

NATURAL SCIENCES TRIPOS Part II

Wednesday 25 May 2016 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, 2** and **one** other question.*

*The approximate number of marks allocated to each question or part of a question is indicated in the right margin. This paper contains **four** sides, 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

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

1 Attempt all parts of this question. Answers should be concise and relevant formulae may be assumed without proof.

(a) Find the magnitude of the energy splitting of the ground state of Ce^{3+} , which has electronic configuration $\dots(4f)^1$, in a magnetic field of 1 T.

$$\left[\text{Note that the Landé } g\text{-factor is } g = \frac{3}{2} + \frac{S(S+1) - L(L+1)}{2J(J+1)} \right] \quad [4]$$

(b) A system has degenerate stationary states $|a\rangle$, $|b\rangle$ and $|c\rangle$ with energy E_0 . A perturbation \hat{H}_1 gives matrix elements

$$\langle a | \hat{H}_1 | b \rangle = \langle b | \hat{H}_1 | c \rangle = \langle c | \hat{H}_1 | a \rangle = t \text{ with } t \text{ real, and}$$

$\langle a | \hat{H}_1 | a \rangle = \langle b | \hat{H}_1 | b \rangle = \langle c | \hat{H}_1 | c \rangle = 0$. Find the energy values of the perturbed system to first order in perturbation theory. [4]

(c) Make an order-of-magnitude comparison between (i) the ground-state energy density of electromagnetic waves in vacuum for wavelengths down to 1 Å and (ii) the binding energy of the electron in a hydrogen atom, divided by the volume of the hydrogen atom. [Note that in (i), each allowed wavevector and polarisation contributes $\hbar\omega/2$ to the ground-state energy.] [4]

(a) (Bookwork to remember use of Landé g -factor and to remember Hund's rules.)

$\ell = 3$, $s = 1/2$. By Hund's third rule, $j = 5/2$. This gives $g_j = 3/2 - 45/70 = 0.86$. The splitting is $g_j \mu_B B = 9 \times 10^{-24} \text{ J} = 0.05 \text{ meV}$.

(b) (Problem in degenerate perturbation theory.)

$$\langle m \hat{H} n \rangle = \begin{pmatrix} E_0 & t & t \\ t & E_0 & t \\ t & t & E_0 \end{pmatrix}_{mn} = H_{mn}$$

Note symmetry and try eigenvector (111):

$$H \begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix} = (E_0 + 2t) \begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix}$$

$$\Rightarrow \text{First energy} = E_0 + 2t$$

Then, either do a polynomial division of the determinant, $|H - EI|/(E - (E_0 + 2t))$ to get a quadratic equation, or simply guess the other two eigenvectors from the symmetry of H :

$$H \begin{pmatrix} 1 \\ e^{\pm i2\pi/3} \\ e^{\pm i4\pi/3} \end{pmatrix} = [E_0 + 2t \cos(\pm 2\pi/3)] \begin{pmatrix} 1 \\ e^{\pm i2\pi/3} \\ e^{\pm i4\pi/3} \end{pmatrix} = (E_0 - t) \begin{pmatrix} 1 \\ e^{\pm i2\pi/3} \\ e^{\pm i4\pi/3} \end{pmatrix}$$

$$\Rightarrow \text{Second energy (doubly degenerate)} = E_0 - t.$$

(c) (Bookwork to remember energy per mode of a harmonic oscillator and energy of hydrogen atom, problem to sum up over modes.)

Zero-point energy per mode = $\hbar\omega$ (2 polarisations).

$$E_0 = \hbar \frac{V}{(2\pi)^3} \int_0^{k_c} \omega(k) 4\pi k^2 dk = \frac{4\pi V}{4(2\pi)^3} \hbar c k_c^4 = (\text{for } k_c = 2\pi/a) = 2\pi^2 V \hbar c a^{-4}$$

Hence, the energy density is $2\pi^2 \hbar c a^{-4}$. Alternatively, for a rough estimate, consider a box with dimension a , three modes possible, giving a similar energy density of $3\hbar c \frac{2\pi}{a} \frac{1}{a^3}$.

The binding energy of the hydrogen atom is $\frac{1}{2} \frac{e^2}{4\pi\epsilon_0 a_0}$, which, if we take the hydrogen atom to occupy a space of $a^3 = 1 \text{ \AA}^3$ and write $a_0 \simeq 0.5a$, gives an energy density of $E_1/a^3 = \frac{e^2}{4\pi\epsilon_0} a^{-4}$.

The ratio between the two energy densities is $\frac{e^2}{8\pi^3\epsilon_0\hbar c} = \frac{1}{2\pi^2}\alpha$ (fine-structure constant), so it is about $4 \cdot 10^{-4}$. The zero-point energy is about 3000 times larger than the chemical binding energy.

2 *Attempt this question. Credit will be given for well-structured and clear explanations, including appropriate diagrams and formulae. Detailed mathematical derivations are not required.*

Write brief notes on **two** of the following:

[13]

- (a) the WKB method, with an example of its application;
- (b) stimulated and spontaneous emission;
- (c) Fermi's golden rule and its application to scattering within the Born approximation.

- (a) • Find approximate bound-state solutions to Schrödinger equations of the form $-\frac{\hbar^2}{2m}\psi'' = (E - V(x))\psi$ by noting that $\psi(x) \simeq e^{ik(x)x}$ with $\hbar^2 k^2/(2m) = (E - V)$ would solve the differential equation for constant V . Hence, rewrite the differential equation as $\psi'' = -k(x)^2\psi$ and express approximate solutions as $A(x)e^{i\phi(x)}$, where the phase $\phi = \pm \int^x k(x')dx'$.
- Substituting these solutions into the differential equation gives $A(x) \propto k(x)^{-1/2}$.
 - This approximation is valid, if $V(x)$ varies 'slowly', so that the fractional change in wavenumber, $\Delta k/k$ over one wavelength is small:
 $|k'/k| \ll |k| \implies |\Delta k/k| \ll 2\pi$
 - Where $k(x) \rightarrow 0$, the approximation breaks down. These are the classical turning points, at which $V(x) = E$. Beyond these, have exponentially decaying solutions. Connection formulae can be found by matching the exponentially decaying solutions to the oscillatory solutions between turning points. For bound states in 1D, this gives the quantisation condition $\int_a^b k(x)dx = (n + \frac{1}{2})\pi$

(TURN OVER)

- Example: quantum harmonic oscillator. Can find energy levels as $\hbar\omega(n + 1/2)$ and sketch a resulting wavefunction.
- (b)
- Consider atomic transitions in the presence of an electromagnetic field. Atomic states are $|1\rangle$ and $|2\rangle$, with $E_1 - E_2 = \hbar\omega$. We have atom in state 1 and $n(\mathbf{k})$ photons of frequency ω and wavevector \mathbf{k} , or the atom in state 2 and $n(\mathbf{k}) + 1$ photons of frequency ω and wavevector \mathbf{k} .
 - Transition rate from 1 to 2, $\Gamma_{1 \rightarrow 2}$ can be found by applying Fermi's golden rule to the system atom+field. We find that $\Gamma_{1 \rightarrow 2} \propto (n(\mathbf{k}) + 1)$. This can be interpreted as a *stimulated* contribution to the transition rate, which is proportional to the number of photons, $n(\mathbf{k})$, and a *spontaneous* contribution, which gives the additional zero-point contribution 1 in the bracket.
 - For the inverse process from 2 to 1 (lower energy state to higher energy state), the rate is proportional to the number of photons associated with state 2, only, and there is no zero-point term, so only stimulated transitions are possible.
 - The detailed calculation of transition rates also involves matrix elements of the dipole moment between initial and final states. These give rise to selection rules.
 - The total stimulated rate is equal to the spontaneous rate times the photon number at frequency ω , which can be obtained by summing over all \mathbf{k} with the same frequency, i.e. a spherical shell. This gives $\Gamma_{\text{stimulated}}/\Gamma_{\text{spontaneous}} \propto u(\omega)/\omega^3$, where $u(\omega)$ is the energy density of the electromagnetic field at frequency ω .
 - The same expression can be obtained by Einstein's argument, which equates the transition rates $1 \rightarrow 2$ and $2 \rightarrow 1$ in thermal equilibrium, writing the decay rates in terms of temperature-independent coefficients, and substituting Planck's black-body formula for $u(\omega)$.
- (c)
- Fermi's golden rule can be derived from time-dependent perturbation theory. It states that the transition rate from one stationary state of an unperturbed Hamiltonian, state 0, to another stationary state k , in the presence of a perturbing potential $U(\mathbf{r})e^{-i\omega t}$ is $\Gamma_{0 \rightarrow k} = \frac{2\pi}{\hbar} |\langle 0|U|k \rangle|^2 \delta(E_0 - E_k + \hbar\omega)$.
 - This implies that the transition rate depends on the matrix element of the perturbing potential between the initial and final states, and transitions are only induced if the frequency of oscillation of the perturbation matches the energy difference between initial and final states.
 - Fermi's golden rule has numerous applications, e.g. in calculating atomic transitions in the presence of electromagnetic fields, or in scattering theory.
 - If the transitions occur into a continuum of states, with density of states $g(E_k)$, then integrating over E_k to obtain the total transition rate pulls out $g(E_k)$, giving $\Gamma_{0 \rightarrow k} = \frac{2\pi}{\hbar} |\langle 0|U|k \rangle|^2 g(E_k)$.
 - Applying this to a scattering problem, we take the initial state as a plane wave with wavevector \mathbf{k} , and the final state as a plane wave with wavevector \mathbf{k}' . The scattering event is induced by a time-independent potential $V(\mathbf{r})$. Because the potential is time independent, the collision must be elastic, i.e.

the final state has the same energy as the initial state. Hence $k = k'$. The matrix element is proportional to $\int V(\mathbf{r})e^{(\mathbf{k}-\mathbf{k}')\cdot\mathbf{r}}d^3\mathbf{r}$, which gives the Fourier transform of the potential. The density of states comes from considering a segment $d\Omega$ of a spherical shell in k -space, where $d\Omega$ is an infinitesimal solid angle: $g(E)dE = d\Omega k^2 dk V / (2\pi)^3$, where dE/dk is also $\hbar v$ the velocity of the incoming particles and thereby linked to the incoming particle flux.

- The scattering rate is then expressed in terms of the differential scattering cross section $\frac{d\sigma}{d\Omega}(\mathbf{k}')$, which gives the fraction of the incoming particles that is scattered into a solid angle $d\Omega$ surrounding \mathbf{k}' . The velocity entering the density of states cancels against the incoming flux, giving a differential scattering cross-section which is simply proportional to the magnitude of the matrix element, squared.
 - This is equivalent to the Born approximation, because the full scattering problem is treated in the weak potential limit, in which the state of the outgoing particle only admixes very weakly to the incoming state. Moreover, it applies particularly to elastic scattering at high energies, when the particles' de Broglie wavelength is short in comparison to the spatial extent of the perturbing potential.
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(TURN OVER)

3 Attempt **either** this question or question 4.

The state of a system of two identical spin- $\frac{1}{2}$ particles, which occupy two spatial states $|a\rangle$, $|b\rangle$, can be expressed as a combination of products of normalised single-particle states such as $|1, a \uparrow\rangle |2, b \downarrow\rangle$. Show that the two-particle wavefunction can be written as a product of spatial and spin factors involving either singlet or triplet spin states. Comment on the exchange symmetry of the spin and spatial wavefunction in each case.

[6]

[Here, and for what follows, you may wish to use the short-hand notation $|ab\rangle \equiv |1, a\rangle |2, b\rangle$, and $\langle ab| \equiv \langle 1, a| \langle 2, b|$.]

(Bookwork)

Start with

$$|a \uparrow b \uparrow\rangle = |\psi_1\rangle$$

$$|a \uparrow b \downarrow\rangle = |\psi_2\rangle$$

$$|a \downarrow b \uparrow\rangle = |\psi_3\rangle$$

$$|a \downarrow b \downarrow\rangle = |\psi_4\rangle$$

Antisymmetrise $|\psi_1\rangle$ and $|\psi_4\rangle$:

$$|\phi_1\rangle = \frac{1}{\sqrt{2}} (|a \uparrow b \uparrow\rangle - |b \uparrow a \uparrow\rangle) = \frac{1}{\sqrt{2}} (|ab\rangle - |ba\rangle) |\uparrow\uparrow\rangle$$

$$|\phi_4\rangle = \frac{1}{\sqrt{2}} (|a \downarrow b \downarrow\rangle - |b \downarrow a \downarrow\rangle) = \frac{1}{\sqrt{2}} (|ab\rangle - |ba\rangle) |\downarrow\downarrow\rangle$$

Make linear combinations of $|\psi_2\rangle$ and $|\psi_3\rangle$, antisymmetrise those:

$$\frac{1}{\sqrt{2}} (|\psi_2\rangle + |\psi_3\rangle) \rightarrow \frac{1}{\sqrt{2}} (|ab\rangle - |ba\rangle) \frac{1}{\sqrt{2}} (|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle)$$

$$\frac{1}{\sqrt{2}} (|\psi_2\rangle - |\psi_3\rangle) \rightarrow \frac{1}{\sqrt{2}} (|ab\rangle + |ba\rangle) \frac{1}{\sqrt{2}} (|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)$$

Hence, arrive at four antisymmetric basis states. Three are space-antisymmetric, spin-symmetric (triplet):

$$\begin{aligned} & \frac{1}{\sqrt{2}} (|ab\rangle - |ba\rangle) |\uparrow\uparrow\rangle \\ & \frac{1}{\sqrt{2}} (|ab\rangle - |ba\rangle) \frac{1}{\sqrt{2}} (|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle) \\ & \frac{1}{\sqrt{2}} (|ab\rangle - |ba\rangle) |\downarrow\downarrow\rangle \end{aligned}$$

One is space-symmetric, spin-antisymmetric (singlet):

$$\frac{1}{\sqrt{2}} (|ab\rangle + |ba\rangle) \frac{1}{\sqrt{2}} (|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)$$

In a simple model for the H_2 molecule, consider two normalised spatial states $|a\rangle$, $|b\rangle$, which are orthogonal to each other and resemble the hydrogen 1s orbitals centred on the positions \mathbf{R}_a and \mathbf{R}_b of the two protons: $\langle \mathbf{r}|a\rangle = \phi(\mathbf{r} - \mathbf{R}_a)$, $\langle \mathbf{r}|b\rangle = \phi(\mathbf{r} - \mathbf{R}_b)$. The electronic Hamiltonian can be written as

$$\hat{H} = \hat{H}_1 + \hat{H}_2 + \hat{H}_{1,2} \quad ,$$

where \hat{H}_1 acts only on electron 1, \hat{H}_2 acts only on electron 2, and $\hat{H}_{1,2}$ expresses the Coulomb repulsion between the two electrons.

Write out $\langle a|\hat{H}_1|a\rangle$ and $\langle ab|\hat{H}_{1,2}|ab\rangle$ in integral form. Show that $\langle aa|\hat{H}_1|ab\rangle = 0$ and that $U = \langle aa|\hat{H}_{1,2}|aa\rangle > 0$.

[4]

(Should be familiar, but requires the Hamiltonian for an electron subject to the potential produced by a proton, and for the interaction between two electrons)

$$\begin{aligned} \langle a|\hat{H}_1|a\rangle &= \int d^3\mathbf{r}_1 \psi_a^*(\mathbf{r}_1) \left(\frac{-\hbar^2}{2m} \nabla^2 - \frac{e^2}{4\pi\epsilon_0 |\mathbf{R}_a - \mathbf{r}_1|} - \frac{e^2}{4\pi\epsilon_0 |\mathbf{R}_b - \mathbf{r}_1|} \right) \psi_a(\mathbf{r}_1) \\ \langle ab|\hat{H}_{1,2}|ab\rangle &= \int d^3\mathbf{r}_1 d^3\mathbf{r}_2 \psi_a^*(\mathbf{r}_1) \psi_b^*(\mathbf{r}_2) \psi_a(\mathbf{r}_1) \psi_b(\mathbf{r}_2) \frac{e^2}{4\pi\epsilon_0 |\mathbf{r}_1 - \mathbf{r}_2|} \end{aligned}$$

Also, $\langle aa|\hat{H}_1|ab\rangle = \langle a|\hat{H}_1|a\rangle \langle a|b\rangle$, because \hat{H}_1 only acts on electron 1. The states a and b are orthogonal, and therefore the second bracket contracts to zero, giving zero overall.

Finally, $U = \langle aa|\hat{H}_{1,2}|aa\rangle = \int d^3\mathbf{r}_1 d^3\mathbf{r}_2 |\psi_a(\mathbf{r}_1)|^2 |\psi_a(\mathbf{r}_2)|^2 \frac{e^2}{4\pi\epsilon_0 |\mathbf{r}_1 - \mathbf{r}_2|}$. All the factors in the integrand are positive, and therefore the integral must be positive.

We consider only singlet spin states and introduce the following terms and simplifications, from which the values of other matrix elements follow by symmetry.

$$\begin{aligned} \langle ab|\hat{H}_1|ab\rangle &= \langle a|\hat{H}_1|a\rangle \langle b|b\rangle = E_0 \\ \langle a|\hat{H}_1|b\rangle &= t < 0 \text{ is real} \\ \langle ab|\hat{H}_{1,2}|ab\rangle &\simeq 0 \text{ neglect} \\ \langle ab|\hat{H}_{1,2}|ba\rangle &\simeq 0 \text{ neglect} \\ \langle aa|\hat{H}_{1,2}|bb\rangle &\simeq 0 \text{ neglect} \end{aligned}$$

Show that the energy of the trial state $|\psi\rangle = \frac{1}{\sqrt{2}}(|ab\rangle + |ba\rangle)$ is $E_\psi = 2E_0$. [5]

(TURN OVER)

(H_2 is covered at length in lectures, but actually going through such a calculation is a challenging problem.)

$$\begin{aligned}
 |\psi\rangle &= \frac{1}{\sqrt{2}} (|ab\rangle + |ba\rangle) \\
 E_\psi &= \frac{1}{2} \left[\langle ab|\hat{H}_1|ab\rangle + \langle ab|\hat{H}_2|ab\rangle + \langle ba|\hat{H}_1|ab\rangle + \langle ba|\hat{H}_2|ab\rangle + \right. \\
 &\quad + \langle ab|\hat{H}_1|ba\rangle + \langle ab|\hat{H}_2|ba\rangle + \langle ba|\hat{H}_1|ba\rangle + \langle ba|\hat{H}_2|ba\rangle + \\
 &\quad \left. + \langle ab|\hat{H}_{1,2}|ab\rangle + \langle ba|\hat{H}_{1,2}|ab\rangle + \langle ab|\hat{H}_{1,2}|ba\rangle + \langle ba|\hat{H}_{1,2}|ba\rangle \right] = \\
 &= \frac{1}{2} [E_0 + E_0 + 0 + 0 + 0 + 0 + E_0 + E_0 + 0 + 0 + 0 + 0] = 2E_0
 \end{aligned}$$

(Note that for every term, its complex conjugate also appears, and that $\langle ba|\hat{H}_1|ab\rangle = \langle b|\hat{H}_1|a\rangle \langle ab\rangle = 0$ because of orthogonality of basis states.)

Show that the trial state formed from the bonding molecular orbital $|\phi\rangle = 1/2 (|1, a\rangle + |1, b\rangle) (|2, a\rangle + |2, b\rangle)$ has energy $E_\phi = 2E_0 + 2t + U/2$. [6]

(As before, but a rather lengthy calculation, unless the contributions of single-particle terms to the energy are added for each electron instead of working out the energy associated with the product wavefunction, as given below.)

$$\begin{aligned}
 |\phi\rangle &= \frac{1}{2} (|aa\rangle + |ab\rangle + |ba\rangle + |bb\rangle) \\
 E_\phi &= \frac{1}{4} \left[\langle aa|\hat{H}_1|aa\rangle + \langle ab|\hat{H}_1|ab\rangle + \langle ba|\hat{H}_1|ba\rangle + \langle bb|\hat{H}_1|bb\rangle + \right. \\
 &\quad + \text{analogous with } \hat{H}_2 + \\
 &\quad + \langle aa|\hat{H}_1|ba\rangle + \langle ab|\hat{H}_1|bb\rangle + \langle ba|\hat{H}_1|aa\rangle + \langle bb|\hat{H}_1|ab\rangle + \\
 &\quad + \text{analogous with } \hat{H}_2 + \\
 &\quad \left. + \langle \phi|\hat{H}_{1,2}|\phi\rangle \right] \\
 &= 2(E_0 + t) + \langle \phi|\hat{H}_{1,2}|\phi\rangle
 \end{aligned}$$

Find $\langle \phi|\hat{H}_{1,2}|\phi\rangle$ by noting that only $\langle aa|\hat{H}_{1,2}|aa\rangle$ and $\langle bb|\hat{H}_{1,2}|bb\rangle$ contribute, giving $\frac{1}{4}(U + U) = U/2$.

$$\implies E_\phi = 2(E_0 + t) + U/2$$

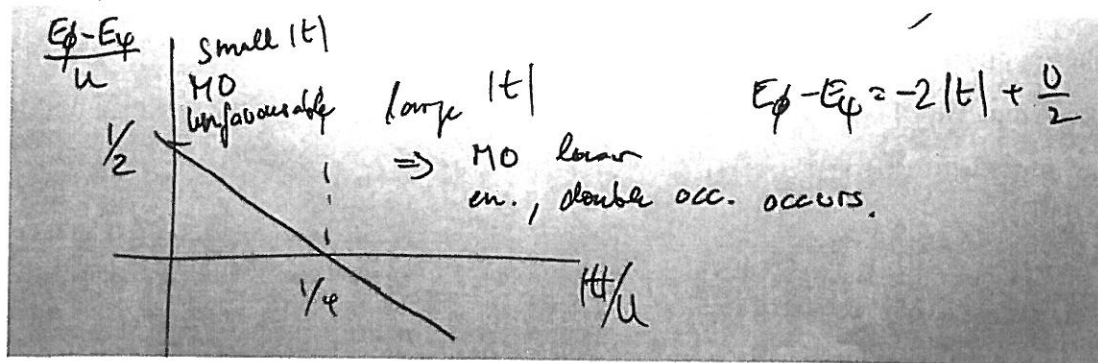
(Could obtain this more quickly by working out $\langle (\hat{H}_1 + \hat{H}_2) \phi \rangle$ first, as $2\frac{1}{2} \langle a + b | \hat{H}_1 | a + b \rangle$).

Sketch $(E_\phi - E_\psi)/U$ vs. $|t|/U$ and state how $|t|$ and U vary with separation. Comment on the character of the ground state wavefunction, and how this affects

the nature of the bond, as the separation between the atoms in the H_2 molecule is varied.

[4]

(This may come as a genuinely new idea to most, although the notion that double-occupancy varies in the ground state wavefunction is present in the lecture course.)



At large separation, $|t| \rightarrow 0$, whereas U remains constant. This favours state ψ , the valence bond state, over state ϕ , the bonding molecular orbital state. The bond at large separations cannot be considered covalent. The valence bond state avoids double occupancy of the atomic basis states. Hence, the probability of finding the basis states doubly occupied goes to zero for large separation, whereas it is 50% (MO solution) for small separation.

(TURN OVER

4 Attempt either this question or question 3.

A spin- $\frac{1}{2}$ particle confined to move in 2D is described by a wavefunction $\psi(\mathbf{r}) \begin{pmatrix} \alpha \\ \beta \end{pmatrix}$ and subject to the Hamiltonian

$$\hat{H} = c \frac{\hbar}{i} \left(\hat{\sigma}_x \frac{\partial}{\partial x} + \hat{\sigma}_y \frac{\partial}{\partial y} \right) + V \hat{\sigma}_z ,$$

where c and V are constants and $\hat{\sigma}_x, \hat{\sigma}_y, \hat{\sigma}_z$ are the Pauli spin matrices (see below). Show that travelling wave states $e^{i\mathbf{k}\cdot\mathbf{r}} \begin{pmatrix} \alpha(\mathbf{k}) \\ \beta(\mathbf{k}) \end{pmatrix}$ are eigenstates of this Hamiltonian and find their dispersion $E(|\mathbf{k}|)$. Sketch $E(|\mathbf{k}|)$ vs. $|\mathbf{k}|$ for $V > 0$, $V = 0$ and $V < 0$.

[8]

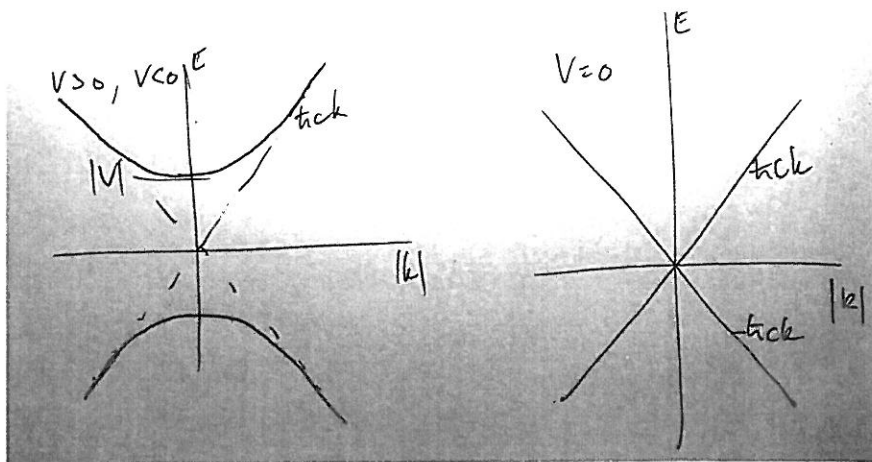
(Typical problem requiring standard approach, but made slightly unusual because of involvement of spin matrices.)

Substituting plane wave states $\begin{pmatrix} \alpha_{\mathbf{k}} \\ \beta_{\mathbf{k}} \end{pmatrix} e^{i\mathbf{k}\cdot\mathbf{r}}$, obtain matrix equation

$$\begin{pmatrix} V & \hbar c(k_x - ik_y) \\ \hbar c(k_x + ik_y) & -V \end{pmatrix} \begin{pmatrix} \alpha_{\mathbf{k}} \\ \beta_{\mathbf{k}} \end{pmatrix} = E_{\mathbf{k}} \begin{pmatrix} \alpha_{\mathbf{k}} \\ \beta_{\mathbf{k}} \end{pmatrix}$$

From the secular determinant, find

$$E_{\mathbf{k}} = \pm \sqrt{V^2 + \hbar^2 c^2 (k_x^2 + k_y^2)}$$



Consider the case $V = 0$. Show that the expectation value of the spin, $(\langle \hat{S}_x(\mathbf{k}) \rangle, \langle \hat{S}_y(\mathbf{k}) \rangle, \langle \hat{S}_z(\mathbf{k}) \rangle)$, is parallel to the wavevector \mathbf{k} .

[6]

(Problem, requiring standard methods)

For $V = 0$, substituting $E_{\mathbf{k}} = \pm \hbar c k$ into the eigenvector equation:

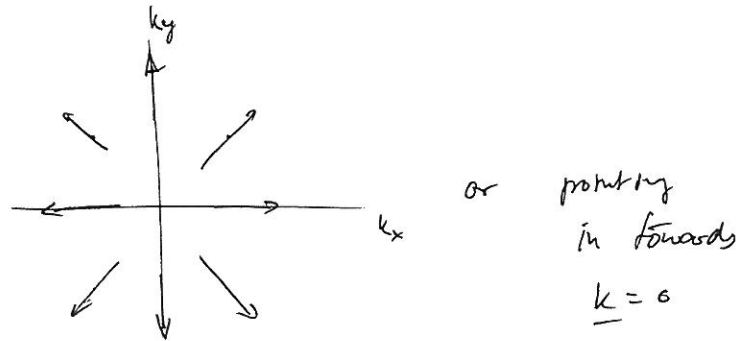
$$\hbar c(k_x - ik_y)\beta_{\mathbf{k}} = \pm \alpha_{\mathbf{k}} \hbar c k$$

Writing $k_x = k\Re e^{i\phi}$, $k_y = k\Im e^{i\phi}$, find $\beta_k = \pm e^{i\phi}\alpha_k$, so that the eigenvectors are $\frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ \pm e^{i\phi} \end{pmatrix}$

Find the expectation value of the spin:

$$\begin{aligned}\langle S_x \rangle &= \frac{\hbar}{2} \langle \hat{\sigma}_x \rangle = \frac{\hbar}{4} (1 \pm e^{-i\phi}) \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} 1 \\ \pm e^{i\phi} \end{pmatrix} = \\ &= \pm \frac{\hbar}{2} \cos \phi \\ \langle S_y \rangle &= \frac{\hbar}{2} \langle \hat{\sigma}_y \rangle = \frac{\hbar}{4} (1 \pm e^{-i\phi}) \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \begin{pmatrix} 1 \\ \pm e^{i\phi} \end{pmatrix} = \\ &= \pm \frac{\hbar}{2} \sin \phi \\ \langle S_z \rangle &= \frac{\hbar}{2} \langle \hat{\sigma}_z \rangle = \frac{\hbar}{4} (1 \pm e^{-i\phi}) \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \begin{pmatrix} 1 \\ \pm e^{i\phi} \end{pmatrix} = \\ &= 0\end{aligned}$$

The spin points along the direction of the wavevector (outwards or inwards, depending on the solution):



In the above Hamiltonian, V now is taken to depend on y :

$$\hat{H} = c \frac{\hbar}{i} \left(\hat{\sigma}_x \frac{\partial}{\partial x} + \hat{\sigma}_y \frac{\partial}{\partial y} \right) + V(y) \hat{\sigma}_z, \quad ,$$

with $V(y) < 0$ for $y < 0$ and $V(y) > 0$ for $y > 0$. Show that the state

$$\psi(x, y) = e^{ik_x x} \exp \left[-\frac{1}{\hbar c} \int_0^y V(y') dy' \right] \begin{pmatrix} 1 \\ -1 \end{pmatrix}$$

is an eigenstate of this Hamiltonian. Sketch its variation along the y direction, if $V(y)$ takes positive and negative, constant, values for $y > 0$ and $y < 0$, respectively.

[7]

(TURN OVER)

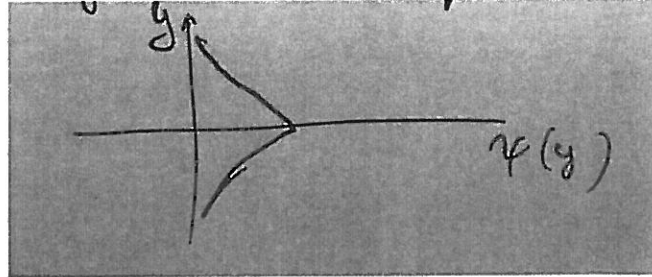
(Unseen, but not very hard to do.)

Take the spatial derivatives first: $\frac{\partial}{\partial x}\psi = ik_x\psi$, $\frac{\partial}{\partial y}\psi = -\frac{V(y)}{\hbar c}\psi$ (differentiation w.r.t. the limit of the integral brings out the integrand evaluated at the limit).

Hence, applying the full hamiltonian to ψ gives

$$\hat{H}\psi(x, y) = \begin{pmatrix} V(y) & \hbar ck_x + V(y) \\ \hbar ck_x - V(y) & -V(y) \end{pmatrix} \begin{pmatrix} 1 \\ -1 \end{pmatrix} e^{ik_x x} \exp\left[-\frac{1}{\hbar c} \int_0^y V(y') dy'\right] = (-i\hbar ck_x)\psi(x, y)$$

$\Rightarrow \psi(x, y)$ is an eigenstate. Variation along the y -direction:

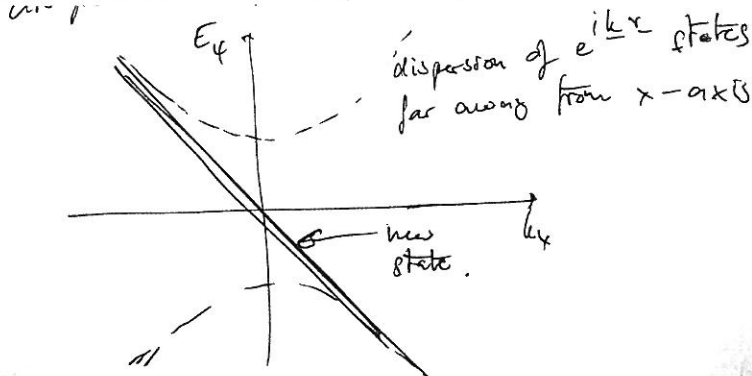


Sketch the dispersion $E(k_x)$ of this eigenstate. Comment on the propagation along the x and y directions of wavepackets built from such eigenstates.

[4]

(Interpreting dispersion relations is familiar)

The new state has the dispersion $E_\psi = -\hbar ck_x$:



This state is bound to the interface, or edge, between $V > 0$ and $V < 0$. The new state cannot propagate along the y -direction, but it travels along the x -direction. The associated group velocity, given by $\partial E / (\hbar \partial k_x)$ is negative, so wavepackets built from a range of k_x -values move towards the left in this geometry.

The Pauli spin matrices are

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

END OF PAPER