PAPER 3 (Advanced Quantum Physics) – ANSWERS

1 (a) *Carbon has electronic structure* $(1s)^2(2s)^2(2p)^2$. *Derive all possible spectroscopic terms* ($^{2S+1}L_J$) *for the partially filled shell within the LS coupling scheme.* [4]

[Similar questions covered in the lectures and in the examples sheet.]

- The two electrons each have $s = 1/2$ and $\ell = 1$. The total spin can $S = 0, 1$. The total orbital angular momentum can be $L = 0, 1, 2$.
- The combinations are restricted by the Pauli principle. This can be implemented in various ways. One method:
  $S = 0$ is anti-symmetric under exchange for the electrons, so the spatial (orbital) wave function must be symmetric, allowing $L = 0, 2$. From these, we obtain $S = 0, L = 0, J = 0$ and $S = 0, L = 1, J = 2$: $^1S_0$, $^1D_2$.
  $S = 1$ is symmetric under exchange for the electrons, so the spatial (orbital) wave function must be anti-symmetric, allowing $L = 1$. From these, we obtain $S = 1, L = 1, J = 0, 1, 2$: $^3P_{0,1,2}$.

(b) *Estimate the Stark shift of the ground state of a KRb molecule in a weak electric field of strength* $\mathcal{E} = 1\,kV\,cm^{-1}$. *The molecule may be viewed as a rigid rotor with moment of inertia* $I = 7.52 \times 10^{-45}\,kg\,m^2$ *and electric dipole moment* $d = 1.89 \times 10^{-30}$ *Cm.* [4]

[You may assume that the z-component of the dipole moment has matrix element $\langle \ell = 1, m_\ell = 0 \,|\, \hat{d}_z \,|\, \ell = 0, m_\ell = 0 \rangle = d/\sqrt{3}$, with ℓ, m_ℓ labelling the molecule's angular momentum and its projection along z.]

[Related Stark shift of Hydrogen is covered in detail in lectures and examples.]

- For the rigid rotor, the energy spectrum is [1]

$$E_\ell = \frac{\hbar^2 \ell(\ell+1)}{2I}$$

- The Stark shift of the ground state is given by second order perturbation theory as [2]

$$\Delta E = -\sum_{\ell \neq 0} \frac{|\langle \ell, 0 | \mathcal{E} \hat{d}_z | 0, 0 \rangle|^2}{E_\ell}$$

Only $\ell = 1$ contributes (selection rules) leading to

$$\Delta E = -\frac{|\langle 1, 0 | \mathcal{E} \hat{d}_z | 0, 0 \rangle|^2}{E_1}$$

- Putting in the values we find [1]

$$\Delta E = -8.03 \times 10^{-27}\text{J} = -12\text{MHz}$$

(c) *The electric field in a single mode cavity is described by the operator* $\hat{\mathcal{E}} = \mathcal{E}_0(\hat{a} + \hat{a}^\dagger)$ *where* $\hat{a}^{(\dagger)}$ *are the usual ladder operators, with* $[\hat{a}, \hat{a}^\dagger] = 1$. *The cavity is in a (normalised) coherent state* $|\alpha\rangle$, *such that* $\hat{a}|\alpha\rangle = \alpha|\alpha\rangle$ *with* α *a complex number. Show that the uncertainty in the electric field is* $\Delta\mathcal{E} = \mathcal{E}_0$. [4]

[Derivation of a result quoted in lectures/handout, using methods explained there.]

$$\Delta\mathcal{E}^2 = \langle\mathcal{E}^2\rangle - \langle\mathcal{E}\rangle^2$$

$$\begin{aligned}
\langle\mathcal{E}\rangle &= \mathcal{E}_0\langle\alpha|(\hat{a} + \hat{a}^\dagger)|\alpha\rangle \\
\hat{a}|\alpha\rangle &= \alpha|\alpha\rangle \\
\langle\alpha|\hat{a}|\alpha\rangle &= \alpha \\
\langle\alpha|\hat{a}^\dagger|\alpha\rangle &= \langle\alpha|\hat{a}|\alpha\rangle^* = \alpha^* \\
\langle\mathcal{E}\rangle &= \mathcal{E}_0\,(\alpha + \alpha^*)
\end{aligned}$$

$$\begin{aligned}
\langle\mathcal{E}^2\rangle &= \mathcal{E}_0^2\langle\alpha|(\hat{a}^2 + \hat{a}^{\dagger 2} + \hat{a}\hat{a}^\dagger + \hat{a}^\dagger\hat{a})|\alpha\rangle \\
&= \mathcal{E}_0^2\langle\alpha|(\hat{a}^2 + \hat{a}^{\dagger 2} + 2\hat{a}^\dagger\hat{a} + 1)|\alpha\rangle \\
&= \mathcal{E}_0^2\left(\alpha^2 + \alpha^{*2} + 2|\alpha|^2 + 1\right)
\end{aligned}$$

$$\begin{aligned}
\Delta\mathcal{E}^2 &= \langle\mathcal{E}^2\rangle - \langle\mathcal{E}\rangle^2 \\
&= \mathcal{E}_0^2\left(\alpha^2 + \alpha^{*2} + 2|\alpha|^2 + 1 - \alpha^2 - \alpha^{*2} - 2|\alpha|^2\right) \\
&= \mathcal{E}_0^2
\end{aligned}$$

2 *Write notes on* **two** *of the following:* *[each part carries equal credit]* [13]

(a) *The JWKB approximation.*

(b) *The fine structure of the Hydrogen atom.*

(c) *The operating principles of a three-level laser.*

[All standard bookwork.]

(a) The JWKB approximation.

- This is a semiclassical method for solution of the one-dimensional Schrodinger equation.
- One writes

$$\psi(x) = e^{i\sigma(x)/\hbar}$$

and derives a differential equation for the phase $\sigma(x)/\hbar$. This is solved by an expansion in the gradients, or equivalently an expansion in $1/\hbar$.

- The WKB result is obtained from the two lowest terms in this expansion. These leads to the WKB wave function

$$\psi(x) = \frac{C_1}{\sqrt{p(x)}} e^{(i/\hbar)\int^x p\,dx'} + \frac{C_2}{\sqrt{p(x)}} e^{-(i/\hbar)\int^x p\,dx'}$$

where

$$p(x) = \sqrt{2m(E - V(x))}$$

- The approximation is accurate for particles with high kinetic energy. Specifically, it is accurate for

$$\frac{1}{2\pi} |\partial_x \lambda(x)| \ll 1$$

where $\lambda(x) = h/p(x)$ is the local wavelength.

- A variant exists for particles with large negative kinetic energy: where the travelling waves are replaced by exponentially growing/decaying evanescent waves.
- This condition fails at the classical turning points, where the kinetic energy is zero.
- In the vicinity of these points, the WKB solutions between the classically forbidden and classically allowed regions, can be matched by the "connection formulas".

(b) The fine structure of the Hydrogen atom.

- The fine structure corrections are the corrections to the energy levels of the H atom arising from the relativistic motion of the electron.

- The size of the corrections is characterised by the fine structure constant, set by $\alpha \simeq (v/c)$ where v is the typical velocity of the electron, $v \simeq \frac{\hbar}{m a_0}$ with a_0 the Bohr radius. Hence the fine structure constant

$$\alpha = \frac{e^2}{4\pi\epsilon_0}\frac{1}{\hbar c} \simeq \frac{1}{137}$$

–relativistic corrections to the kinetic energy;

$$\hat{H}_1 = -\frac{1}{8}\frac{(\hat{\boldsymbol{p}}^2)^2}{m^3c^2}$$

The correction can be calculated by first order perturbation theory.

–coupling between spin and orbital degrees of freedom;

$$\hat{H}_2 = \frac{1}{2m^2c^2}\frac{Ze^2}{4\pi\epsilon_0}\frac{1}{r^3}\,\hat{\boldsymbol{S}}\cdot\hat{\boldsymbol{L}}$$

Physically, the origin of the spin-orbit interaction can be understood from the following considerations. As the electron is moving through the electric field of the nucleus then, in its rest frame, it will experience this as a magnetic field. There will be an additional energy term in the Hamiltonian associated with the orientation of the spin magnetic moment with respect to this field.
This causes the spin and orbital angular momenta to be coupled, such that the states are described by the total angular momentum J.

–a contribution known as the Darwin term.
This arises from the "Zitterbewegung" of the electron – trembling motion – which smears the effective potential felt by the electron. Such effects lead to a perturbation of the form,

$$\hat{H}_3 = \frac{\hbar^2}{8m^2c^2}\nabla^2 V = \frac{e^2}{4\pi\epsilon_0}\,\frac{\hbar^2}{8(mc)^2}\,4\pi\delta^{(3)}(\boldsymbol{r})\,,$$

- The contributions from these corrections can be found by first order perturbation theory – or degenerate perturbation theory for the spin-orbit coupling.
- These corrections lift the (accidental) degeneracy of the H atom, by which states with the same principal quantum number n are degenerate for all angular momenta $\ell = 0, \ldots n-1$.
- The energy levels depend on n and the total angular momentum J (spin and orbital angular momenta are coupled.)

(c) The operating principles of the three-level laser

- The term "laser" is an acronym for "light amplification by stimulated emission of radiation".

- The laser consists of a resonant optical cavity, and a lasing medium (gain mechanism).
- Laser operation arises from the build-up of photons in (one) optical modes, which stimulate emission from atoms in their excited states to emit into this same mode.
- For a net emission from the atoms, requires a population inversion for atomic levels corresponding to the laser transition.
- The population inversion cannot be achieved for just two levels. The minimal set-up that can achieve this is the three-level laser.
- Pumping is applied, to excite atoms from the ground state (level 1) to an excited state (level 3).
- The level 3 has fast relaxation to level 2. Provided the pumping is strong enough, and the relaxation fast enough, this can lead to a population inversion between levels 2 and 1. (More atoms in level 2 than in level 1.)
- Laser action then occurs, with stimulated emission of photons causing atoms in level 2 to de-exicte to level 1.
- Some relevant rate equations, defining the processes should be stated. Relevant parameters include: the number of atoms in each level, the number of photons in the cavity, the pumping rate, the (stimulated) emission rate, and the cavity decay rate.
- When the pumping rate is sufficient that the unsaturated inversion exceeds the cavity loss rate, the steady state solutions allow for a non-zero number of photons in the cavity: this is the threshold for laser action.
- An example of this sort of laser is the Ruby laser, where pumping is provided by irradiation by white light.

3 [A variant of the solution studied in lecture/handout/examples for a particle in a uniform magnetic field. The first 12 marks are for the application of standard bookwork.]

A particle of mass m and charge q moves in the xy-plane subject to a magnetic field B normal to this plane. The field has a gradient in the x-direction, with $B(x) = \alpha x$.

Starting from the general expression for the Hamiltonian in the presence of a vector potential, show that, with an appropriate choice of gauge, the Hamiltonian for the particle can be written

$$\hat{H} = \frac{1}{2m}\left[\hat{p}_x^2 + \left(\hat{p}_y - \frac{1}{2}q\alpha\hat{x}^2\right)^2\right]$$

where $\hat{p}_{x,y}$ are the momentum operators and $\hat{x}$ the position operator in the x-direction. [8]

•Choosing $\boldsymbol{A} = (0, \frac{1}{2}\alpha x^2, 0)$, one should define and check that

$$\boldsymbol{B} \equiv \nabla \times \boldsymbol{A} = -\left(\frac{\partial A_y}{\partial z} - \frac{\partial A_z}{\partial y}, \frac{\partial A_z}{\partial x} - \frac{\partial A_x}{\partial z}, \frac{\partial A_x}{\partial y} - \frac{\partial A_y}{\partial x}\right) = (0, 0, \alpha x)$$

as required. [4]

•Use

$$\hat{H} = \frac{1}{2m}(\hat{p} - qA)^2$$

to obtain required result [4]

$$\hat{H} = \frac{1}{2m}\left[\hat{p}_x^2 + \left(\hat{p}_y - \frac{1}{2}q\alpha\hat{x}^2\right)^2\right]$$

For periodic boundary conditions in the y-direction over a length L_y, explain why the energy eigenstates in position representation can be written as $\Psi(x, y) = e^{iky}\Phi(x)$ and state the allowed values of k. [2]

•The momentum p_y commutes with the Hamiltonian, so energy eigenstates are also eigenstates of $\hat{p}_y$. Hence the wave function factorizes as [1]

$$\Psi = e^{iky}\Phi(x)$$

since e^{iky} has $p_y = \hbar k$.

•PBC require that [1]

$$k = \frac{2\pi}{L_y} \times \text{integer}$$

.

Hence show that the energy eigenvalues follow from the solution of the one-dimensional Schrodinger equation with an effective potential [2]

$$V(x) = \frac{1}{2m}\left(\hbar k - \frac{1}{2}q\alpha x^2\right)^2 .$$

Using the fact that $e^{iky}\Phi(x)$ is an eigenstate of $\hat{p}_y$

$$\begin{aligned}
\hat{H}\Psi &= E\Psi \\
\hat{p}_y e^{iky}\Phi(x) &= \hbar k e^{iky}\Phi(x) \\
\hat{H}e^{iky}\Phi(x) &= \frac{1}{2m}\left[\hat{p}_x^2 + \left(\hbar k - \frac{1}{2}q\alpha x^2\right)^2\right] e^{iky}\Phi(x) = E e^{iky}\Phi(x) \\
\frac{1}{2m}\left[\hat{p}_x^2 + \left(\hbar k - \frac{1}{2}q\alpha x^2\right)^2\right]\Phi(x) &= E\Phi(x)
\end{aligned}$$

one obtains a 1D Schrodinger equation with the stated potential. [2]

Sketch the form of the potential in the cases $k/(q\alpha) > 0$ and $k/(q\alpha) < 0$. [2]

$k/(q\alpha) > 0$: two minima (where $V = 0$) at $x = \pm\sqrt{2\hbar k/(q\alpha)}$. [1]

$k/(q\alpha) < 0$: one minimum (where $V = \hbar^2 k^2/(2m)$) at $x = 0$. [1]

Sketch the wave functions $\Phi(x)$ for the two lowest energy states, when $k/(q\alpha)$ is large and negative, and when $k/(q\alpha)$ is large and positive. [3]

Sketches should indicate that [3]

- The two states have definite parity: even and odd, respectively, with zero and one node.
- For large positive $k/(q\alpha)$ the wave function is concentrated close to the two (widely spaced) minima.
- and be qualitatively correct (no extra nodes, discontinuities/cusps, etc..)

Explain why the energies of the two lowest energy states are nearly degenerate for large positive $k/(q\alpha)$. By expanding $V(x)$ close to one of its minima, show that each of these energies is approximately

$$E_k = \frac{1}{m}\left(\frac{\hbar^3 q\alpha k}{2}\right)^{1/2} .$$

[6]

- For large positive $k/(q\alpha)$ the two lowest states are strongly localised at the widely spaced minima $\pm x_k$, where $x_k^2 \equiv \frac{2\hbar k}{q\alpha}$. The energy difference of these two states is the tunnel splitting, which is strongly suppressed. Hence the two states are near degenerate. [2]

•Expanding near $+x_k \equiv \frac{2\hbar k}{q\alpha}$ we find [2]

$$\begin{aligned} V(x) &= \frac{1}{2m}\left(\frac{q\alpha}{2}\right)^2 \left[x^2 - x_k^2\right]^2 \\ &= \frac{1}{2m}\left(\frac{q\alpha}{2}\right)^2 [x - x_k]^2 [x + x_k]^2 \\ &\simeq \frac{1}{2m}\left(\frac{q\alpha}{2}\right)^2 [x - x_k]^2 [2x_k]^2 \\ &\simeq \frac{q^2\alpha^2 x_k^2}{2m} [x - x_k]^2 \end{aligned}$$

•This is a SHO with frequency ω_k where

$$\frac{1}{2}m\omega_k^2 = \frac{q^2\alpha^2 x_k^2}{2m}$$

Hence

$$\omega_k = \frac{q\alpha}{m}x_k = \frac{q\alpha}{m}\sqrt{\frac{2\hbar k}{q\alpha}}$$

The ground state has energy [2]

$$\begin{aligned} E_0 &= (1/2)\hbar\omega_k = \frac{1}{2}\frac{\hbar q\alpha}{m}\sqrt{\frac{2\hbar k}{q\alpha}} \\ &= \frac{1}{2}\frac{\hbar q\alpha}{m}\sqrt{\frac{2\hbar k_y}{q\alpha}} \\ &= \frac{1}{m}\left(\frac{\hbar^3 q\alpha k}{2}\right)^{1/2} \end{aligned}$$

Calculate the group velocity in the y-direction of wave packets formed from these states. [2]

•A wave packet with drift with group velocity [2]

$$v_g = \frac{1}{\hbar}\frac{dE_0}{dk}$$

which is in the $+y$ direction. (This can be interpreted in terms of semiclassical trajectory of the charged particle, performing cyclotron orbits with slightly different radius of curvature at different x-positions.)

4 [A variant of a question from the handout, but applied to a different physical situation. The first 12 marks are for standard bookwork.]

A quantum mechanical system has eigenstates $|\psi_n\rangle$ with energies $\hbar\omega_n$ ($\omega_0 \leq \omega_1 \leq \omega_2 \ldots$). At time $t = -\infty$ the system is in the ground state $|\psi_0\rangle$. A weak perturbation $\hat{V}(t)$ is applied. Representing the state in terms of the unperturbed eigenstates as

$$|\Psi(t)\rangle = \sum_n c_n(t) e^{-i\omega_n t} |\psi_n\rangle$$

show that the coefficients c_n, for $n \neq 0$, are approximately

$$c_n(t) = \frac{1}{i\hbar} \int_{-\infty}^{t} e^{i(\omega_n - \omega_0)t'} \langle \psi_n | \hat{V}(t') | \psi_0 \rangle dt'$$

making clear any assumptions that you make. [12]

Standard bookwork, which should include

- State the time-dependent S.E. for $\hat{H} + \hat{V}(t)$.
- Apply to the expansion of the function.
- Use that $|\psi_n\rangle$ are eigenstates of $\hat{H}$.
- In first order P.T., approximate that $c_0 \simeq 1$.

An electron in a semiconductor quantum well can be represented as a particle in a box, with position x in the range $0 < x < w$, within which the potential is initially zero. Initially the electron is in its ground state $|\psi_0\rangle$. At $t = 0$, a uniform electric field $\mathcal{E}$ along the x-direction is applied, with

$$\mathcal{E}(t) = \mathcal{E}_0 e^{-t/\tau} \qquad t \geq 0$$

Explain why, in first-order perturbation theory, the electric field cannot excite the electron into the second excited state $|\psi_2\rangle$. [2]

- The electric field provides a potential that is odd under parity $x \to -x$. Hence, the selection rule on the matrix element requires the quantum number n to change from even (for the ground state) to an odd value, such that the parity of the eigenstates changes. Transition from $n = 0$ to $n = 2$ is forbidden.

Denoting the electron mass by m_e and charge by $-e$, find an expression for the probability that at $t = \infty$ the electron is in the first excited state, $|\psi_1\rangle$. [6]

- The normalised states are [2]

$$\psi_n = \sqrt{\frac{2}{w}} \sin\left[\frac{\pi(n+1)x}{w}\right]$$

with energies

$$E_n = \hbar\omega_n = \frac{\hbar^2\pi^2(n+1)^2}{2m_e w^2}$$

•The transition probability is [4]

$$\begin{aligned} P_{0\to1} \equiv |c_1|^2 &= \frac{1}{\hbar^2}\left|\int_0^\infty e^{i(\omega_1-\omega_0)t'}\langle\psi_1| - e\mathcal{E}_0\hat{x}|\psi_0\rangle e^{-t'/\tau}dt'\right|^2 \\ \int_0^\infty e^{i(\omega_1-\omega_0)t'}e^{-t'/\tau}dt' &= \frac{-1}{i(\omega_1-\omega_0)-1/\tau} \\ \langle\psi_1|\hat{x}|\psi_0\rangle &= \frac{2}{w}\int_0^w \sin(2\pi x/w)x\sin(\pi x/w)\,dx \\ \text{using formula given} &= \frac{2}{w}\times\frac{-8w^2 1}{\pi^2 1\times 9} \end{aligned}$$

Putting all together

$$\begin{aligned} P_{0\to1} \equiv |c_1|^2 &= \frac{e^2\mathcal{E}_0^2}{\hbar^2}\frac{1}{(\omega_1-\omega_0)^2+1/\tau^2}\frac{256w^2}{81\pi^4} \\ &= \frac{e^2\mathcal{E}_0^2}{\hbar^2}\frac{1}{\left[\frac{\hbar\pi^2}{2m_e w^2}(4-1)\right]^2+1/\tau^2}\frac{256w^2}{81\pi^4} \\ &= \frac{e^2\mathcal{E}_0^2 w^2}{\frac{9\hbar^4\pi^4}{4m_e^2w^4}+\frac{\hbar^2}{\tau^2}}\frac{256}{81\pi^4} \end{aligned}$$

If, instead, the electron had started in the state $|\psi_1\rangle$ at $t = -\infty$, describe the effects of the above weak electric field pulse. [5]

•The electron can end up in any state ψ_m with m even. [1]

•The probabilty for transition to the ground state $m = 0$ is *identical* to the above result. $P_{1\to0} = P_{0\to1}$. [2]

•For the other cases (m even) the result is: [2]

$$P_{1\to m} = \frac{e^2\mathcal{E}_0^2 w^2}{\frac{\hbar^4\pi^4}{4m_e^2w^4}[(1+m)^2-4]^2+\frac{\hbar^2}{\tau^2}}\frac{256(1+m)^2}{(m-1)^2(m+3)^2\pi^4}$$

[You can use the result $\int_0^w x\sin\frac{2\pi x}{w}\sin\frac{(m+1)\pi x}{w}dx = \frac{-8w^2(1+m)}{\pi^2(m-1)^2(3+m)^2}$ for *even* m.]

END OF PAPER