

## NATURAL SCIENCES TRIPOS Part II

Wednesday 30 May 2018

9.00 am to 11.00 am

PHYSICS (3)

PHYSICAL SCIENCES: HALF SUBJECT PHYSICS (3)

ADVANCED QUANTUM PHYSICS

Candidates offering this paper should attempt a total of **three** questions. The questions to be attempted are 1 and **two** questions from Section B.

The approximate number of marks allocated to each question or part of a question is indicated in the right margin. This paper contains five sides, including this coversheet, and is accompanied by a handbook giving values of constants and containing mathematical formulae which you may quote without proof.

STATIONERY REQUIREMENTS

2 × 20 Page Answer Book Metric graph paper Rough workpad Yellow master coversheet SPECIAL REQUIREMENTS

Mathematical Formulae handbook Approved calculator allowed

You may not start to read the questions printed on the subsequent pages of this question paper until instructed that you may do so by the Invigilator.

## ADVANCED QUANTUM PHYSICS

## SECTION A

Answers should be concise and relevant formulae may be assumed without proof.

- 1 Attempt all parts of this question.
  - (a) Two distinguishable spin-one particles combine into an overall S=0, m=0 singlet state. The overall spin state is a linear combination of two-particle product states:  $|S=0, m=0\rangle = \alpha |\chi_1\chi_2\rangle + \beta |\eta_1\eta_2\rangle + \gamma |\psi_1\psi_2\rangle$ .

Find the three product states. By applying spin raising and lowering operators on the overall singlet state, find a possible combination of the coefficients  $\alpha$ ,  $\beta$  and  $\gamma$ .

[Note that 
$$\widehat{J}^{\pm}|j,m\rangle = \sqrt{j(j+1) - m(m\pm 1)}|j,m\pm 1\rangle$$
] [4]

- (b) Why does an electric field applied across a symmetric quantum well give rise to a relative shift in energy levels proportional to the square of the electric field?
- (c) Na *D*-lines are produced by the transition of the single valence electron from a p- to an s-state. The lines split in an applied magnetic field. Draw an energy level diagram and indicate the allowed transitions. Indicate which of the allowed transitions produces the shortest wavelength.

  [The Law 16 of frequence  $a = \frac{3}{2} + \frac{S(S+1)-L(L+1)}{2}$ ]

[The Landé g-factor is  $g = \frac{3}{2} + \frac{S(S+1)-L(L+1)}{2J(J+1)}$ ]

[4]

[4]

(a) We construct the singlet state:  $|\psi\rangle|S=0, m=0\rangle=\alpha|1,-1\rangle+\beta|-1,1\rangle+\gamma|0,0\rangle$ , where the states on the right hand side are specified by the  $m_s$ -values for each particle, as the overall spin of each particle is fixed at 1.

Applying the spin raising operator produces:

$$\widehat{S}^{+}|\psi\rangle = 0 = (\widehat{S}_{1}^{+} + \widehat{S}_{2}^{+})|\psi\rangle = \beta\widehat{S}_{1}^{+}|-1,1\rangle + \alpha\widehat{S}_{2}^{+}|1,-1\rangle + \gamma\widehat{S}_{1}^{+}|0,0\rangle + \gamma\widehat{S}_{2}^{+}|0,0\rangle = (1)$$

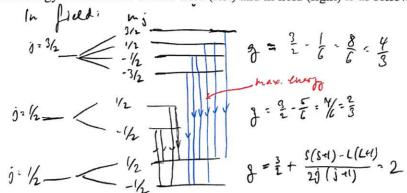
$$= \sqrt{2}\left[\beta|0,1\rangle + \alpha|1,0\rangle + \gamma|1,0\rangle + \gamma|0,1\rangle\right]$$
(2)

This implies that  $\alpha=\beta=-\gamma$ . Normalisation then gives us  $|\psi\rangle=\frac{1}{\sqrt{3}}\left[|1,-1\rangle+|-1,1\rangle-|0,0\rangle\right]$ 

(b) As the well is symmetric, the well potential V(x) commutes with the spatial inversion operator  $\widehat{P}$ . Hence, stationary states can be found, which are also eigenstates of  $\widehat{P}$ . On the other hand,  $\widehat{P}x = -x\widehat{P}$ . This means that the first-order energy shift caused by the perturbing field -qEx is zero:  $\langle \psi | x | \psi \rangle = \langle \widehat{P}\psi | \widehat{P}x | \psi \rangle = -\langle \widehat{P}\psi | x | \widehat{P}\psi \rangle = -\langle \psi | x | \psi \rangle = 0$ .

There remains the second-order shift, which goes as  $\Delta E_n = \sum_m \frac{|\langle \psi_m | q E x | \psi_n \rangle|^2}{E_n - E_m}$  and is therefore quadratic in the applied field E.

(c) The energy level scheme in zero field (left) and in field (right) is as follows:



We work out the g-factors for the three sets of states (s orbital, j = 1/2-p, j = 3/2-p) as 2, 2/3 and 4/3. The allowed transitions are determined from the selection rules, which rule out  $m_j = 3/2 \rightarrow m_j = -1/2$  and  $m_j = -3/2 \rightarrow m_j = 1/2$ . Because the splitting of the s states is larger than that of the p states, the shortest wavelength is associated with the transition  $m_j = 1/2 \rightarrow m_j = -1/2$ , as shown in the diagram above.

## SECTION B

Attempt two questions from this section

B2 A particle with mass m and charge q constrained to move in one dimension is subject to a potential  $V(x) = \frac{m}{2}\omega_0^2x^2$ , where  $\omega_0$  is the classical frequency of oscillation. Show that the matrix element of the position operator  $\widehat{x}$  between ground state  $|0\rangle$  and first excited state  $|1\rangle$  has the magnitude

$$\left|\langle 1|\widehat{x}|0\rangle\right| = \sqrt{\frac{\hbar}{2m\omega_0}}$$

[An appropriate ladder operator is  $\widehat{a} = \widehat{x} \sqrt{\omega_0 m/(2\hbar)} + i\widehat{p}/\sqrt{2\hbar\omega_0 m}$ .]

The particle starts out in its ground state for  $t \to -\infty$ , but is subjected to a gradually increasing uniform electric field E, which produces a weak perturbation  $\widehat{V}_1(t) = -qE\widehat{x}e^{t/\tau}$ , where  $\tau$  defines a time-scale. Show that the probability of finding the particle in the first excited state at t=0 is

$$p_1(0) = \left| \frac{qE}{\hbar} \langle 1 | \widehat{x} | 0 \rangle \int_{-\infty}^{0} e^{i\omega_0 t'} e^{t'/\tau} dt' \right|^2.$$

[7]

[5]

[7]

Find how  $p_1(0)$  depends on  $\tau$ , illustrating your answer with a suitable sketch and analysing both limiting cases  $\omega_0 \tau >> 1$  and  $\omega_0 \tau << 1$ .

The ladder operators are (using the hint)  $\widehat{a} = \widehat{x} \sqrt{\omega_0 m/(2\hbar)} + i\widehat{p}/\sqrt{2\hbar\omega_0 m}$  and  $\widehat{a}^{\dagger} = \widehat{x} \sqrt{\omega_0 m/(2\hbar)} - i\widehat{p}/\sqrt{2\hbar\omega_0 m}$ . We can therefore write the matrix element as

$$\langle 1|\widehat{x}|0\rangle = \langle 1|\widehat{a}+\widehat{a}^{\dagger}|0\rangle \; \sqrt{\frac{\hbar}{2m\omega_0}} \; .$$

The lowering operator will annihilate the ground state, the raising operator moves  $|n\rangle$  to  $(n+1)|n+1\rangle$ , which here gives simply  $\widehat{a}^{\dagger}|0\rangle$  to  $|1\rangle$ , giving the required expression for the magnitude of the matrix element.

If we express a general state in terms of evolving stationary states of the unperturbed Hamiltonian:  $|\psi(t)\rangle = \sum_n c_n(t)e^{-iE_nt/\hbar}|n\rangle$ , where  $E_n = (n+1/2)\hbar\omega_0$  are the energy levels of the unperturbed Hamiltonian, then the time-dependent Schrödinger equation becomes

$$i\hbar\frac{\partial}{\partial t}\left|\psi(t)\right\rangle = i\hbar\sum e^{-iE_nt/\hbar}\left(E_nc_n(t)+\dot{c}_n(t)\right)\left|n\right\rangle = \left(\widehat{H}_0+\widehat{V}_1(t)\right)\left|\psi\right\rangle = \sum \left(E_n+\widehat{V}_1(t)\right)e^{-iE_nt/\hbar}c_n(t)\left|n\right\rangle \;.$$

Making all the  $c_n = 0$  apart from  $c_0$ , cancelling the terms on both sides related to  $E_n$  and left multiplying with  $\langle 1 |$  produces

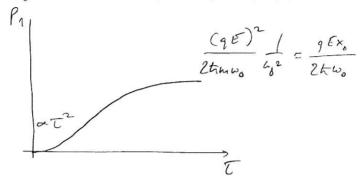
$$\dot{c}_1(t) = \frac{1}{i\hbar} e^{i(E_1-E_0)t/\hbar} \left<1\right| \widehat{V}_1(t) \left|0\right> c_0 \; . \label{eq:continuous}$$

Putting  $c_0 = 1$  for  $t \to -\infty$  and integrating up, noting that  $E_1 - E_0 = \hbar \omega_0$ , then gives the required answer for the probability  $p_1 = |c_1|^2$ .

The integral is  $\frac{1}{i\omega_0+1/\tau}$ , and so

$$p_1(0) = \frac{(qE)^2}{2\hbar m\omega_0} \frac{1}{\omega_0^2 + 1/\tau^2} = \frac{(qE)^2}{2\hbar m\omega_0} \frac{\tau^2}{(\omega_0\tau)^2 + 1} \; .$$

For short  $\tau$ , so that  $\omega_0 \tau << 1$ , this rises  $\propto \tau^2$ , but it saturates at  $\frac{(qE)^2}{2\hbar m \omega_0^3}$  for long  $\tau$ , when  $\omega_0 \tau >> 1$ . For a static *E*-field, the average position in the ground state would be shifted to  $x_0 = qE/k = qE/(m\omega_0^2)$ . Hence, we can view  $p_1$  for large  $\tau$  as  $qEx_0/(2\hbar\omega_0)$ .



B3 For spin- $\frac{1}{2}$  particles, show that if the spin state  $|\chi\rangle = \alpha |\uparrow\rangle + \beta |\downarrow\rangle$  is expressed in terms of angles  $\theta$ ,  $\phi$  as  $\alpha = \cos(\theta/2)$ ,  $\beta = e^{i\phi}\sin(\theta/2)$ , then  $\theta$  and  $\phi$  give the direction of  $\langle \chi | \widehat{S} | \chi \rangle$  in spherical polars. Explain why the two angles contain enough information to specify the spin state, up to a phase factor.

[5]

A spin- $\frac{1}{2}$  particle is described by a two-component spinor wavefunction  $\psi(r) = \phi(r) \begin{pmatrix} \alpha \\ \beta \end{pmatrix}$ . It is subject to the Hamiltonian

$$\widehat{H} = v \frac{\hbar}{i} \left( \sigma_x \frac{\partial}{\partial x} + \sigma_y \frac{\partial}{\partial y} + \sigma_z \frac{\partial}{\partial z} \right) \quad ,$$

where v is a constant and  $\sigma_x$ ,  $\sigma_y$ ,  $\sigma_z$  are the Pauli matrices (see hint below). Show that travelling wave states

 $\psi_k(\mathbf{r}) = e^{ik \cdot \mathbf{r}} \begin{pmatrix} \cos(\theta/2) \\ e^{i\phi} \sin(\theta/2) \end{pmatrix}$ 

with  $k = \pm k (\sin \theta \cos \phi, \sin \theta \sin \phi, \cos \theta)$  are eigenstates of  $\widehat{H}$ . Find the dispersion E(k), sketch it as a function of k and show that it is gapless. Sketch the spin orientation of eigenstates in the plane  $k_z = 0$ .

[8]

A perturbing potential added to the Hamiltonian above has matrix elements  $V_{mn}$  between spinor states with the same wavevector, whereas the matrix elements are zero between states with different wavevectors. Explain why all Hermitian 2-by-2 matrices can be expressed as a linear superposition of the Pauli matrices and the identity matrix I:  $V = a\sigma_x + b\sigma_y + c\sigma_z + dI$ , with real coefficients a, b, c, d. Use this fact to show that the perturbed Hamiltonian, like the original Hamiltonian, has a gapless spectrum.

[6]

The Pauli matrices are

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \ \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \ \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

(Typical problem requiring standard approach, but made slightly unusual because of involvement of spin matrices.)

We calculate the expectation value of  $\widehat{S}$  using the Pauli spin matrices given in the hint:

$$\langle \chi | \widehat{S} | \chi \rangle = \frac{1}{2} \langle \chi | \tau | \chi \rangle = (\alpha^*, \beta^*) \begin{pmatrix} (0, 0, 1) & (1, -i, 0) \\ (1, i, 0) & (0, 0, -1) \end{pmatrix} \begin{pmatrix} \alpha \\ \beta \end{pmatrix} = \frac{1}{2} (2\Re(\alpha^*\beta), 2\Im(\alpha^*\beta), |\alpha|^2 - |\beta|^2)$$

Substituting  $\alpha = \cos(\theta/2)$ ,  $\beta = e^{i\phi}\sin(\theta/2)$ , this gives  $\frac{1}{2}(\sin\theta\cos\phi, \sin\theta\sin\phi, \cos\theta)$ , as it should. The spin state is specified by two complex numbers. By taking out the phase of  $\alpha$  into the phase pre-factor, which we are told not to worry about, we have a real number for  $\alpha$  and a complex number (two real numbers) for  $\beta$ . The constraint on the magnitude brings the number of degrees of freedom down to two, so two angles can be sufficient.

Substituting plane wave states  $\begin{pmatrix} \alpha_k \\ \beta_k \end{pmatrix} e^{ik \cdot r}$ , obtain matrix equation

$$\begin{pmatrix} \overline{\hbar} v k_z & \overline{\hbar} v (k_x - i k_y) \\ \overline{\hbar} v (k_x + i k_y) & -\overline{\hbar} v k_z \end{pmatrix} \begin{pmatrix} \alpha_k \\ \beta_k \end{pmatrix} = E_k \begin{pmatrix} \alpha_k \\ \beta_k \end{pmatrix}$$

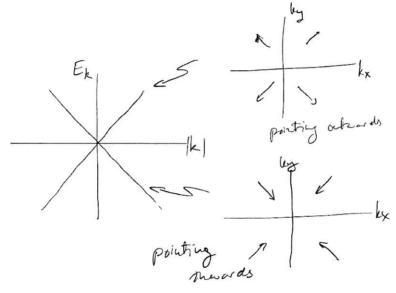
By expressing k in spherical polars, as suggested in the question, this can also be written as

$$\pm \hbar v k \begin{pmatrix} \cos \theta & \sin \theta e^{-i\phi} \\ \sin \theta e^{i\phi} & -\cos \theta \end{pmatrix} \begin{pmatrix} \cos(\theta/2) \\ e^{i\phi} \sin \theta/2 \end{pmatrix} = \pm \hbar v k \begin{pmatrix} \cos(\theta/2) \\ e^{i\phi} \sin(\theta/2) \end{pmatrix} = E_k \begin{pmatrix} \cos(\theta/2) \\ e^{i\phi} \sin(\theta/2) \end{pmatrix}$$

Alternatively, from the secular determinant, find

$$E_k = \pm \hbar v \sqrt{k_x^2 + k_y^2 + k_z^2}$$

and deduce the eigenstates, but this is more laborious.



A Hermitian 2-by-2 matrix has two real numbers on the diagonal and one independent complex number off-diagonal, so four real numbers specify a Hermitian 2-by-2 matrix. The space of Hermitian 2-by-2 matrices must be four-dimensional. If we find four independent basis elements, they will span the space. The four Pauli matrices plus the identity matrix are linearly independent, hence we can use them to build any Hermitian 2-by-2 matrix.

We can write the action of the perturbed Hamiltonian on  $\psi_k(\mathbf{r}) = e^{i\mathbf{k}\cdot\mathbf{r}} \begin{pmatrix} \alpha \\ \beta \end{pmatrix}$  as

$$\widehat{H}\psi_k = \Big((\overline{\hbar} v k_x + a)\sigma_x + (\overline{\hbar} v k_y + b)\sigma_y + (\overline{\hbar} v k_z + c)\sigma_z + dI\Big)\binom{\alpha}{\beta}e^{ik\cdot r}$$

The effect of the perturbation is therefore simply to shift the node of the dispersion in k-space and to shift the energies vertically by an amount d. The structure of the dispersion curve and its gapless nature remain unchanged.

B4 A ring of N atoms, each carrying an unpaired electron with spin  $\frac{1}{2}$ , has the Hamiltonian

$$\widehat{H} = -\frac{J}{\hbar^2} \sum_{i=1}^{N} \widehat{S}_{i} \cdot \widehat{S}_{j+1}$$

where an arbitrary atom has been labelled as atom 1, and we interpret the index N+1 as pointing back to atom 1. J is a positive constant. The eigenstates of any  $\widehat{S}_z$  are  $|\uparrow\rangle$  and  $|\downarrow\rangle$ , and a small applied field along the z-axis makes the ground state the state  $|\psi_0\rangle$ , in which all spins are up. We denote by  $|\psi_n\rangle$  the state in which all spins are up apart from that at position n, which is down.

Show that

$$\widehat{S}_{j} \cdot \widehat{S}_{j+1} = \frac{1}{2} \left( \widehat{S}_{j}^{+} \widehat{S}_{j+1}^{-} + \widehat{S}_{j}^{-} \widehat{S}_{j+1}^{+} \right) + \widehat{S}_{j}^{z} \widehat{S}_{j+1}^{z}, \text{ and hence that}$$

$$\widehat{S}_{j} \cdot \widehat{S}_{j+1} | \psi_{n} \rangle = \frac{\hbar^{2}}{4} | \psi_{n} \rangle \quad \text{if } n \neq j \text{ and } n \neq j+1, \text{ and}$$

$$\widehat{S}_{j} \cdot \widehat{S}_{j+1} | \psi_{j} \rangle = \frac{\hbar^{2}}{4} \left[ 2 \left| \psi_{j+1} \right\rangle - \left| \psi_{j} \right\rangle \right], \quad \widehat{S}_{j} \cdot \widehat{S}_{j+1} | \psi_{j+1} \rangle = \frac{\hbar^{2}}{4} \left[ 2 \left| \psi_{i} \right\rangle - \left| \psi_{i+1} \right\rangle \right]$$
[6]

Find an expression for the energy  $E_0$  of the ground state  $|\psi_0\rangle$  in terms of J and N.

[3]

[7]

Show that the states  $|\psi_q\rangle = \sum_{n=1}^N e^{iqna} |\psi_n\rangle$ , where a is the straight-line distance between the atoms and q denotes a wavenumber, are eigenstates of the Hamiltonian. Find the allowed values of q and the associated energies E(q).

Sketch the dispersion  $E(q) - E_0$  of these so-called 'spin waves' for  $-2\pi/a < q < 2\pi/a$ , assuming large N. [3]

We write  $S^{\pm} = S^x \pm iS^y$  and hence  $S^x = \frac{1}{2}(S^+ + S^-)$ ,  $S^y = \frac{1}{2i}(S^+ - S^-)$ . Taking the dot product then produces

$$S_{j}^{x}S_{j+1}^{x} + S_{j}^{y}S_{j+1}^{y} + S_{j}^{z}S_{j+1}^{z} = \frac{1}{4}(S_{j}^{+} + S_{j}^{-})(S_{j+1}^{+} + S_{j+1}^{-}) - \frac{1}{4}(S_{j}^{+} - S_{j}^{-})(S_{j+1}^{+} - S_{j+1}^{-}) + S_{j}^{z}S_{j+1}^{z} + S_{j}^{z}S_{j+1$$

The ++ and -- terms cancel, and the cross-terms +- and -+ combine to give the required expression.

If  $j \neq n$  and  $j \neq n+1$ , then both spin operators see an up-spin. Raising operators would annihilate this state, so only the  $S_z$  operators produce an outcome, namely  $S_z |\uparrow\rangle = \frac{\hbar}{2} |\uparrow\rangle$ , so together the two  $S_z$  operators give  $\hbar^2/4$  times the original state  $\psi_n$ .

if j=n, then the first spin operator meets a down-spin, the second meets an up-spin. The second operator product  $S_j^- S_{j+1}^+$  will annihilate the state, but the first operator product produces  $\frac{1}{2}S_j^+ S_{j+1}^- |-1/2, 1/2\rangle = \frac{1}{2}\hbar \sqrt{\frac{1}{2}\frac{3}{2} - \frac{-1}{2}\frac{1}{2}} \cdot \hbar \sqrt{\frac{1}{2}\frac{3}{2} - \frac{1}{2}\frac{-1}{2}} |1/2, -1/2\rangle = \frac{\hbar^2}{2} |\psi_{j+1}\rangle$ . The result of the  $S^z$  operators is  $-\hbar^2/4\psi_j$ , negative sign now because the two spins are antiparallel.

If j + 1 = n, then the first spin operator meets an up-spin, the second meets a down-spin. Now the product  $S_j^+ S_{j+1}^-$  annihilates the spin state, but the other one produces

 $\frac{1}{2}S_{j}^{-}S_{j+1}^{+}|1/2,-1/2\rangle = \frac{1}{2}\hbar|-1/2,+1/2\rangle = \frac{\hbar^{2}}{2}|\psi_{j}\rangle.$  The result of the  $S^{z}$  operators is  $-\hbar^{2}/4\psi_{j+1}$ . In the ground state, only the  $S^{z}$  operators produce non-zero outcomes, namely a total of  $N\frac{\hbar^{2}}{4}$ , as there are N repetitions of the j, j+1 term in the Hamiltonian.

We can check that  $|\psi_q\rangle$  is an eigenstate of  $\widehat{H}$  by checking equality for every component of the eigenvector equation  $\widehat{H}|\psi_q\rangle=E(q)|\psi_q\rangle$ :

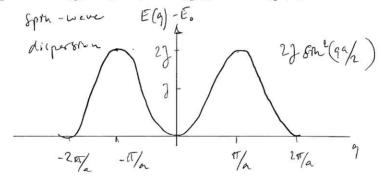
$$\left\langle \psi_{n} \left| \widehat{H} \right| \psi_{q} \right\rangle = E(q) \left\langle \psi_{n} \left| \psi_{q} \right\rangle = -\frac{J}{\hbar^{2}} \sum_{j=1}^{N} \sum_{m=1}^{N} e^{iqma} \left\langle \psi_{n} \left| \widehat{S}_{j} \cdot \widehat{S}_{j+1} \right| \psi_{m} \right\rangle =$$

$$= E(q) e^{iqna} = -\frac{J}{\hbar^{2}} e^{iqna} \frac{\hbar^{2}}{4} \left[ \underbrace{N-2}_{N-2 \text{ terms in } j\text{-sum with } j+1 \neq n \neq j} - \underbrace{2}_{2 \text{ terms with } m=j=n \text{ or } m=j+1=n} \right] -$$

$$- \frac{J}{\hbar^{2}} \left[ \underbrace{e^{iq(n+1)a} \frac{\hbar^{2}}{2}}_{\text{from } m=n+1} + \underbrace{e^{iq(n-1)a} \frac{\hbar^{2}}{2}}_{\text{from } m=n-1} \right] = \frac{J}{4} e^{iqna} \left( 4 - N - 2e^{iqa} - 2e^{-iqa} \right)$$

Hence we obtain  $E(q) = J(1-\cos(qa)) + E_0$ , and because the same result is obtained for projection along all basis states  $|\psi_n\rangle$  from which the eigenstate has been constructed,  $|\psi_q\rangle$  must be an eigenstate. The allowed values of q are given by the periodic boundary conditions:  $e^{iqNa} = 1 \implies q = \frac{2\pi}{Na} \times \text{integer}$ .

The dispersion is  $E(q) - E_0 = J(1 - \cos(qa)) = 2J \sin^2(qa/2)$ .



**END OF PAPER** 

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