{-i\phi} \\ \sin\theta e^{i\phi} & -\cos\theta \end{pmatrix}$

Eigenstates $\begin{pmatrix} \cos\frac{1}{2}\theta \\ \sin\frac{1}{2}\theta e^{i\phi} \end{pmatrix}; \begin{pmatrix} \sin\frac{1}{2}\theta \\ -\cos\frac{1}{2}\theta e^{i\phi} \end{pmatrix}$ for eigenvalues $+\frac{1}{2}\hbar; -\frac{1}{2}\hbar$ respectively.

+x: $\frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix} = (\chi_+ + \chi_-)/\sqrt{2}; -x: \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -1 \end{pmatrix} = (\chi_+ - \chi_-)/\sqrt{2};$

+y: $\frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ i \end{pmatrix} = (\chi_+ + i\chi_-)/\sqrt{2}; -y: \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -i \end{pmatrix} = (\chi_+ - i\chi_-)/\sqrt{2};$

where χ_{\pm} are the wavefunctions corresponding to z-component of spin $= \pm\frac{1}{2}\hbar$. Wavefunctions can of course be multiplied by any overall phase factor.

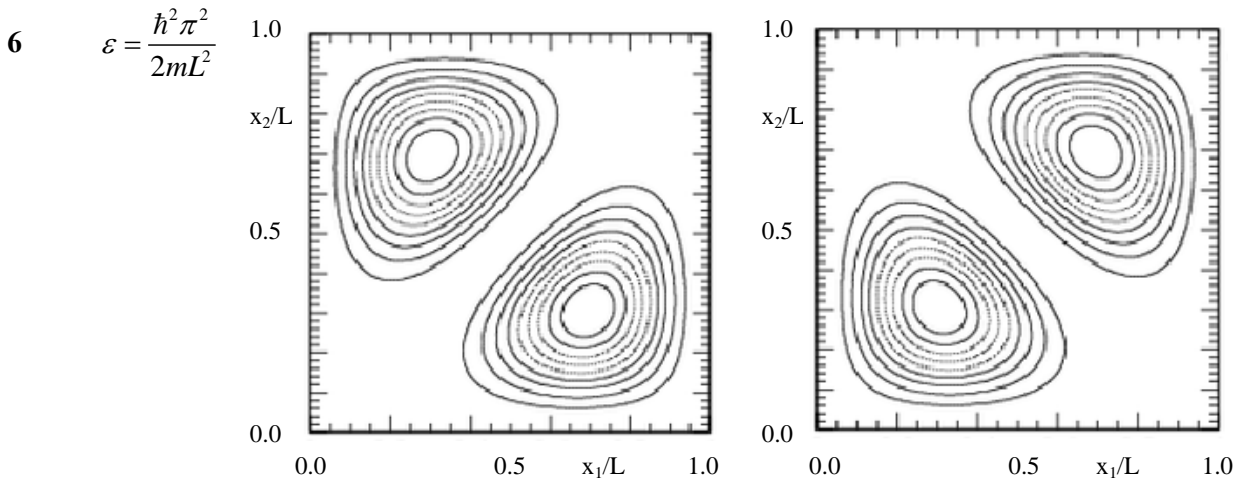
4 a) $|3,2\rangle = \sqrt{\frac{1}{3}}|1,0;2,2\rangle + \sqrt{\frac{2}{3}}|1,1;2,1\rangle, |2,2\rangle = \sqrt{\frac{2}{3}}|1,0;2,2\rangle - \sqrt{\frac{1}{3}}|1,1;2,1\rangle$

b) States $\chi_+(1)\chi_+(2), \chi_-(1)\chi_-(2)$ and $(\chi_+(1)\chi_-(2) + \chi_-(1)\chi_+(2))/\sqrt{2}$ all have $S=1$; $(\chi_+(1)\chi_-(2) - \chi_-(1)\chi_+(2))/\sqrt{2}$ has $S=0$.

Probability of obtaining $S=1$ is $\frac{3+2\sqrt{2}}{6} = 0.971$.

5 Energies $\frac{\hbar^2}{2} \left(\frac{1}{I_x} + \frac{1}{I_y} \right), \frac{\hbar^2}{2} \left(\frac{1}{I_x} + \frac{1}{I_z} \right), \frac{\hbar^2}{2} \left(\frac{1}{I_y} + \frac{1}{I_z} \right)$

with eigenvectors $\begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}, \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 0 \\ 1 \end{pmatrix}, \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 0 \\ -1 \end{pmatrix}$ respectively.



7 $E \leq \sqrt{\frac{5}{14}} \hbar \omega = 0.598 \hbar \omega$, corresponding to $a^2 = \sqrt{\frac{35}{2}} \frac{\hbar}{m\omega}$.

8 $E \leq -R_\infty = -13.6$ eV, i.e. the exact ground state energy is obtained (because the correct functional form for the wavefunction was chosen).

10 $E = \alpha - \gamma\beta$ or $E = \alpha + \frac{1}{2}\beta \left(\gamma \pm \sqrt{\gamma^2 + 8} \right)$.

11 (a) $C^2 = 1/2(1 + S^2)$

(b) $\psi^{VB} = C[(1 + S)\sigma_g(\mathbf{r}_1)\sigma_g(\mathbf{r}_2) - (1 - S)\sigma_u^*(\mathbf{r}_1)\sigma_u^*(\mathbf{r}_2)]$

(c) $\psi_\perp = [(1 + S^2)\psi^{IB} - 2S\psi^{VB}]/(1 - S^2)$, where $\psi^{IB} = C[\psi_a(\mathbf{r}_1)\psi_a(\mathbf{r}_2) + \psi_b(\mathbf{r}_1)\psi_b(\mathbf{r}_2)]$

(d) IB:VB \sim 1:0.88 in ψ_\perp

12 $\frac{1}{2} \hbar \omega + \frac{3\hbar^2}{4m^2\omega^2} \lambda$

13 2s: $\frac{b^2}{6a_0^2} R_\infty$; 2p: $\frac{b^4}{240a_0^4} R_\infty$, where b is the nuclear radius and a_0 the Bohr radius.

15 (c) $E_2^{(1)} = \pm \frac{\lambda \hbar}{2m\omega}$

16 $\mu_p = 1.42 \times 10^{-26} \text{ JT}^{-1}$

17 $1.3 \mu\text{m}$

21 $k = \frac{qBa}{\hbar}, \quad \frac{qB}{2\pi\hbar}$

22 (c) $E = W \pm b, E = -W \pm \sqrt{4W^2 + b^2}$

25 No probability of being in 2s, 2p_{±1}; probability of being in 2p₀ is $\frac{(\mathcal{E}_0 e a_0 128 \sqrt{2}/243)^2}{(\Delta E^2 + \hbar^2/\tau^2)}$

where ΔE is the difference in energy between 1s and 2p states $= \frac{3}{4} R_\infty$.

26 $\text{Prob} = |c_1|^2 = \left(\frac{\lambda}{\hbar\omega} \right)^2 \frac{\hbar}{2m\omega} \left| 1 + \frac{1 - \exp(i\omega T)}{i\omega T} \right|^2$

27 (i) $\text{Prob} = \frac{1}{\hbar^2} |\langle \psi_n | \hat{V} | \psi_1 \rangle|^2 t^2$ (ii) $\text{Prob} = \frac{4}{\hbar^2 \Delta\omega^2} |\langle \psi_n | \hat{V} | \psi_1 \rangle|^2 \sin^2 \left(\frac{\Delta\omega t}{2} \right), \Delta\omega = \omega_n - \omega_1 - \omega$

28 $\frac{d\sigma}{d\Omega} = \left[\frac{2mV_0}{\hbar^2 K^3} (\sin Ka - Ka \cos Ka) \right]^2$ Low energy limit: $\sigma = 4\pi \left(\frac{2mV_0 a^3}{3\hbar^2} \right)^2$

29 1.6 ns

30 Rotating dipole moment during the transition \Rightarrow circularly polarised radiation.
Dipole = $128ea_0/243$

$$31 \quad p(n) = \frac{\langle n \rangle^n e^{-\langle n \rangle}}{n!}$$

$$32 \quad \Delta N = \frac{RN_0}{A_{10}} \frac{A_{10} - \frac{g_2}{g_1} A_{21}}{A_{21} + B_{21}u(\omega)}$$

34 (2s)(3p): $^1P_1, ^3P_{0,1,2}$; (2p)²: $^1S_0, ^1D_2, ^3P_{0,1,2}$; (3d)²: $^1S_0, ^1D_2, ^1G_4, ^3P_{0,1,2}, ^3F_{2,3,4}$; (3d)¹⁰: 1S_0 ; (3d)⁹: $^2D_{\frac{3}{2}, \frac{5}{2}}$. Sm ground state 7F_0

35 (i) $3p \rightarrow 3s, 4p \rightarrow 3s, 5p \rightarrow 3s, 6p \rightarrow 3s$
(ii) $4s \rightarrow 3p, 5s \rightarrow 3p, 6s \rightarrow 3p, 7s \rightarrow 3p$
(iii) $3d \rightarrow 3p, 4d \rightarrow 3p, 5d \rightarrow 3p, 6d \rightarrow 3p$

(a) 0.29 meV; (b) 5.2 eV; (c) about equal

38

$$L = 2, S = 1, J = 3, m_J = 3 \Rightarrow \Delta E = 4\mu_B B$$

$$L = 2, S = 1, J = 3, m_J = 2 \Rightarrow \Delta E = \frac{8}{3}\mu_B B$$

$$L = 2, S = 1, J = 2, m_J = 2 \Rightarrow \Delta E = \frac{7}{3}\mu_B B$$

39 In general, observe seven lines, displaced by $\pm 2\mu_B B, \pm \frac{3}{2}\mu_B B, \pm \frac{1}{2}\mu_B B$ and 0 w.r.t. unperturbed transition.

View perpendicular to B – three lines ($0, \pm \frac{1}{2}$) plane polarised parallel to B and four lines ($\pm 2, \pm \frac{3}{2}$) plane polarised perpendicular to B .

Fluorescence – three lines, circularly polarised, two polarised in same sense as original, one in the other sense.