**<u>ONE HOUR THIRTY MINUTES</u>**

A list of constants is enclosed.

**UNIVERSITY OF MANCHESTER**

Fundamentals of Solid State Physics

[redacted] 2024, [redacted]

Answer **<u>ALL</u>** parts of question 1 and **<u>TWO</u>** other questions

---

The use of calculators is permitted, as long as they cannot store text and have no graphing capability.

---

The numbers are given as a guide to the relative weights of the different parts of each question.

**1.** a) What is a typical value of the lattice constant of a crystal? Give reasons for your answer.

[4 marks]

b) List all the 5 Bravais lattices in 2D. Which Bravais lattice does a honeycomb lattice belong to? Sketch the honeycomb lattice and its primitive unit cell.

[6 marks]

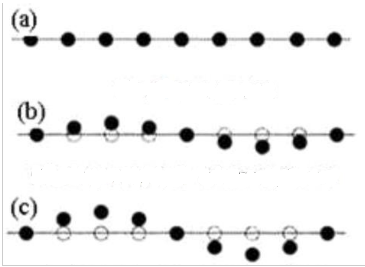
c) Write down expressions for $2p\sigma$ and $2p\sigma*$ molecular orbitals. Explain any notation you use.

[5 marks]

d) i) Define phonons in a lattice.

[2 marks]

ii) The following diagrams show vibrational states of a 1D lattice.




What is the number of phonons in (a)?
The vibrations in (b) and (c) have the same frequency. Which has the greater number of phonons and why?

[4 marks]

e) For a sample of intrinsic gallium arsenide at room temperature, the conductivity is $1.0 \times 10^{-6}\ \Omega^{-1}\mathrm{m}^{-1}$, the electron and hole mobilities are, respectively 0.85 and 0.04 $\mathrm{m}^2\mathrm{V}^{-1}\mathrm{s}^{-1}$. Calculate the electron and hole densities.

[4 marks]

**2.** a) i) Write down an expression for the exchange integral in the molecular-orbital (MO) theory of $H_2^+$. Explain any notation you use.

[5 marks]

ii) Sketch the energy of $H_2^+$ in the bonding MO as a function of the separation between the two protons. Identify the dissociation energy and bond length of the molecule in your sketch.

[5 marks]

b) i) Consider a linear chain of identical atoms of mass $M$ and lattice constant $a$, where the forces between nearest neighbours and next-nearest neighbours are included. Take the spring constants for the nearest-neighbour and next-nearest-neighbour interactions to be $S_1$ and $S_2$ respectively. Show that the dispersion relation, $\omega(k)$, for lattice vibrations of the chain is given by

$$M\omega^2 = 2S_1[1 - \cos(ka)] + 2S_2[1 - \cos(2ka)].$$

[8 marks]

ii) By considering the limit $ka \ll 1$, find the speed of sound in the 1D lattice. You may find the following expansion useful

$$\cos x = 1 - \frac{1}{2}x^2 + \cdots, \quad \text{for } x \ll 1.$$

[4 marks]

iii) What is the largest energy of a phonon in the 1D lattice?

[3 marks]

**3.** a) The electron density of iron is $1.7 \times 10^{29}$ m$^{-3}$. Calculate the Fermi energy and Fermi temperature of iron. Discuss briefly the physical implications of this Fermi temperature.

[6 marks]

b) The valence electrons in a calcium atom are in the shell $(4s)^2$. Describe, with the aid of a sketch for the density of states as a function of energy, how the nearly-free electron model is modified to account for the metallic conductivity of solid calcium.

[4 marks]

c) The calcium atoms are arranged in a face-centred cubic lattice. An X-ray experiment, using a wavelength of 1.54 Å, measures the first-order scattering from (200) planes of the crystal at a scattering angle of 32.2°.

i) Sketch a conventional unit cell, showing the alignment of the (200) plane in the unit cell, and the incident and scattered X-ray beams.

[4 marks]

ii) Calculate the (200) interplanar distance and determine the lattice constant. What is the value of the nearest-neighbour distance between two calcium atoms?

[6 marks]

iii) Calculate the mass density of solid calcium, given that the atomic mass of calcium is 40.1 u.

[5 marks]

**4.** a) i) Write down the ground-state electronic configuration of the molecular ion $O_2^+$ and calculate its bond order. Will this ion have shorter or longer bond length than $O_2$? Explain your answer.

[5 marks]

ii) An $O_2$ molecule absorbs light of wavelength 145 nm. Determine its electronic energy in eV. Estimate its vibrational and rotational energies in eV.

[6 marks]

b) Define a hole in a semiconductor and give its charge.

The energy spectrum of an electron in a valence band of a semiconductor is given by

$$E(k) = -Ak^2,$$

where $A = 2.0 \times 10^{-38}$ Jm$^2$. Calculate the effective mass of the electron in terms of electron mass $m_e$.

A hole is created in the valence band. Determine its effective mass.

[6 marks]

c) i) Write down the expression for the donor binding energy $\Delta E$ as measured from the conduction band edge for a doped semiconductor and explain any notation you use.

[3 marks]

ii) For the semiconductor Indium phosphide (InP), the effective electron mass $m_e^* = 0.08m_e$ and the relative permittivity $\epsilon = 12.4$. Calculate the absolute value of the donor binding energy for electrons doped into InP. Comment on the implication of your results on the conductivity given that the bandgap of InP is 1.5 eV.

[5 marks]

**END OF EXAMINATION PAPER**

**ONE HOUR THIRTY MINUTES**

A list of constants is enclosed.

**UNIVERSITY OF MANCHESTER**

Advanced Quantum Mechanics

[redacted] 2024, [redacted] - [redacted]

Answer **TWO** questions

---

The use of calculators is permitted, as long as they cannot store text and have no graphing capability.

---

The numbers are given as a guide to the relative weights of the different parts of each question.

You may assume the following formulae in any question *if proof is not explicitly requested*:

**Special integrals**

$$\int_{-\infty}^{\infty} x^{2n} e^{-ax^2} dx = \frac{1\cdot 3\cdot 5\cdots(2n-1)}{(2a)^n}\sqrt{\frac{\pi}{a}}, \qquad \int_0^{\infty} x^n e^{-ax} dx = \frac{n!}{a^{n+1}}, \quad a > 0.$$

**4-vectors**
Use notation $x^\mu = (x^0, \mathbf{r})$ for 4-position and $p^\mu = (E/c, \mathbf{p})$ for 4-momentum. In electromagnetism $A^\mu = (\Phi/c, \mathbf{A})$ for 4-potential.

**Klein-Gordon equation** in scalar $S$ and vector $(V_0/c, \mathbf{V})$ potential field

$$\left[(\hat{\mathbf{p}} - \mathbf{V})^2 c^2 + (mc^2 + S)^2\right]\Psi = (i\hbar\partial_t - V_0)^2\Psi.$$

**Dirac equation** in scalar $S$ and vector $(V_0/c, \mathbf{V})$ potential field

$$\left[\boldsymbol{\alpha}\cdot(\hat{\mathbf{p}} - \mathbf{V})c + \beta(mc^2 + S)\right]\Psi = (i\hbar\partial_t - V_0)\Psi.$$

**Standard spinor solutions** to the free massive Dirac equation

$$u_s(E,\mathbf{p}) = \sqrt{E+mc^2}\begin{pmatrix}\phi_s \\ \frac{c\boldsymbol{\sigma}\cdot\mathbf{p}}{E+mc^2}\phi_s\end{pmatrix}, \quad \phi_1 = \begin{pmatrix}1\\0\end{pmatrix} \text{ and } \phi_2 = \begin{pmatrix}0\\1\end{pmatrix};$$

**Standard matrices**

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

$$\alpha_i = \begin{pmatrix}0 & \sigma_i\\ \sigma_i & 0\end{pmatrix}, \quad \beta = \begin{pmatrix}I_2 & 0\\ 0 & -I_2\end{pmatrix}, \quad \Sigma_i = \begin{pmatrix}\sigma_i & 0\\ 0 & \sigma_i\end{pmatrix};$$

$$\gamma_0 = \begin{pmatrix}I_2 & 0\\ 0 & -I_2\end{pmatrix}, \quad \gamma_1 = \begin{pmatrix}0 & \sigma_x\\ -\sigma_x & 0\end{pmatrix}, \quad \gamma_2 = \begin{pmatrix}0 & \sigma_y\\ -\sigma_y & 0\end{pmatrix}, \quad \gamma_3 = \begin{pmatrix}0 & \sigma_z\\ -\sigma_z & 0\end{pmatrix}.$$

**Space-time metric** We use the metric $\eta_{\mu\nu} = \mathrm{diag}(1,-1,-1,-1)$.

**Laplacian operator** in terms of angular momentum operator $\hat{\mathbf{L}}$

$$\nabla^2 = \frac{1}{r}\frac{\partial^2}{\partial r^2}r - \frac{\hat{\mathbf{L}}^2}{\hbar^2 r^2}.$$

**Solution to Dirac equation** in spherical vector potential $(V_0(r)/c, \vec{0})$

$$\psi^\kappa_{jm}(\mathbf{r}) = \begin{pmatrix} f^\kappa_j(r)\mathcal{Y}^\kappa_{jm}(\theta,\phi) \\ i g^\kappa_j(r)\mathcal{Y}^{-\kappa}_{jm}(\theta,\phi)\end{pmatrix} \quad \text{with } F = rf \text{ and } G = rg,$$

$$\hbar c\left[\frac{d}{dr} - \frac{\kappa}{r}\right] G^\kappa_j(r) = -\left(E - V_0(r) - mc^2\right) F^\kappa_j(r),$$

$$\hbar c\left[\frac{d}{dr} + \frac{\kappa}{r}\right] F^\kappa_j(r) = \left(E - V_0(r) + mc^2\right) G^\kappa_j(r).$$

**1.** a) Show that the angular momentum operator $\hat{L}_x$ is the generator of infinitesimal rotations about the $x$-axis for a spinless particle. Derive an expression in terms of $\hat{L}_x$ for the operator $\hat{U}_\beta$ that represents a finite rotation of angle $\beta$ about the $x$-axis.

[8 marks]

b) For a spinless particle with non-zero orbital angular momentum, write down the operator $\hat{U}_{\alpha,\beta,\gamma}$ representing a rotation with Euler angles $(\alpha, \beta, \gamma)$.

Within the space of states with angular momentum quantum number $l = 1$, the operators $\hat{L}_x$, $\hat{L}_y$, and $\hat{L}_z$ may be written in matrix representation as

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

Show that for the choice of Euler angles $(0, 0, \gamma)$ the $\hat{L}_x$ eigenstate

$$\frac{1}{\sqrt{2}} \begin{pmatrix} -1 \\ 0 \\ 1 \end{pmatrix},$$

can be transformed into an eigenstate of $\hat{L}_y$ for an appropriate value of $\gamma$. Give the corresponding Wigner $D$-matrix.

[7 marks]

c) A charged quantum rotor of angular momentum quantum number $l = 1$ is placed in a uniform magnetic field oriented along the $z$-axis. The Hamiltonian is given by

$$\hat{H}_0 = \alpha \hat{L}_z,$$

where $\alpha$ is a positive constant. Initially the rotor is in the ground state of $\hat{H}_0$. At time $t = 0$ a weak magnetic field is switched on in the $x$-direction, which subsequently decays in time. The Hamiltonian of the rotor is now

$$\hat{H}(t) = \hat{H}_0 + \beta \hat{L}_x \exp(-t/\tau),$$

where $\beta$ and $\tau$ are positive constants, with $\beta \ll \alpha$.

i) Using first-order perturbation theory, calculate the transition probability $P(t)$ to the first excited state of the rotor as a function of time.

[7 marks]

ii) Determine the long-time limit $P(\infty)$ and find a condition on $\tau$ to ensure its validity.

[3 marks]

**2.** a) Consider a free relativistic spin-1/2 particle of mass $m$. Define the Dirac four-current $j^\mu = (c\rho, \mathbf{j})$ and show that the Dirac equation implies the continuity equation,

$$\frac{\partial}{\partial t}\rho + \nabla \cdot \mathbf{j} = 0.$$

[4 marks]

b) Now consider a relativistic electron moving in the $x$-$y$ plane with a uniform applied magnetic field in the $z$-direction, given by $\mathbf{B} = (0, 0, B)$.

i) Show that this magnetic field can be described by the vector potential $\mathbf{A} = (0, xB, 0)$ and prove that the following identity holds for this potential:

$$[\boldsymbol{\sigma} \cdot (\hat{\mathbf{p}} + e\mathbf{A})]^2 = (\hat{\mathbf{p}} + e\mathbf{A})^2 + e\hbar\sigma_z B.$$

[4 marks]

ii) The Hamiltonian for a non-relativistic electron in the same potential is

$$\hat{H}_{\text{NR}} = \frac{1}{2m}(\hat{\mathbf{p}} + e\mathbf{A})^2,$$

which has eigenvalues

$$E_n = \left(n + \frac{1}{2}\right)\hbar\omega_c.$$

Here, $n = 0, 1, 2, \ldots$ and $\omega_c = eB/m$ is the cyclotron frequency.

Express the Dirac equation for this electron in terms of the upper components only. Find the energy eigenvalues by treating the upper components as simultaneous eigenstates of $\hat{H}_{\text{NR}}$ and of the spin operator $\hat{S}_z$.

[8 marks]

iii) For the weak-field case, $\hbar\omega_c \ll mc^2$, show that the energy levels of the relativistic electron are given by

$$E_n^{\uparrow} = mc^2 + (n+1)\hbar\omega_c, \quad E_n^{\downarrow} = mc^2 + n\hbar\omega_c, \quad n = 0, 1, 2 \ldots$$

for spin-up and spin-down electrons, respectively.

[2 marks]

c) A beam of massless relativistic particles with charge $q = e$, energy $E_p$, and in the spin-up eigenstate of $\hat{S}_z$ (spinor $\phi_1$) is moving in the positive $z$-direction and encounters an electrostatic step potential defined by

$$e\Phi(z) = \begin{cases} 0 & \text{for } z < 0, \\ V_0 & \text{for } z > 0. \end{cases}$$

Show that for $E_p > V_0$ all particles are transmitted.

[7 marks]

**3.** a) Consider a non-relativistic spinless particle of charge $q$ and mass $m$ in the 4-potential $A^\mu = (\Phi/c, \mathbf{A})$.

i) Write down the electromagnetic gauge transformation for the potentials $\Phi$ and $\mathbf{A}$ in terms of a differentiable function $\lambda(\mathbf{r}, t)$.

[2 marks]

ii) The particle is placed in a homogenous oscillatory electric field of frequency $\omega$ directed along the $z$-axis, with $E_z = E_0 \cos(\omega t)$. In two different gauges the electric field may be considered as arising purely from the potential $\Phi$, or purely from the potential $\mathbf{A}$. Write down the corresponding potentials and find a function $\lambda(\mathbf{r}, t)$ that transforms from the first to the second. Given that $|\psi_1\rangle$ is a solution to the time-dependent Schrödinger equation in the first case, show that

$$|\psi_2\rangle = \exp(iq\lambda(\mathbf{r}, t)/\hbar)|\psi_1\rangle,$$

is a solution in the second case. [8 marks]

b) Now consider a relativistic spinless particle of charge $e$ that is bound to a nucleus by a Coulomb-like *scalar* potential $S(r) = -Z\hbar c\alpha/r$, where $\alpha$ is the fine-structure constant.

i) Write down the time-independent Klein-Gordon equation for the eigenstates of the particle with energy $E$.

[2 marks]

ii) By considering an eigenstate of total angular momentum with quantum number $l$, show that the eigenvalue equation for the radial part $\psi(r)$ of the wave function of the particle can be written as

$$\left[2mE' + \hbar^2\left(\frac{1}{r}\frac{\partial^2}{\partial r^2}r - \frac{l'(l'+1)}{r^2}\right) + \frac{2m\hbar c Z\alpha}{r}\right]\psi(r) = 0. \qquad (1)$$

Express $E'$ and $l'(l'+1)$ in terms of $E$ and $l$.

[6 marks]

iii) The eigenvalues of equation (1) can be written in the form

$$E' = -\frac{1}{2}mc^2\left(\frac{Z\alpha}{n'}\right)^2,$$

where $n'$ is related to $l$ and the principal quantum number $n = 1, 2, 3\ldots$ by

$$n' = n - (l + 1/2) + \sqrt{(l + 1/2)^2 + (Z\alpha)^2}.$$

Find the energy levels $E_{n,l}$ of the particle and discuss whether or not there are any restrictions on the allowed values of $Z\alpha$. Considering the limit $Z\alpha \ll 1$ find the first *relativistic* energy correction for the case $l = 0$.

[7 marks]



**END OF EXAMINATION PAPER**

**ONE HOUR THIRTY MINUTES**

A list of constants is enclosed.

**UNIVERSITY OF MANCHESTER**

Introduction to Quantum Mechanics

16th January 2024, 2.00 p.m. - 3.30 p.m.

Answer **ALL** parts of question 1 and **TWO** other questions

---

The use of calculators is permitted, as long as they cannot store text or perform algebra, and have no graphing capability.

---

The numbers are given as a guide to the relative weights of the different parts of each question.

# Formula Sheet

In plane polar coordinates, $(r, \phi)$, the Laplacian operator is given by

$$\nabla^2 = \frac{\partial^2}{\partial r^2} + \frac{1}{r}\frac{\partial}{\partial r} + \frac{1}{r^2}\frac{\partial^2}{\partial \phi^2}\,,$$

and the angular momentum operator is given by

$$\hat{L}_z = -i\hbar\frac{\partial}{\partial \phi}\,.$$

In spherical polar coordinates, $(r, \theta, \phi)$, the Laplacian operator is given by

$$\nabla^2 = \frac{\partial^2}{\partial r^2} + \frac{2}{r}\frac{\partial}{\partial r} + \frac{1}{r^2}\frac{\partial^2}{\partial \theta^2} + \frac{1}{r^2}\frac{\cos\theta}{\sin\theta}\frac{\partial}{\partial \theta} + \frac{1}{r^2\sin^2\theta}\frac{\partial^2}{\partial \phi^2}\,,$$

and the angular momentum operators are given by

$$\hat{L}^2 = -\hbar^2\left(\frac{\partial^2}{\partial \theta^2} + \frac{\cos\theta}{\sin\theta}\frac{\partial}{\partial \theta} + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial \phi^2}\right),$$

$$\hat{L}_z = -i\hbar\frac{\partial}{\partial \phi}\,.$$

You may use the following integral without proof:

$$\int_0^\infty x^n\,\mathrm{e}^{-x}\,\mathrm{d}x = n! \quad \text{for integer } n \geq 0.$$

**1.** a) A particle of mass $m$ is moving in two dimensions in a potential $V(\mathbf{r})$. Write down the time-independent Schrödinger equation of the particle. Explain any symbols you have used.

[4 marks]

b) i) Write down the definition of the momentum operator $\hat{p}_x$ in one dimension. Show that the function

$$\psi(x) = e^{i\alpha x},$$

with constant $\alpha$, is an eigenfunction of $\hat{p}_x$. Determine the eigenvalue of $\psi(x)$.

ii) A particle is moving in one-dimensional free space and is described by a spatial function

$$\phi(x) = \cos(\beta x),$$

where $\beta$ is a constant. What are the possible outcomes of a measurement of the particle's momentum and what are their probabilities?

[5 marks]

c) Two operators, $\hat{A}$ and $\hat{B}$, can act on wavefunctions $\Psi$. Define the commutator of the two operators and explain what the expression $[\hat{A}, \hat{B}]\Psi$ represents.

Show that the commutator of the position and momentum operators in one dimension is given by

$$[\hat{x}, \hat{p}_x] = i\hbar\,.$$

What is the implication of this result for measurements of these quantities?

[6 marks]

d) Diatomic molecules of nitric oxide gas, NO, absorb infrared light of wavelength $5.4 \times 10^{-6}$ m. Use this to estimate the effective spring constant of the bond in a nitric oxide molecule.

You may assume that the atomic masses of nitrogen and oxygen are 14.0 and 16.0 respectively.

[5 marks]

e) Sketch the hydrogen energy-level diagram up to $n = 3$.

Explain which transitions are allowed between these states by the emission or absorption of a single photon and indicate these on your diagram.

Explain why the $2s$ state is much longer-lived than any of the other excited states.

[5 marks]

**2.** The Hamiltonian operator for a particle moving in three dimensions in a central potential $V(r)$ is given by

$$\hat{H} = \frac{-\hbar^2}{2m}\nabla^2 + V(r).$$

a) Use this, and information on the Formula Sheet, to show that the total angular momentum operator, $\hat{L}^2$, and its component, $\hat{L}_z$, both commute with this Hamiltonian. Explain the physical consequence of these commutations.

[5 marks]

b) Consider separable energy eigenfunctions,

$$\psi(r,\theta,\phi) = R(r)Y_\ell^m(\theta,\phi),$$

where the spherical harmonics $Y_\ell^m(\theta,\phi)$ are eigenfunctions of $\hat{L}^2$ and $\hat{L}_z$.

i) Show that the radial function $R(r)$ depends on the angular momentum quantum number $\ell$. Write down the energy eigenvalue equation satisfied by $R(r)$.

[5 marks]

ii) Explain why the $\phi$ dependence of $Y_\ell^m(\theta,\phi)$ must be equal to $\mathrm{e}^{im\phi}$, where $m$ is an integer.

[3 marks]

c) The Hamiltonian of a three-dimensional simple harmonic oscillator of classical angular frequency $\omega$ and mass $m$ is given by

$$\hat{H} = \frac{-\hbar^2}{2m}\nabla^2 + \frac{1}{2}m\omega^2 r^2.$$

i) Show that the function $\psi_0(r,\theta,\phi) = A\,\mathrm{e}^{-r^2/2a^2}$ is an eigenfunction of $\hat{L}^2$ and $\hat{L}_z$, and write down its eigenvalues.
Show that this function is also an energy eigenfunction, provided $a = \sqrt{\hbar/m\omega}$, and calculate its energy.

[7 marks]

ii) Show that the function $\psi_1(r,\theta,\phi) = B\,r\sin\theta\cos\phi\,\mathrm{e}^{-r^2/2a^2}$ is an eigenfunction of $\hat{L}^2$ and calculate its eigenvalue.
Show that this function is not an eigenfunction of $\hat{L}_z$.
If a system was in the state described by $\psi_1$ and the value of $L_z$ was measured, what values could be obtained?

[5 marks]

**3.** a) Consider the following wavefunctions of a hydrogen atom

$$\begin{aligned}
\psi_A(r,\theta,\phi) &= A\frac{r}{a_0}\mathrm{e}^{-r/2a_0}\sin\theta\,\mathrm{e}^{i\phi}, \\
\psi_B(r,\theta,\phi) &= B\frac{r}{a_0}\left(6-\frac{r}{a_0}\right)\mathrm{e}^{-r/3a_0}\sin\theta\,\mathrm{e}^{i\phi}, \\
\psi_C(r,\theta,\phi) &= C\left(\frac{r}{a_0}\right)^2\mathrm{e}^{-r/3a_0}\sin\theta\cos\theta\,\mathrm{e}^{i\phi},
\end{aligned}$$

where $A$, $B$, $C$ and $a_0$ are constants.

i) Deduce by inspection the values of the quantum numbers $(n, \ell, m_\ell)$ for each of these eigenfunctions.

[6 marks]

ii) Show that the states $\psi_A$, $\psi_B$ and $\psi_C$ are all orthogonal to each other.

[6 marks]

b) Explain why deuterium (the hydrogen isotope with atomic mass = 2) has a different ground state energy to standard hydrogen (with atomic mass = 1). Calculate the ratio of their ground state energies.

[3 marks]

c) The spin-orbit coupling operator $\hat{V}_{\mathrm{SO}}$ for a hydrogen atom is given by

$$\hat{V}_{\mathrm{SO}} = f(r)\hat{\mathbf{S}}\cdot\hat{\mathbf{L}}\,,$$

with the function $f(r)$ defined as

$$f(r) = \frac{\alpha\hbar}{2m_e^2c}\frac{1}{r^3},$$

where $\alpha = 1/137$ and all symbols have their usual meanings.

i) The hydrogen atom is in the $3d$ state. Determine the possible values of the total angular momentum quantum number $j$. Hence determine the eigenvalues of the operator $\hat{\mathbf{S}}\cdot\hat{\mathbf{L}}$.

[6 marks]

ii) Estimate the spin-orbit energy splitting in eV between the states with the $j$ values found in Part (i).
You may use the result that the expectation value for the $3d$ state of hydrogen is

$$\left\langle\frac{1}{r^3}\right\rangle = \frac{1}{405a_0^3},$$

where $a_0$ is the Bohr radius.

[4 marks]

**4.** a) Briefly state the physical meanings of the quantum numbers $(n, \ell, m_\ell, m_s)$ of a hydrogen atom. Specify their values for a hydrogen atom in its ground state, and their allowed values for excited states.

[5 marks]

b) The operator $\hat{P}$ is defined for a system containing two identical particles as the operator that exchanges all properties (position $\mathbf{r}$ and spin $\mathbf{s}$) of the two particles:

$$\hat{P}\Psi(\mathbf{r}_1, \mathbf{s}_1, \mathbf{r}_2, \mathbf{s}_2) = \Psi(\mathbf{r}_2, \mathbf{s}_2, \mathbf{r}_1, \mathbf{s}_1),$$

for which you may use the shorthand $\hat{P}\Psi(1, 2) = \Psi(2, 1)$.

i) Find the eigenvalues of $\hat{P}$.

[5 marks]

ii) Which of the eigenvalues in Part (i) do electron states have?
If two electrons are in a state with separable position and spin wavefunctions,

$$\Psi(\mathbf{r}_1, \mathbf{s}_1, \mathbf{r}_2, \mathbf{s}_2) = \psi(\mathbf{r}_1, \mathbf{r}_2)\chi(\mathbf{s}_1, \mathbf{s}_2),$$

what does this eigenvalue imply about the functions $\psi$ and $\chi$?

[2 marks]

iii) In a helium atom, the spin wavefunction of the two electrons can be anti-symmetric (parahelium) or symmetric (orthohelium).
Write down the ground-state electronic configurations of parahelium and ortho-helium. Which has the lower energy? Explain why.

[5 marks]

iv) In both orthohelium and parahelium, an electronic configuration $(1s)(2s)$ is possible. Which has the lower energy? Explain why.

[5 marks]

c) Explain why the ground state electronic configuration of lithium, Li, is $(1s)^2(2s)$.

[3 marks]

**END OF EXAMINATION PAPER**

**ONE HOUR THIRTY MINUTES**

A list of constants is enclosed.

**UNIVERSITY OF MANCHESTER**

Advanced Quantum Mechanics

32nd January 2023, 2.00 p.m. - 3.30 p.m.

Answer **TWO** questions

---

Electronic calculators may be used, provided that they cannot store text.

---

The numbers are given as a guide to the relative weights of the different parts of each question.

You may assume the following formulae in any question *if proof is not explicitly requested*:

**Special integrals**

$$\int_{-\infty}^{\infty} x^{2n} e^{-ax^2} dx = \frac{1 \cdot 3 \cdot 5 \cdots (2n-1)}{(2a)^n} \sqrt{\frac{\pi}{a}}, \qquad \int_0^{\infty} x^n e^{-ax} dx = \frac{n!}{a^{n+1}}, \quad a > 0.$$

**4-vectors**
Use notation $x^\mu = (x^0, \mathbf{r})$ for 4-position and $p^\mu = (E/c, \mathbf{p})$ for 4-momentum. In electromagnetism $A^\mu = (\Phi/c, \mathbf{A})$ for 4-potential.

**Klein-Gordon equation** in scalar $S$ and vector $(V_0/c, \mathbf{V})$ potential field

$$\left[(\hat{\mathbf{p}} - \mathbf{V})^2 c^2 + (mc^2 + S)^2\right] \Psi = (i\hbar\partial_t - V_0)^2 \Psi.$$

**Dirac equation** in scalar $S$ and vector $(V_0/c, \mathbf{V})$ potential field

$$\left[\boldsymbol{\alpha} \cdot (\hat{\mathbf{p}} - \mathbf{V})c + \beta(mc^2 + S)\right] \Psi = (i\hbar\partial_t - V_0)\Psi.$$

**Standard spinor solutions** to the free massive Dirac equation

$$u^{(s)}(E, \mathbf{p}) = \sqrt{E + mc^2} \begin{pmatrix} \phi^s \\ \frac{c\boldsymbol{\sigma}\cdot\mathbf{p}}{E+mc^2}\phi^s \end{pmatrix}, \quad \phi^1 = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \text{ and } \phi^2 = \begin{pmatrix} 0 \\ 1 \end{pmatrix};$$

**Standard matrices**

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

$$\alpha_i = \begin{pmatrix} 0 & \sigma_i \\ \sigma_i & 0 \end{pmatrix}, \quad \beta = \begin{pmatrix} I_2 & 0 \\ 0 & -I_2 \end{pmatrix}, \quad \Sigma_i = \begin{pmatrix} \sigma_i & 0 \\ 0 & \sigma_i \end{pmatrix};$$

$$\gamma_0 = \begin{pmatrix} I_2 & 0 \\ 0 & -I_2 \end{pmatrix}, \quad \gamma_1 = \begin{pmatrix} 0 & \sigma_x \\ -\sigma_x & 0 \end{pmatrix}, \quad \gamma_2 = \begin{pmatrix} 0 & \sigma_y \\ -\sigma_y & 0 \end{pmatrix}, \quad \gamma_3 = \begin{pmatrix} 0 & \sigma_z \\ -\sigma_z & 0 \end{pmatrix}.$$

**Space-time metric** We use the metric $\eta_{\mu\nu} = \mathrm{diag}(1, -1, -1, -1)$.

**Laplacian operator** in terms of angular momentum operator $\hat{\mathbf{L}}$

$$\nabla^2 = \frac{1}{r}\frac{\partial^2}{\partial r^2} r - \frac{\hat{\mathbf{L}}^2}{\hbar^2 r^2}.$$

**Solution to Dirac equation** in spherical vector potential $(V_0(r)/c, \vec{0})$

$$\psi^\kappa_{jm}(\mathbf{r}) = \begin{pmatrix} f^\kappa_j(r)\mathcal{Y}^\kappa_{jm}(\theta, \phi) \\ i g^\kappa_j(r)\mathcal{Y}^{-\kappa}_{jm}(\theta, \phi) \end{pmatrix} \quad \text{with } F = rf \text{ and } G = rg,$$

$$\hbar c \left[\frac{d}{dr} - \frac{\kappa}{r}\right] G^\kappa_j(r) = -\left(E - V_0(r) - mc^2\right) F^\kappa_j(r),$$

$$\hbar c \left[\frac{d}{dr} + \frac{\kappa}{r}\right] F^\kappa_j(r) = \left(E - V_0(r) + mc^2\right) G^\kappa_j(r).$$

**1.** a) State the selection rules for electric-dipole transitions in light atoms and explain any notation that you use. State whether each of the following transitions in nitrogen [(i),(ii)] or carbon [(iii)] could be electric-dipole transitions, and justify your answers:

i) $(2s)^2(2p)^3\ {}^4S_{3/2} \to (2s)^2(2p)^2(3d)\ {}^4P_{5/2}$
ii) $(2s)^2(2p)^2(3s)\ {}^4D_{3/2} \to (2s)^2(2p)^2(3d)\ {}^4P_{5/2}$
iii) $(2s)^2(2p)(3d)\ {}^1D_2 \to (2s)^2(2p)^2\ {}^1S_0$

[4 marks]

b) Show that the momentum operator $\hat{\mathbf{p}}$ is the generator of infinitesimal translations in space. Derive an expression in terms of $\hat{\mathbf{p}}$ for the operator $\hat{U}_{\mathbf{a}}$ representing a finite translation $\mathbf{r} \to \mathbf{r} - \mathbf{a}$. Show that $\hat{U}_{\mathbf{a}}$ is unitary.

[7 marks]

c) Write down the operator $\hat{U}_{\alpha,\beta,\gamma}$ representing a rotation with Euler angles $(\alpha, \beta, \gamma)$ for a spin-1/2 particle with zero orbital angular momentum. Determine the corresponding Wigner D-matrix. Use this Wigner D-matrix to show that a $2\pi$ rotation of an eigenstate of $\hat{S}_z$ about the $x$-axis changes the sign of the state.

[9 marks]

d) Consider a free relativistic electron of mass $m$. Show that the orbital angular momentum operator $\hat{\mathbf{L}}$ is not a constant of the motion.

[5 marks]

**2.** a) A spin-1/2 system subject to a static field is described by the Hamiltonian

$$\hat{H}_0 = \frac{\hbar\gamma}{2}\sigma_z.$$

At time $t = 0$ a weak rotating field in the $xy$ plane is switched on and the Hamiltonian becomes $\hat{H} = \hat{H}_0 + \hat{V}(t)$, where

$$\hat{V}(t) = \frac{\hbar\Omega}{2}(\sigma_x \cos\omega t + \sigma_y \sin\omega t).$$

Both $\gamma$ and $\Omega$ are independent of $t$. Initially, at time $t = 0$, the spin system is in the ground-state of $H_0$. Assuming $\Omega$ to be weak and taking $\hat{V}(t)$ as a perturbation, use first-order time-dependent perturbation theory to derive the transition rate (probability per unit time) for the system to make a transition to the excited state of $\hat{H}_0$ in the large-$t$ limit. You may find the asymptotic behaviour of the following function useful:

$$t\frac{\sin^2(xt/2)}{(xt/2)^2} = t\,\mathrm{sinc}^2(xt/2) \to 2\pi\delta(x), \quad \text{as } t \to \infty.$$

[12 marks]

b) i) Write down the time-dependent Schrödinger equation for a non-relativistic spinless particle of mass $m$ and charge $q$ in the 4-potential $A^\mu = (\Phi/c, \mathbf{A})$. Under a gauge transformation the 4-potential transforms as:

$$\mathbf{A} \to \mathbf{A} + \nabla\lambda(\mathbf{r}, t), \qquad \Phi \to \Phi - \frac{\partial\lambda(\mathbf{r}, t)}{\partial t}.$$

Write down the corresponding gauge transformation operator for the wave function of the particle. Show that the time-dependent Schrödinger equation transforms as expected using this gauge transformation operator.

[6 marks]

ii) Consider the particle moving in a uniform magnetic field $\mathbf{B}$ that points in the $z$-direction and is described by the 4-potential $(0, \mathbf{A})$. Show that the field can be described by the vector potential $\mathbf{A} = (-yB, 0, 0)$. Using the time-independent Schrödinger equation, find the eigenvalues (Landau levels) of the Hamiltonian for the motion in the $xy$ plane and express the eigenfunctions in terms of the eigenfunctions $\Phi_n(y)$ of a simple harmonic oscillator.

[7 marks]

**3.** a) i) Define the action of the parity operator $\hat{P}$ on an arbitrary state represented by the position space wave function $\psi(\mathbf{r}, t)$. Calculate the eigenvalues of $\hat{P}$ and comment on the symmetry of its eigenstates.

[5 marks]

ii) By considering a matrix element of the momentum operator $\hat{\mathbf{p}}$ of the form

$$\langle\phi|\hat{\mathbf{p}}|\psi\rangle = \int d\mathbf{r}\, \phi^*(\mathbf{r}, t)\, \hat{\mathbf{p}}\, \psi(\mathbf{r}, \mathbf{t}),$$

for arbitrary $|\phi\rangle$ and $|\psi\rangle$, show that the passive parity transformation of $\hat{\mathbf{p}}$ is

$$\hat{P}^\dagger\, \hat{\mathbf{p}}\, \hat{P} = -\hat{\mathbf{p}}.$$

[5 marks]

b) Consider a spinless particle of charge $e$ in a vector potential field $(e\Phi(r)/c, \mathbf{0})$, where

$$e\Phi(r) = \begin{cases} 0, & \text{for } r \leq R \\ \infty & \text{for } r > R, \end{cases}$$

defines an infinite electrostatic spherical potential of radius $R$.

i) Write down the time-independent Klein-Gordon equation for the eigenstates of the particle.

[3 marks]

ii) By considering an eigenstate of total angular momentum with quantum number $l$, find the eigenvalue equation for the radial part $R(r)$ of the wave function of the particle.

[4 marks]

iii) Using suitable boundary conditions, find the ground-state wave function and the ground-state energy of the particle. The ground-state wave function does not need to be normalised and you might find it helpful to make the substitution $R(r) = u(r)/r$. Briefly discuss the non-relativistic limit for the ground-state energy.

[8 marks]

**END OF EXAMINATION PAPER**

**<u>ONE HOUR THIRTY MINUTES</u>**

A list of constants is enclosed.

**UNIVERSITY OF MANCHESTER**

Fundamentals of Solid State Physics

32nd May/June 2023, xx - xx

Answer **<u>ALL</u>** parts of question 1 and **<u>TWO</u>** other questions

---

Electronic calculators may be used, provided that they cannot store text.

---

The numbers are given as a guide to the relative weights of the different parts of each question.

**1.** a) What is the Born-Oppenheimer approximation for molecules? Why is it a valid approximation?

[3 marks]

b) Write down an expression for the Coulomb integral in the molecular-orbital theory of $H_2^+$. Explain any notation you use.

[4 marks]

c) The electronic configuration of a magnesium atom is $[\mathrm{Ne}](2s)^2$. Explain, with the aid of a sketch for the energy band structure in the nearly-free electron model, why solid magnesium shows metallic conductivity.

[5 marks]

d) Write down a model potential for the pair-wise interaction between ions of an ionic solid. Explain the physical origin of each term.

[4 marks]

e) i) Given that the phonons in a 3D monatomic solid can be represented by a plane wave of form, $e^{i\mathbf{k}\cdot\mathbf{r}}$, show that the density of states for the phonons is related to their energy by

$$g(E) \propto E^2,$$

where the phonon energy $E = \hbar v_p k$ and $v_p$ is the speed of sound.

[5 marks]

ii) Consider a mole of this monatomic solid for which the density of states for the phonons is written as $g(E) = AE^2$. Find the constant $A$ in terms of the Debye temperature $\Theta_D$ and the gas constant $R$.

[4 marks]

**2.** a) i) The molar volume of sodium is $23.8 \times 10^{-6}$ m$^3$, the electron mobility at room temperature is $5.3 \times 10^{-3}\,\mathrm{m^2V^{-1}s^{-1}}$, and the atomic electronic configuration is $[\mathrm{Ne}](3s)^1$. Estimate the value of the electrical conductivity of sodium at room temperature.

[5 marks]

ii) Estimate also the value of the electronic thermal conductivity of sodium at room temperature. You may assume the following value for the Lorenz number

$$L_D \approx 1.67 \times 10^{-8}\,\mathrm{W\Omega K^{-2}}.$$

[3 marks]

b) An electron moving in a 1D solid of lattice constant $a$ is described by a Hamiltonian $\hat{H}$. A crystal orbital of the electron is given by

$$\psi_k = \sum_n e^{ikna}\phi_n(x),$$

where $n$ is summed over all lattice sites, $k$ is the wavenumber, $\phi_n$ is the atomic orbital at site $n$.

i) Using the tight-binding approximation, show that the energy spectrum of the electron is given by

$$E(k) = \alpha + 2\beta\cos(ka),$$

and find the expressions for $\alpha$ and $\beta$ as integrals involving $\hat{H}$.

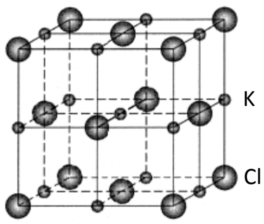
[10 marks]

ii) State the physical meanings of $\alpha$ and $\beta$. Given that $\beta$ is always negative, sketch $E(k)$ for $-\pi/a < k < \pi/a$. Discuss the nature of bonding contributed by the electron in the limits $k \to 0$ and $k \to \pm\pi/a$.

[7 marks]

**3.** a) KCl has the following crystal structure. State the nature of bonding in the solid and the Bravais lattice type. How many atoms are there in the basis?

[6 marks]




b) How many acoustic and optical vibrational branches (modes per basis) are there in a KCl crystal?

[3 marks]

c) An X-ray experiment, using a wavelength of 1.54 Å, measures the first-order scattering from (200) planes of a KCl crystal at a scattering angle of 28.4°.

i) Sketch the experimental arrangement, showing the alignment of the (200) plane in the unit cell, and the incident and scattered X-ray beams.

[4 marks]

ii) Calculate the (200) interplanar distance. What is the value of the lattice parameter of the conventional unit cell?

[7 marks]

iii) Calculate mass density of KCl, given the atomic mass is 39.1 u for K and 35.4 u for Cl.

[5 marks]

**4.** a) i) State the law of equipartition of energy. What does this predict for the molar heat capacity of a monatomic solid?

[4 marks]

ii) Sketch the form of a typical experimental plot of the molar heat capacity $C_V$ as a function of temperature, from absolute zero to room temperature. Explain the limiting value of $C_V$ at absolute zero.

[5 marks]

b) i) The electron density in the conduction band of a semiconductor at temperature $T$ is given by

$$n = 2\left(\frac{2\pi m_e^* k_B T}{h^2}\right)^{3/2} \exp\left(\frac{E_F - E_C}{k_B T}\right),$$

where $m_e^*$ is the electron effective mass, $E_F$ the Fermi energy, and $E_C$ the energy of the conduction band edge. Making a simplifying assumption that the effective masses of electrons in the conduction band and of holes in the valence band of Ge are both equal to $0.1m_e$ and the energy gap $E_G = 0.7$ eV, calculate the hole density in the valence band of intrinsic Ge at 1000 K.

[6 marks]

ii) Germanium ($Z = 32$) is doped by substituting arsenic (As, $Z = 33$) atoms. Identify the type of doping. Sketch an energy-level diagram to illustrate the band structure at $T = 0$ K of Ge doped with As atoms. Mark on your diagram the positions of the conduction and valence band edges and the Fermi energy.

[5 marks]

iii) The dopant ionization energy in As-doped Ge is 5.5 meV. Assuming the semiconductor is in the impurity range with impurity density $10^{25}$ m$^{-3}$, estimate the carrier density of the semiconductor at 300 K. Use your answers in (i) and (iii) to comment on the properties of the doped and intrinsic Ge.

[5 marks]

**END OF EXAMINATION PAPER**

**<u>ONE HOUR THIRTY MINUTES</u>**

A list of constants is enclosed.

**UNIVERSITY OF MANCHESTER**

Introduction to Quantum Mechanics

18th January 2023, 9:45a.m. - 11:15a.m.

Answer **<u>ALL</u>** parts of question 1 and **<u>TWO</u>** other questions

---

Electronic calculators may be used, provided that they cannot store text.

---

The numbers are given as a guide to the relative weights of the different parts of each question.

# Formula Sheet

In plane polar coordinates, $(r, \phi)$, the Laplacian operator is given by

$$\nabla^2 = \frac{\partial^2}{\partial r^2} + \frac{1}{r}\frac{\partial}{\partial r} + \frac{1}{r^2}\frac{\partial^2}{\partial \phi^2}\,,$$

and the angular momentum operator is given by

$$\hat{L}_z = -i\hbar\frac{\partial}{\partial \phi}\,.$$

In spherical polar coordinates, $(r, \theta, \phi)$, the Laplacian operator is given by

$$\nabla^2 = \frac{\partial^2}{\partial r^2} + \frac{2}{r}\frac{\partial}{\partial r} + \frac{1}{r^2}\frac{\partial^2}{\partial \theta^2} + \frac{1}{r^2}\frac{\cos\theta}{\sin\theta}\frac{\partial}{\partial \theta} + \frac{1}{r^2\sin^2\theta}\frac{\partial^2}{\partial \phi^2}\,,$$

and the angular momentum operators are given by

$$\hat{L}^2 = -\hbar^2\left(\frac{\partial^2}{\partial \theta^2} + \frac{\cos\theta}{\sin\theta}\frac{\partial}{\partial \theta} + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial \phi^2}\right),$$

$$\hat{L}_z = -i\hbar\frac{\partial}{\partial \phi}\,.$$

You may use the following integral without proof:

$$\int_0^\infty x^n\,\mathrm{e}^{-x}\,\mathrm{d}x = n! \quad \text{for integer } n \geq 0.$$

**1.** a) Electrons with a kinetic energy of 3 eV are passing through a slit of width 1.2 nm. Are the wave properties of these electrons important? Give your reason.

[3 marks]

b) A particle is in the following mixed state

$$\Psi(x,t) = \frac{1}{\sqrt{5}}\Psi_1(x,t) + \frac{2}{\sqrt{5}}\Psi_2(x,t),$$

where $\Psi_n(x,t) = \psi_n(x)\mathrm{e}^{-iE_nt/\hbar}$ are stationary states.

What are the possible outcomes of a measurement of the particle's energy?

Determine the expectation value of the energy of the particle.

[4 marks]

c) Specify the allowed values of the quantum numbers $(n, \ell, m_\ell, m_s)$ of a hydrogen atom. Briefly state their physical meanings.

Calculate how many different states have the same quantum number $n$.

Explain briefly why different states with the same value of $n$ do not all have the same energy.

[7 marks]

d) State the definition of the Hermitian conjugate, $\hat{A}^\dagger$, of an operator $\hat{A}$, and the definition of a Hermitian operator.

Show that the momentum operator $\hat{p}_x$ is a Hermitian operator.

[7 marks]

e) Write down the atomic ground-state electronic configuration of carbon ($Z = 6$). Determine the total $S$, $L$ and $J$ of its ground state and write down the corresponding spectroscopic term symbol.

[4 marks]

**2.** a) Consider a 1D simple quantum harmonic oscillator of classical angular frequency $\omega$. Draw on one sketch, the potential energy function, energy levels, and wavefunctions of the three lowest energy states.

[8 marks]

b) Vibrations of a diatomic molecule such as carbon monoxide can be considered to be approximately simple harmonic. With the help of a sketch of the potential energy as a function of the distance between a carbon atom and an oxygen atom, explain why this is the case.

What feature of this function determines the effective spring constant?

Explain briefly why the bond energy (the energy required to separate the atoms in a diatomic molecule from each other) is different quantum mechanically from the one that would be expected from a classical calculation with the same potential energy function.

[6 marks]

c) Now consider a 1D oscillator consisting of a mass on a spring that can be extended elastically, but not compressed, corresponding to a potential energy function:

$$V(x) = \begin{cases} \frac{1}{2}m\omega^2 x^2 & \text{if } x > 0, \\ \infty & \text{if } x \leq 0. \end{cases}$$

Write down the full set of energy eigenvalues of this oscillator and sketch the eigenfunction of its ground state. Find the first excitation energy (i.e. the difference between the energies of the ground state and first excited state). Briefly state the reasoning behind your results.

[6 marks]

d) One of the energy eigenfunctions of a 2D simple harmonic oscillator is given by

$$\psi_{1,0} = A\frac{x}{a}\exp\left(\frac{-(x^2+y^2)}{2a^2}\right),$$

where $A$ and $a$ are constants. By writing the Cartesian coordinates $x$ and $y$ in plane polar coordinates, show that this is not an eigenfunction of angular momentum.

Determine the values of angular momentum that could be obtained from a measurement of this state.

[5 marks]

**3.** a) Use the following commutation relations

$$\left[\hat{L}_x, \hat{L}_y\right] = i\hbar\hat{L}_z, \quad \left[\hat{L}_y, \hat{L}_z\right] = i\hbar\hat{L}_x, \quad \left[\hat{L}_z, \hat{L}_x\right] = i\hbar\hat{L}_y,$$

to show that $\left[\hat{L}^2, \hat{L}_z\right] = 0$. What is the significance of this result?

Explain why $\hat{L}^2$ and $\hat{L}_z$ also commute with the Hamiltonian for a central potential.

[7 marks]

b) Use the expression for $\hat{L}^2$ in spherical polar coordinates on the Formula Sheet to show that the spherical harmonic

$$Y(\theta, \phi) = \sqrt{\frac{15}{8\pi}} \sin\theta \cos\theta \, \mathrm{e}^{i\phi}$$

is an eigenfunction of $\hat{L}^2$ and find the corresponding eigenvalue.

[8 marks]

c) Consider the following wavefunctions of a hydrogen atom

$$\begin{aligned}
\psi_A(r, \theta, \phi) &= A\,\mathrm{e}^{-r/a_0}, \\
\psi_B(r, \theta, \phi) &= B\left(1 - \frac{r}{2a_0}\right)\mathrm{e}^{-r/2a_0}, \\
\psi_C(r, \theta, \phi) &= C\left(\frac{r}{a_0}\right)^2 \mathrm{e}^{-r/3a_0} \sin\theta \cos\theta \, \mathrm{e}^{i\phi},
\end{aligned}$$

where $A$, $B$, $C$ and $a_0$ are constants.

i) Deduce by inspection the values of the quantum numbers $(n, \ell, m_\ell)$ for each of these eigenfunctions.

[4 marks]

ii) Show that the states $\psi_A$ and $\psi_C$ are orthogonal to each other.

[2 marks]

d) A lithium atom has three electrons. Use your knowledge of the energy levels and eigenfunctions of hydrogen to explain why:

The first ionization energy of lithium (the energy required to remove one electron from a neutral lithium atom) is around 5 eV;

The last ionization energy of lithium (the energy required to remove the one remaining electron from a $Li^{2+}$ ion) is around 120 eV.

[4 marks]

**4.** a) The total angular momentum operator is given by

$$\hat{\mathbf{J}} = \hat{\mathbf{L}} + \hat{\mathbf{S}},$$

where $\hat{\mathbf{L}}$ is the orbital angular momentum operator and $\hat{\mathbf{S}}$ is the spin operator.

Explain how the quantum numbers that describe $\hat{\mathbf{J}}$ are related to those that describe $\hat{\mathbf{L}}$ and $\hat{\mathbf{S}}$.

[5 marks]

b) For a state specified by fixed values of $\ell$ and $s$, show that the number of $(m_\ell, m_s)$ combinations is $(2\ell + 1)(2s + 1)$.

Show that the number of $(j, m_j)$ combinations is also $(2\ell + 1)(2s + 1)$.

[6 marks]

c) The spin-orbit operator $\hat{V}_{SO}$ for a hydrogen atom is given by

$$\hat{V}_{SO} = f(r)\,\hat{\mathbf{S}} \cdot \hat{\mathbf{L}}$$

with the function $f(r)$ given by

$$f(r) = \frac{\alpha\hbar}{2m_e^2 c}\frac{1}{r^3},$$

where $\alpha = 1/137$ and all other symbols have their usual meaning.

i) The hydrogen atom is in the $2p$ state. Determine the possible values of the total angular momentum quantum number $j$. Hence determine the eigenvalues of the operator $\hat{\mathbf{S}} \cdot \hat{\mathbf{L}}$.

[6 marks]

ii) Estimate the spin-orbit energy splitting between states with the $j$ values you found in Part (i). You may use the result that the expectation value for the $2p$ state of hydrogen is

$$\left\langle \frac{1}{r^3} \right\rangle = \frac{1}{(3a_0)^3},$$

where $a_0$ is the Bohr radius.

[4 marks]

d) The magnetic energy operator for an electron in a magnetic field $B$, pointing in the $z$ direction, is approximately

$$\hat{V}_{mag} = \frac{eB}{2m_e}\left(\hat{L}_z + 2\hat{S}_z\right).$$

Use this to discuss the number of energy levels the $2p$ orbital of hydrogen is broken into by both strong and weak magnetic fields.

[4 marks]

**END OF EXAMINATION PAPER**

**TWO HOURS**

A list of constants is enclosed.

**UNIVERSITY OF MANCHESTER**

Advanced Quantum Mechanics

33rd June 2022, 00.00 a.m. - 12.00 p.m.

Answer **TWO** questions

---

Electronic calculators may be used, provided that they cannot store text.

---

The numbers are given as a guide to the relative weights of the different parts of each question.

You may assume the following formulae in any question *if proof is not explicitly requested*:

**Special integrals**

$$\int_{-\infty}^{\infty} x^{2n} e^{-ax^2} dx = \frac{1 \cdot 3 \cdot 5 \cdots (2n-1)}{(2a)^n} \sqrt{\frac{\pi}{a}}, \qquad \int_0^{\infty} x^n e^{-ax} dx = \frac{n!}{a^{n+1}}, \quad a > 0.$$

**4-vectors**
Use notation $x^\mu = (x^0, \mathbf{r})$ for 4-position and $p^\mu = (E/c, \mathbf{p})$ for 4-momentum. In electromagnetism $A^\mu = (\Phi/c, \mathbf{A})$ for 4-potential.

**Klein-Gordon equation** in scalar $S$ and vector $(V_0/c, \mathbf{V})$ potential field

$$\left[(\hat{\mathbf{p}} - \mathbf{V})^2 c^2 + (mc^2 + S)^2\right] \Psi = (i\hbar\partial_t - V_0)^2 \Psi.$$

**Dirac equation** in scalar $S$ and vector $(V_0/c, \mathbf{V})$ potential field

$$\left[\boldsymbol{\alpha} \cdot (\hat{\mathbf{p}} - \mathbf{V})c + \beta(mc^2 + S)\right] \Psi = (i\hbar\partial_t - V_0)\Psi.$$

**Standard spinor solutions** to the free massive Dirac equation

$$u^{(s)}(E, \mathbf{p}) = \sqrt{E + mc^2} \begin{pmatrix} \phi^s \\ \frac{c\boldsymbol{\sigma}\cdot\mathbf{p}}{E+mc^2}\phi^s \end{pmatrix}, \quad \phi^1 = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \text{ and } \phi^2 = \begin{pmatrix} 0 \\ 1 \end{pmatrix};$$

**Standard matrices**

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

$$\alpha_i = \begin{pmatrix} 0 & \sigma_i \\ \sigma_i & 0 \end{pmatrix}, \quad \beta = \begin{pmatrix} I_2 & 0 \\ 0 & -I_2 \end{pmatrix}, \quad \Sigma_i = \begin{pmatrix} \sigma_i & 0 \\ 0 & \sigma_i \end{pmatrix};$$

$$\gamma_0 = \begin{pmatrix} I_2 & 0 \\ 0 & -I_2 \end{pmatrix}, \quad \gamma_1 = \begin{pmatrix} 0 & \sigma_x \\ -\sigma_x & 0 \end{pmatrix}, \quad \gamma_2 = \begin{pmatrix} 0 & \sigma_y \\ -\sigma_y & 0 \end{pmatrix}, \quad \gamma_3 = \begin{pmatrix} 0 & \sigma_z \\ -\sigma_z & 0 \end{pmatrix}.$$

**Space-time metric** We use the metric $\eta_{\mu\nu} = \mathrm{diag}(1, -1, -, 1, -1)$.

**Laplacian operator** in terms of angular momentum operator $\hat{\mathbf{L}}$

$$\nabla^2 = \frac{1}{r}\frac{\partial^2}{\partial r^2} r - \frac{\hat{\mathbf{L}}^2}{\hbar^2 r^2}.$$

**Solution to Dirac equation** in spherical vector potential $(V_0(r)/c, \vec{0})$

$$\psi^\kappa_{jm}(\mathbf{r}) = \begin{pmatrix} f^\kappa_j(r)\mathcal{Y}^\kappa_{jm}(\theta, \phi) \\ ig^\kappa_j(r)\mathcal{Y}^{-\kappa}_{jm}(\theta, \phi) \end{pmatrix} \quad \text{with } F = rf \text{ and } G = rg,$$

$$\hbar c \left[\frac{d}{dr} - \frac{\kappa}{r}\right] G^\kappa_j(r) = -\left(E - V_0(r) - mc^2\right) F^\kappa_j(r),$$

$$\hbar c \left[\frac{d}{dr} + \frac{\kappa}{r}\right] F^\kappa_j(r) = \left(E - V_0(r) + mc^2\right) G^\kappa_j(r).$$

**1.** a) Show that the angular momentum operator $\hat{L}_y$ is the generator of rotations about the $y$-axis for a spinless particle. Derive an expression in terms of $\hat{L}_y$ for the operator $\hat{U}_\beta$ representing a finite rotation of angle $\beta$ about the $y$-axis. Show that the operator $\hat{U}_\beta$ is unitary.

[8 marks]

Write down the corresponding $\hat{U}_\beta$ for a particle with spin, and explain any notation you use.

[2 marks]

b) i) State the selection rules for electric dipole transitions in light atoms. Explain any notation you use.

[3 marks]

ii) Sketch the energy levels of hydrogen (non-relativistic and without spin-orbit coupling) up to the quantum number $n = 3$, and mark at least 4 electric dipole transitions.

[2 marks]

iii) State whether each of the following transitions in the oxygen atom could be an electric dipole transition. Give your reasons.

i. $(2s)^2(2p)^4$, ${}^3P_2 \rightarrow (2s)^2(2p)^3(3d)$, ${}^3P_1$
ii. $(2s)^2(2p)^3(3s)$, ${}^3S_1 \rightarrow (2s)^2(2p)^3(3d)$, ${}^3P_1$
iii. $(2s)^2(2p)^2(3d)^2$, ${}^5D_1 \rightarrow (2s)^2(2p)^3(3s)$, ${}^5S_2$
iv. $(2s)^2(2p)^3(3s)$, ${}^3S_1 \rightarrow (2s)^2(2p)^4$, ${}^3P_0$

[2 marks]

c) i) Write down the wave function of a free relativistic spin-1/2 particle of energy $E$. Define a helicity basis for Pauli spinors and express the wave function for a massless particle in terms of the helicity basis.

[4 marks]

ii) The energy bands of a non-relativistic electron in graphene near the Dirac points with momentum $\mathbf{p} = (p_x, p_y)$ can be obtained from the following Hamiltonian matrices as

$$\hat{H}^{\pm} = a \begin{pmatrix} 0 & \pm p_x - ip_y \\ \pm p_x + ip_y & 0 \end{pmatrix}$$

where $a$ is a constant. Find the eigenvalues and confirm that $\hat{H}^+$ and $\hat{H}^-$ have the same eigenvalues. Show that this problem can be cast in the same form as the massless Dirac equation in the helicity basis.

[4 marks]

**2.** a) Consider a non-relativistic electron moving in a two-dimensional $xy$ plane with a perpendicular uniform magnetic field $\mathbf{B}$ described by the 4-potential $(0, \mathbf{A})$ where $\mathbf{A} = (0, xB, 0)$. Write down the time-independent Schrödinger equation of the electron, ignoring its spin ($g = 0$).

[2 marks]

By using a wave function of the form

$$\psi(\mathbf{r}) = e^{ik_y y}\phi(x)$$

with constant $k_y$, find and solve the equation for $\phi(x)$, giving the energy eigenvalues (Landau levels) of the electron.

[4 marks]

Find the degeneracy per unit area of the Landau levels and briefly describe the Quantum Hall Effect in terms of Landau levels.

[6 marks]

b) A relativistic spin-0 $\pi^-$ meson of mass $m$ is bound to a nucleus with $Z$ protons by a Coulomb potential

$$V(r) = -Z\alpha\frac{\hbar c}{r}.$$

We assume that the ground-state wave function of the meson can be written in the form

$$\Psi(\mathbf{r}, t) \propto r^{\epsilon}e^{-\beta r}e^{-iEt/\hbar}.$$

Show that

$$\epsilon = \frac{1}{2}\left(-1 \pm \sqrt{1 - (2Z\alpha)^2}\right), \quad \beta = -\frac{\epsilon E}{\hbar c Z\alpha}$$

and

$$E = \pm mc^2\sqrt{1+\epsilon},$$

where the two $\pm$ signs are independent. Be requiring the correct energy for $Z\alpha = 0$, determine both signs.

[10 marks]

Find expressions for $\epsilon$, $E$ and $\beta$ for small $Z\alpha$, and compare them with the expected non-relativistic results.

[3 marks]

**3.** a) A one-dimensional harmonic oscillator of mass $m$ and angular frequency $\omega$ in its ground state is subject to a small force $F = F_0 e^{-t/\tau}$ for $t > 0$. Find the probability, in the first-order approximation, that the oscillator is in its first excited state in the limit $t \to \infty$. The ground and first excited state wave functions of the oscillator are

$$\phi_0(x) = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} \exp\left(-\frac{m\omega x^2}{2\hbar}\right), \quad \phi_1(x) = \sqrt{\frac{2m\omega}{\hbar}}\, x\phi_0(x)\,.$$

[5 marks]

b) A free spin-1/2 particle is described by the Dirac equation. Define a probability current density $J^\mu = (\rho, \mathbf{j})$ and prove that it satisfies the continuity equation

$$\frac{\partial}{\partial t}\rho + \nabla \cdot \mathbf{j} = 0.$$

[3 marks]

c) A beam of relativistic electrons with mass $m$ and energy $E_p$ is moving in the positive $z$ direction and encounters an electrostatic step potential at $z = 0$:

$$e\Phi = \begin{cases} 0, & z < 0 \\ V_0, & z \geq 0. \end{cases}$$

i) Calculate the probability current density for the incident, reflected, and transmitted beams. Hence determine the reflection coefficient $R$ and transmission coefficient $T$. Show that $R + T = 1$.

[10 marks]

ii) State the conditions for total reflection to occur.

[2 marks]

iii) For the case $V_0 > E_p + mc^2$, show that the wave number for the right-moving wave must be negative. Hence show that the reflection coefficient is greater than unity. Briefly state your resolution of this paradox.

[3 marks]

iv) Determine the reflection and transmission coefficients for a beam of massless neutrinos in the case $V_0 > E_p$.

[2 marks]

**END OF EXAMINATION PAPER**

**<u>ONE HOUR THIRTY MINUTES</u>**

A list of constants is enclosed.

**UNIVERSITY OF MANCHESTER**

Fundamentals of Solid State Physics

32nd May/June 2022, xx - xx

Answer **<u>ALL</u>** parts of question 1 and **<u>TWO</u>** other questions

---

Electronic calculators may be used, provided that they cannot store text.

---

The numbers are given as a guide to the relative weights of the different parts of each question.

**1.** a) Write down $2s\sigma$ and $2s\sigma^*$ molecular orbitals for diatomic molecules in terms of suitable atomic orbitals and explain any notation you use. Which of the two molecular orbitals has lower energy and why?

[5 marks]

b) Solid tungsten has a body-centered cubic crystal structure with one atom in the basis. Sketch its conventional unit cell. How many atoms are there in the cell? What is the number of nearest-neighbours of an atom in the solid? Why is the conventional unit cell often used rather than the primitive unit cell?

[5 marks]

c) Given that the Fermi energy of solid tungsten is 9.75 eV, determine the free electron density in the solid. Given that solid tungsten has mass density of 19.3 g/cm$^3$ and an atomic weight of 183.84, calculate the number of free electrons each tungsten atom contributes.

[6 marks]

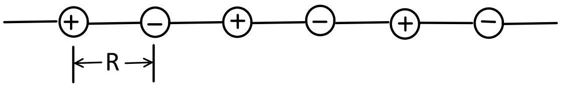
d) List three types of bonding in solids. State the main nature of each bonding and give an example of solids for each bonding.

[6 marks]

e) At room temperature, a sample of intrinsic germanium has a free electron concentration of $2.33 \times 10^{19}$ m$^{-3}$. The electron and hole mobilities are $0.39\,\mathrm{m^2V^{-1}s^{-1}}$ and $0.19\,\mathrm{m^2V^{-1}s^{-1}}$ respectively. Calculate the conductivity of this sample.

[3 marks]

**2.** a) An infinitely long one-dimensional (1D) solid consists of alternating positive and negative ions, with charge $+e$ and $-e$, and mass $m_+$ and $m_-$, respectively, as shown in the following diagram. The nearest neighbour separation is $R$.




i) In addition to the Coulomb interactions between the ions, there is a short-range repulsion between the nearest neighbours only described by the potential, $U = A/R^9$, with positive parameter $A$. Determine the total potential energy per unit cell of the 1D solid. Derive an expression for the equilibrium separation $R$ in terms of $A$ and other parameters of the potentials.

You may find the following summation useful

$$\ln 2 = 1 - \frac{1}{2} + \frac{1}{3} - \frac{1}{4} + \cdots.$$

[6 marks]

ii) Given that the vibrational motion in a 1D solid can be modeled by considering the bonds as springs with a spring constant $K$, write down the equations for the displacements of the ions in a basis (but do not solve them) and explain any notation you use.

[3 marks]

There are two vibrational modes in the solid with the spectra $\omega(k)$ given by

$$\omega^2 = \frac{K}{\mu} \pm K\sqrt{\frac{1}{\mu^2} - \frac{4}{m_- m_+}\sin^2(kR)}, \quad \text{where}\, \mu = \frac{m_- m_+}{m_- + m_+}.$$

Which of these modes is acoustic and which is optical? Find the expressions of $\omega$ of the two modes in the limits $k \to 0$. Determine the sound velocity in terms of the spring constant $K$. Describe briefly the motion of the ions in the basis in the limit $k \to 0$ for the two modes.

[6 marks]

b) i) Write down the electronic configuration for $C_2$ and determine its bond order. After removing one electron, will the molecular ion $C_2^+$ have a shorter or longer bond length? Explain why.

[5 marks]

ii) Molecular $C_2$ can absorb light of wavelength 515 nm and has a bond length of 1.24 Å. Determine the electronic and rotational excitation energies of $C_2$ in eV. From your value of the electronic excitation energy, estimate the vibrational energy-level interval of $C_2$ in eV.

[5 marks]

**3.** a) i) Find the density of states $g(E)$ for free electrons in a metal. Derive an expression for the Fermi energy $E_F$ in terms of the electron concentration $n$.

[7 marks]

ii) The free electron density of copper is $n = 8.5 \times 10^{28}$ m$^{-3}$. Calculate its Fermi velocity $v_F$ and Fermi temperature $T_F$. Describe the significance of this value of $T_F$.

[6 marks]

b) i) Use the Drude model to derive the electronic conductivity of a metal in terms of the electron density $n$ and collision time $\tau$.

[3 marks]

ii) Describe what really happens for the electric resistivity in metals in terms of collisions. Sketch the resistivity as a function of temperature and describe the general behaviours of resistivity in different regions of temperature.

[6 marks]

iii) Calculate the drift velocity $v_D$ of copper with the electron concentration given in (a.ii) for a current density of $10^8$ Am$^{-2}$. Compare the value of $v_D$ with your value of Fermi velocity $v_F$ in (a.ii) and comment on what happens to the Fermi sphere of copper when such a current flows.

[3 marks]

**4.** a) i) Without using formulae or diagrams, describe the main features of electric conductivity in intrinsic silicon. Describe what happens to the conductivities after doping with phosphorous atoms, and with boron atoms.

[7 marks]

ii) The electron and hole mobilities in silicon are $0.12\,\mathrm{m^2V^{-1}s^{-1}}$ and $0.05\,\mathrm{m^2V^{-1}s^{-1}}$ respectively. Two samples of silicon are doped, one with phosphorous atoms of concentration $7.5 \times 10^{21}\ \mathrm{m^{-3}}$, and the other with boron atoms of concentration $1.6 \times 10^{20}\,\mathrm{m^{-3}}$. Assuming that all dopant atoms are ionized, calculate the conductivity in each case. You can ignore the intrinsic conductivity of silicon.

[4 marks]

b) i) Neon forms an fcc solid. Write down the pairwise potential between neon atoms, and state the origin of each term in the potential.

[4 marks]

ii) X-rays of wavelength 1.54 Å are used in a diffraction measurement of the inter-layer distance between (101) planes in solid neon. Sketch the experimental arrangement, showing the relationship between the alignment of the conventional cubic unit cell and the incident and scattered x-ray beams. Mark the scattering angle in your sketch.

[3 marks]

iii) The (101) planes diffract x-rays in first order with a scattering angle of 28.5°. Calculate the inter-layer (101) distance. Determine the lattice constant of the cubic unit cell. What is the nearest-neighbour distance between neon atoms?

[7 marks]

**END OF EXAMINATION PAPER**

**ONE HOUR THIRTY MINUTES**

A list of constants is enclosed.

**UNIVERSITY OF MANCHESTER**

Introduction to Quantum Mechanics

99th January 2022, ?.?? p.m. - ?.?? p.m.

Answer **ALL** parts of question 1 and **TWO** other questions

---

Electronic calculators may be used, provided that they cannot store text.

---

The numbers are given as a guide to the relative weights of the different parts of each question.

# Formula Sheet

In plane polar coordinates, $(r, \phi)$, the Laplacian operator is given by

$$\nabla^2 = \frac{\partial^2}{\partial r^2} + \frac{1}{r}\frac{\partial}{\partial r} + \frac{1}{r^2}\frac{\partial^2}{\partial \phi^2},$$

and the angular momentum operator is given by

$$\hat{L}_z = -i\hbar \frac{\partial}{\partial \phi}.$$

In spherical polar coordinates, $(r, \theta, \phi)$, the Laplacian operator is given by

$$\nabla^2 = \frac{\partial^2}{\partial r^2} + \frac{2}{r}\frac{\partial}{\partial r} + \frac{1}{r^2}\frac{\partial^2}{\partial \theta^2} + \frac{1}{r^2}\frac{\cos\theta}{\sin\theta}\frac{\partial}{\partial \theta} + \frac{1}{r^2\sin^2\theta}\frac{\partial^2}{\partial \phi^2},$$

and the angular momentum operators are given by

$$\hat{L}^2 = -\hbar^2\left(\frac{\partial^2}{\partial \theta^2} + \frac{\cos\theta}{\sin\theta}\frac{\partial}{\partial \theta} + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial \phi^2}\right),$$

$$\hat{L}_z = -i\hbar \frac{\partial}{\partial \phi}.$$

**1.** a) i) The normalized wavefunction of a particle moving in one dimension is $\Psi$. Consider an operator $\hat{A}$ associated with a physical measurement, $A$.
Write down the definition of the expectation value of $\hat{A}$.
Briefly describe the physical meaning of this value and how it is related to the outcomes of particular measurements of $A$.

[5 marks]

ii) Write down the definition of the Hermitian conjugate, $\hat{A}^\dagger$, of the operator $\hat{A}$.
Show that this definition results in the relation $\left(\hat{A}\hat{B}\right)^\dagger = \hat{B}^\dagger\hat{A}^\dagger$.

[5 marks]

b) A quantum rotor has a moment of inertia of $5 \times 10^{-48}\,\mathrm{kg\,m^2}$. What are the values of the three lowest rotational energy eigenvalues, in eV? What is the degeneracy of each of these three energy levels?

[5 marks]

c) A helium atom has states in which each of the two electrons can be in $1s$, $2s$ or $2p$ orbitals.
Explain how the occupation of these states is affected by the spins of the two electrons.
Explain why the ground state of helium has a total electron spin of $S = 0$.
Explain why the first excited state is $(1s)(2s)$ rather than $(1s)(2p)$.

[5 marks]

d) Write down the atomic ground-state electronic configurations of titanium ($Z = 22$) and nickel ($Z = 28$). Determine the total $S$, $L$ and $J$ of each of their ground states and write down the corresponding spectroscopic term symbols.

[5 marks]

**2.** a) Consider a 1D simple quantum harmonic oscillator of classical angular frequency $\omega$.

i) Draw on one sketch, the potential energy function, energy levels, and wavefunctions of the three lowest energy states.

[8 marks]

ii) Calculate the value of the zero-point energy of the oscillator if its classical angular frequency is $2.0 \times 10^{13}\,\mathrm{s}^{-1}$.

[2 marks]

iii) If the particle in the quantum harmonic oscillator is charged, transitions between energy levels can involve the absorption or emission of a single photon.
Explain how the frequency of this photon is related to the classical frequency of the oscillator.

[3 marks]

iv) In a carbon monoxide (CO) molecule, the effective spring constant of the covalent bond has a value of $1860\,\mathrm{N\,m^{-1}}$. Estimate the first excitation energy for vibrational motion of a CO molecule.
You may take the atomic masses of carbon and oxygen to be 12.0 and 16.0 respectively.

[5 marks]

b) Now consider a 2D simple quantum harmonic oscillator of classical angular frequency $\omega$.

i) Write down the general form of a single-valued eigenfunction, $\Phi(\phi)$, of the angular momentum operator $\hat{L}_z$,

$$\hat{L}_z \Phi(\phi) = L_z \Phi(\phi),$$

where $\phi$ is the polar angle, and state the corresponding value of $L_z$.

[2 marks]

ii) The following are all energy eigenfunctions of the 2D quantum harmonic oscillator with the same energy, $3\hbar\omega$:

$$\psi_{2,0} = A\left(2\frac{x^2}{a^2} - 1\right)\mathrm{e}^{-(x^2+y^2)/2a^2}, \quad \psi_{0,2} = A\left(2\frac{y^2}{a^2} - 1\right)\mathrm{e}^{-(x^2+y^2)/2a^2},$$

$$\psi_{1,1} = B\frac{xy}{a^2}\mathrm{e}^{-(x^2+y^2)/2a^2},$$

where $A$, $B$ and $a$ are constants. By writing the Cartesian coordinates $x$ and $y$ in plane polar coordinates, show that these states are not eigenfunctions of angular momentum.
Show that they can all be written as superpositions of states with $L_z = 2\hbar$, 0 and $-2\hbar$.

[5 marks]

**3.** a) For a particle of mass $m$ moving in one dimension, write down the definition of the momentum operator $\hat{p}_x$ and derive the kinetic energy operator $\hat{T}$.
The particle is moving in a region of free space with a wavefunction

$$\psi(x) = A\cos kx,$$

where $A$ and $k$ are constants. Show that $\psi(x)$ is not an eigenfunction of $\hat{p}_x$ but is an eigenfunction of $\hat{T}$.
What are the possible outcomes of a measurement of the particle's momentum?

[9 marks]

b) The magnetic energy operator for an electron in a magnetic field $B$, pointing in the $z$ direction, is given by

$$\hat{V}_{mag} = \frac{eB}{2m_e}\left(\hat{L}_z + g\hat{S}_z\right),$$

where $g$ is the gyromagnetic ratio of the electron, which we will take to be equal to 2, and the other symbols have their usual meanings.

i) When the magnetic field is strong, the quantum numbers $m_\ell$ and $m_s$ can be assumed to be good quantum numbers. Use this to calculate how many energy levels the $2p$ orbital of hydrogen is split into, in a strong magnetic field.
Calculate the spacing between these energy levels. You may state your answer in terms of Bohr magnetons, or electronvolts.

[4 marks]

ii) When the magnetic field is weak, the quantum numbers $m_\ell$ and $m_s$ are not good quantum numbers. Explain what this means and why it is the case.
What are the good quantum numbers in this case?

[4 marks]

iii) When the magnetic field is weak, the magnetic energy operator is equivalent to

$$\hat{V}_{mag} = \frac{eB}{2m_e}\, g_L \hat{J}_z,$$

where $g_L$ is the Landé factor,

$$g_L = 1 + \frac{j(j+1) + s(s+1) - \ell(\ell+1)}{2j(j+1)}.$$

For the $2p$ orbital of hydrogen, what values of $j$ are allowed?
For each of these $j$ values, calculate the spacing between the magnetic energy levels. You may state your answer in terms of Bohr magnetons, or electronvolts.

[6 marks]

iv) How would you decide if a given value of magnetic field would be considered "strong" or "weak" in this context?
*You do not need to provide a quantitative calculation.*

[2 marks]

**4.** a) Consider the following wavefunctions of a hydrogen atom

$$\begin{aligned}\psi_A(r,\theta,\phi) &= A\,\mathrm{e}^{-r/a_0},\\ \psi_B(r,\theta,\phi) &= B\left(1-\frac{r}{2a_0}\right)\mathrm{e}^{-r/2a_0},\\ \psi_C(r,\theta,\phi) &= C\left(\frac{r}{a_0}\right)^3\mathrm{e}^{-r/4a_0}\sin^2\theta\cos\theta\,\mathrm{e}^{2i\phi},\end{aligned}$$

where $A$, $B$, $C$ and $a_0$ are constants.

i) Deduce by inspection the values of the quantum numbers $(n, \ell, m_\ell)$ for each of these eigenfunctions.

[4 marks]

ii) Sketch the radial probability distribution $P(r)$ corresponding to the wavefunction $\psi_B$.

[4 marks]

iii) Show that the states $\psi_A$, $\psi_B$ and $\psi_C$ are all orthogonal to one another. *You may use the result* $\int_0^\infty x^n\,\mathrm{e}^{-x}\,\mathrm{d}x = n!$ *for integer* $n \geq 0$.

[4 marks]

b) i) Write down the quantum operators for the angular momentum components $\hat{L}_x$, $\hat{L}_y$ and $\hat{L}_z$, in terms of $\hat{x}$ and $\hat{p}_x$, etc.

[3 marks]

ii) Given the following commutation relation,

$$\left[\hat{L}_x, \hat{L}_y\right] = i\hbar\hat{L}_z,$$

use the cyclic rule to write down the other two commutation relations between the angular momentum component operators. Hence show that

$$\left[\hat{L}_z, \hat{L}^+\right] = \hbar\hat{L}^+, \tag{1}$$

where $\hat{L}^+ = \hat{L}_x + i\hat{L}_y$.

[5 marks]

iii) Use Eq. (1) to show that the wavefunction defined by

$$\hat{L}^+\psi_C,$$

where $\psi_C$ is given in part (a), is also an eigenfunction of $\hat{L}_z$. Find its eigenvalue.

[5 marks]

**END OF EXAMINATION PAPER**

**ONE HOUR THIRTY MINUTES**

A list of constants is enclosed.

**UNIVERSITY OF MANCHESTER**

Introduction to Quantum Mechanics

17 January 2020, 14.00 - 15.30

Answer **ALL** parts of question 1 and **TWO** other questions

---

Electronic calculators may be used, provided that they cannot store text.

---

The numbers are given as a guide to the relative weights of the different parts of each question.

**1.** a) Show how the method of separation of variables can be used for the time-dependent Schrödinger equation (TDSE) if the potential energy function is time-independent, to give the time-independent Schrödinger equation.
Solve the differential equation for the time dependence and hence write down the general solution of the TDSE.

[7 marks]

b) Two wavefunctions of a system, $\psi_1(x)$ and $\psi_2(x)$, have the same definite energy, but different values of some observable $A$, represented by the operator $\hat{A}$, $A_1$ and $A_2$ respectively. The system is in a mixed state $\psi(x) = a_1\psi_1(x) + a_2\psi_2(x)$, where $a_1$ and $a_2$ are complex numbers. If $A$ is measured, what outcomes are possible and what are their probabilities?
If $A$ is measured a second time, how does the result of the first measurement affect the second measurement?

[5 marks]

c) Show that the commutator of the position and momentum operators is given by

$$[\hat{x}, \hat{p}_x] = i\hbar \,.$$

What is the implication of this result for measurements of these quantities?

[4 marks]

d) The angular momentum operator $\hat{\mathbf{J}}$ is given in terms of the orbital angular momentum operator $\hat{\mathbf{L}}$ and the spin operator $\hat{\mathbf{S}}$ by

$$\hat{\mathbf{J}} = \hat{\mathbf{L}} + \hat{\mathbf{S}} \,.$$

Explain how the quantum numbers $j$ and $m_j$ are related to $\hat{\mathbf{J}}$.
For the case $l = 2$, $s = 1$, enumerate the possible values of $j$ and $m_j$. Show that the number of states is equal to $(2l + 1)(2s + 1)$.

[5 marks]

e) Write down the atomic ground-state electronic configurations of boron ($Z = 5$) and gallium ($Z = 31$). Determine the total $S$, $L$ and $J$ of the ground state of boron and write down the corresponding spectroscopic term symbol.

[4 marks]

**2.** a) Write down the quantum operators for the angular momentum components $\hat{L}_x$, $\hat{L}_y$ and $\hat{L}_z$, in terms of $\hat{x}$ and $\hat{p}_x$, etc. Show that

$$[\hat{L}_x, \hat{L}_y] = i\hbar\hat{L}_z.$$

[6 marks]

b) Show that in polar coordinates $r, \theta, \phi$,

$$\hat{L}_z = -i\hbar\frac{\partial}{\partial\phi}\,.$$

Show that the wavefunction

$$\psi(\phi) = \frac{1}{\sqrt{2\pi}}\,\mathrm{e}^{im\phi}$$

is an eigenfunction of $\hat{L}_z$ and explain why only integer values of $m$ are allowed.

[6 marks]

c) The Hamiltonian of a three-dimensional simple harmonic oscillator of classical angular frequency $\omega$ and mass $m$ is given by

$$\hat{H} = -\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}+\frac{\partial^2}{\partial z^2}\right)+\frac{1}{2}m\omega^2\left(x^2+y^2+z^2\right).$$

i) Write down its energy eigenvalues as a function of quantum numbers $n_x$, $n_y$ and $n_z$. What are the lowest three energy levels and the corresponding degeneracies?

[6 marks]

ii) Show that $\hat{L}_z$ commutes with $\hat{H}$. What is the significance of this? You may use the following formula without proof:

$$\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}+\frac{\partial^2}{\partial z^2}=\frac{\partial^2}{\partial r^2}+\frac{2}{r}\frac{\partial}{\partial r}+\frac{1}{r^2}\left(\frac{\partial^2}{\partial\theta^2}+\cot\theta\frac{\partial}{\partial\theta}+\frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\right).$$

[3 marks]

d) Show that the wavefunction

$$\psi(x,y,z) = A\,x\,\mathrm{e}^{-(x^2+y^2+z^2)/2a^2}$$

is not an eigenfunction of $\hat{L}_z$. What values of $L_z$ could be obtained from a measurement of the oscillator in a state with this wavefunction?

[4 marks]

**3.** a) Two real eigenfunctions of the time-independent Schrödinger equation for an electron in a potential $V(x)$ are $\psi_1(x)$ and $\psi_2(x)$ with eigenvalues $E_1$ and $E_2$ respectively. At time $t = 0$, the electron is in a state

$$\psi(x) = \frac{1}{\sqrt{2}}\Big[\psi_1(x) + \psi_2(x)\Big].$$

i) Write down the electron's wavefunction $\Psi(x, t)$ at time $t > 0$.

[2 marks]

ii) Determine the energy uncertainty $\Delta E$ in the state $\Psi(x, t)$.

[4 marks]

iii) Show that the probability density $|\Psi(x, t)|^2$ is an oscillatory function in time and find the period $\tau$. Calculate $\tau\,\Delta E$ and comment on your value.

[4 marks]

b) The following wavefunctions are energy eigenfunctions of the hydrogen atom,

$$\begin{aligned}
\psi_1(r,\theta,\phi) &= A_1\,\mathrm{e}^{-r/a_0}, \\
\psi_2(r,\theta,\phi) &= A_2\left(\frac{r}{a_0}\right)\mathrm{e}^{-r/2a_0}\sin\theta\,\mathrm{e}^{-i\phi}, \\
\psi_3(r,\theta,\phi) &= A_3\left(\frac{r}{a_0}\right)^2\mathrm{e}^{-r/3a_0}\sin\theta\cos\theta\,\mathrm{e}^{-i\phi},
\end{aligned}$$

where $A_1$, $A_2$ and $A_3$ are normalization constants and $a_0$ is the Bohr radius.

i) Deduce by inspection the values of the quantum numbers $(n, l, m_l)$ for each of these eigenfunctions.

[6 marks]

ii) What are the energy eigenvalues of these three states in eV? If a hydrogen atom makes a transition from state $\psi_2$ to state $\psi_1$ by emitting a photon, calculate the frequency of the photon.

[5 marks]

iii) Show that these states are all orthogonal to one another.

[4 marks]

**4.** a) Give the definition of a Hermitian operator that acts on wavefunctions in one dimension. Show that the momentum operator is Hermitian.

[5 marks]

b) The operator $\hat{P}$ is defined for a system containing two identical particles as the operator that exchanges all properties (position $\mathbf{r}$ and spin $\mathbf{s}$) of the two particles:

$$\hat{P}\Psi(\mathbf{r}_1, \mathbf{s}_1, \mathbf{r}_2, \mathbf{s}_2) = \Psi(\mathbf{r}_2, \mathbf{s}_2, \mathbf{r}_1, \mathbf{s}_1),$$

for which you may use the shorthand $\hat{P}\Psi(1,2) = \Psi(2,1)$. By applying $\hat{P}$ twice to $\Psi(1,2)$, find its eigenvalues, $\lambda$.

[5 marks]

c) Which of these eigenvalues do electron states have?
If two electrons are in a state with separable position and spin wavefunctions,

$$\Psi(\mathbf{r}_1, \mathbf{s}_1, \mathbf{r}_2, \mathbf{s}_2) = \psi(\mathbf{r}_1, \mathbf{r}_2)\chi(\mathbf{s}_1, \mathbf{s}_2),$$

what does this eigenvalue imply about the functions $\psi$ and $\chi$?

[2 marks]

d) Explain briefly how first order perturbation theory can be used to estimate the energy levels of helium from hydrogen atom wavefunctions.

[3 marks]

e) In a helium atom, the spin wavefunction of the two electrons can be antisymmetric (parahelium) or symmetric (orthohelium).
Write down the ground-state configurations of parahelium and orthohelium. Which has the lower energy? Explain why.

[5 marks]

f) In both orthohelium and parahelium, a configuration $1s2s$ is possible. Which has the lower energy? Explain why.

[5 marks]

**END OF EXAMINATION PAPER**

**ONE HOUR THIRTY MINUTES**

A list of constants is enclosed.

**UNIVERSITY OF MANCHESTER**

Advanced Quantum Mechanics

28 May 2019, 09:45 - 11:15

Answer any **TWO** questions

---

Electronic calculators may be used, provided that they cannot store text.

---

The numbers are given as a guide to the relative weights of the different parts of each question.

You may assume the following formulae in any question *if proof is not explicitly requested*:

**Special integrals**

$$\int_{-\infty}^{\infty} x^{2n} e^{-ax^2} dx = \frac{1 \cdot 3 \cdot 5 \cdots (2n-1)}{(2a)^n} \sqrt{\frac{\pi}{a}}, \qquad \int_0^{\infty} x^n e^{-ax} dx = \frac{n!}{a^{n+1}}, \quad a > 0.$$

**4-vectors**
Use notation $x^\mu = (x^0, \mathbf{x})$ for 4-position and $p^\mu = (E/c, \mathbf{p})$ for 4-momentum. In electromagnetism $A^\mu = (\Phi/c, \mathbf{A})$ for 4-potential.

**Klein-Gordon equation** in scalar $S$ and vector $(V_0/c, \mathbf{V})$ potential field

$$\left[(\hat{\mathbf{p}} - \mathbf{V})^2 c^2 + (mc^2 + S)^2\right] \Psi = (i\hbar\partial_t - V_0)^2 \Psi.$$

**Dirac equation** in scalar $S$ and vector $(V_0/c, \mathbf{V})$ potential field

$$\left[\boldsymbol{\alpha} \cdot (\hat{\mathbf{p}} - \mathbf{V})c + \beta(mc^2 + S)\right] \Psi = (i\hbar\partial_t - V_0)\Psi.$$

**Standard spinor solutions** to the free massive Dirac equation

$$u^{(s)}(E, \mathbf{p}) \; = \; \sqrt{E + mc^2} \begin{pmatrix} \phi^s \\ \frac{c\boldsymbol{\sigma}\cdot\mathbf{p}}{E+mc^2}\phi^s \end{pmatrix}, \quad \phi^1 = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \text{ and } \phi^2 = \begin{pmatrix} 0 \\ 1 \end{pmatrix};$$

$$v^{(s)}(-|E|, -\mathbf{p},) \; = \; \sqrt{|E| + mc^2} \begin{pmatrix} \frac{c\boldsymbol{\sigma}\cdot\mathbf{p}}{|E|+mc^2}\chi^s \\ \chi^s \end{pmatrix}, \quad \chi^1 = \begin{pmatrix} 0 \\ 1 \end{pmatrix} \text{ and } \chi^2 = \begin{pmatrix} -1 \\ 0 \end{pmatrix}.$$

**Standard matrices**

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

$$\alpha_i = \begin{pmatrix} 0 & \sigma_i \\ \sigma_i & 0 \end{pmatrix}, \quad \beta = \begin{pmatrix} I_2 & 0 \\ 0 & -I_2 \end{pmatrix}, \quad \Sigma_i = \begin{pmatrix} \sigma_i & 0 \\ 0 & \sigma_i \end{pmatrix};$$

$$\gamma_0 = \begin{pmatrix} I_2 & 0 \\ 0 & -I_2 \end{pmatrix}, \quad \gamma_1 = \begin{pmatrix} 0 & \sigma_x \\ -\sigma_x & 0 \end{pmatrix}, \quad \gamma_2 = \begin{pmatrix} 0 & \sigma_y \\ -\sigma_y & 0 \end{pmatrix}, \quad \gamma_3 = \begin{pmatrix} 0 & \sigma_z \\ -\sigma_z & 0 \end{pmatrix}.$$

**Space-time metric** We use the metric $\eta_{\mu\nu} = \mathrm{diag}(1, -1, -, 1, -1)$.

**Laplacian operator** in terms of angular momentum operator $\hat{\mathbf{L}}$

$$\nabla^2 = \frac{1}{r}\frac{\partial^2}{\partial r^2} r - \frac{\hat{\mathbf{L}}^2}{\hbar^2 r^2}.$$

**Solution to Dirac equation** in spherical vector potential $(V_0(r)/c, \mathbf{0})$

$$\psi^\kappa_{jm}(\mathbf{r}) \; = \; \begin{pmatrix} f^\kappa_j(r)\mathcal{Y}^\kappa_{jm}(\theta, \phi) \\ ig^\kappa_j(r)\mathcal{Y}^{-\kappa}_{jm}(\theta, \phi) \end{pmatrix} \quad \text{with } F = rf \text{ and } G = rg,$$

$$\hbar c\left[\frac{d}{dr} - \frac{\kappa}{r}\right] G^\kappa_j(r) \; = \; -\left(E - V_0(r) - mc^2\right) F^\kappa_j(r),$$

$$\hbar c\left[\frac{d}{dr} + \frac{\kappa}{r}\right] F^\kappa_j(r) \; = \; \left(E - V_0(r) + mc^2\right) G^\kappa_j(r).$$

**1.** a) Consider a spinless non-relativistic particle of charge $q$ and mass $m$ moving in a space with a 4-potential $(\Phi/c, \mathbf{A})$.

i) The 4-potential transforms under a gauge transformation according to $\mathbf{A} \to \mathbf{A} + \nabla\lambda$, $\Phi \to \Phi - \partial\lambda/\partial t$, where $\lambda$ is a function of space and time. Write down the corresponding gauge transformation operator for the wave function of the particle, and demonstrate that the operator is unitary. Show that the time-dependent Schrödinger equation of the particle is invariant under the gauge transformation.

[5 marks]

ii) Now consider the particle moving in a space with a uniform magnetic field $\mathbf{B}$ described by the 4-potential $(0, \mathbf{A})$ where $\mathbf{A} = (0, xB, 0)$. Write down the time-independent Schrödinger equation of the particle. By using a wave function of the form

$$\psi(\mathbf{r}) = e^{ik_y y + ik_z z}\phi(x)$$

with constants $k_y$ and $k_z$, find and solve the equation for $\phi(x)$, giving the energy eigenvalues of the particle.

[6 marks]

b) i) The two components of the angular momentum operator with quantum number $l = 1$ can be written as

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

Write down the eigenvalues and eigenvectors of $\hat{L}_z$. Use the angular momentum commutation relations to derive the $\hat{L}_y$ matrix.

[4 marks]

ii) Consider a charged quantum rotor of angular-momentum quantum number $l = 1$. The rotor is placed in a uniform magnetic field along the $z$-axis with the Hamiltonian given by

$$\hat{H}_0 = \alpha \hat{L}_z,$$

where $\alpha$ is a positive constant. Initially the rotor is in the ground state of $\hat{H}_0$. At $t = 0$, a weak rotating magnetic field of angular frequency $\omega$ is switched on in the $xy$ plane. The Hamiltonian of the rotor is now

$$\hat{H}(t) = \hat{H}_0 + \beta\left(\cos\omega t\, \hat{L}_x + \sin\omega t\, \hat{L}_y\right),$$

where $\beta$ is a constant ($|\beta| \ll \alpha$). Use first-order perturbation theory to calculate the probability of transition to the first excited state as a function of time. Find the resonant frequency. Determine the transition probability at the resonant frequency and comment on the validity of your result in the long-time limit in this case.

[10 marks]

**2.** a) List all the excited states of helium for the configurations $(1s)(nl)$ with $n = 1, 2, 3$. Write down the corresponding term symbols ${}^{2S+1}L$ for these states. Sketch the corresponding energy levels and mark all the possible electric dipole transitions.

[7 marks]

b) A spin 1/2 particle of mass $m$, subjected to a modified vector potential, is described by the following Dirac equation:

$$\left[c\boldsymbol{\alpha}\cdot\hat{\mathbf{p}} + imc\omega(\beta\boldsymbol{\alpha})\cdot\mathbf{r} + mc^2\beta\right]\Psi = E\Psi, \text{ where } \Psi = \begin{pmatrix}\phi\\ \chi\end{pmatrix}.$$

i) Show that $\phi$ and $\chi$ satisfy the following equations

$$\begin{aligned}(E^2 - m^2c^4)\phi &= 2mc^2\left[\frac{\hat{\mathbf{p}}^2}{2m} + \frac{m\omega^2}{2}\mathbf{r}^2 - \frac{3}{2}\hbar\omega - 2\frac{\omega}{\hbar}\hat{\mathbf{L}}\cdot\hat{\mathbf{S}}\right]\phi,\\ (E^2 - m^2c^4)\chi &= 2mc^2\left[\frac{\hat{\mathbf{p}}^2}{2m} + \frac{m\omega^2}{2}\mathbf{r}^2 + \frac{3}{2}\hbar\omega + 2\frac{\omega}{\hbar}\hat{\mathbf{L}}\cdot\hat{\mathbf{S}}\right]\chi,\end{aligned}$$

where $\hat{\mathbf{S}} = \hbar\boldsymbol{\sigma}/2$.

[8 marks]

ii) We can represent $\phi$ as $|n, l, s, j\rangle$ and $\chi$ as $|n', l', s, j\rangle$, where these are spin-1/2 eigenstates of a *three-dimensional* harmonic oscillator

$$\left(\frac{\hat{\mathbf{p}}^2}{2m} + \frac{m\omega^2}{2}\mathbf{r}^2\right)|n, l, s, j\rangle = \hbar\omega\left(n + \frac{3}{2}\right)|n, l, s, j\rangle,$$

where $l$ has the following allowed values:

$$l = \begin{cases} 0, 2, \cdots, n & \text{for even } n,\\ 1, 3, \cdots, n & \text{for odd } n.\end{cases}$$

Find the energy eigenvalues for the two equations satisfied by $\phi$ and $\chi$ *separately* in terms of $n, n', l, l'$ and $j$.

[3 marks]

iii) By considering $n' = n \pm 1$, what are the relations between $n$ and $n'$, and $l$ and $l'$, in order that $\Psi$ is a solution of the given Dirac equation? (Hint: there are two possibilities.)

[5 marks]

iv) The eigenenergies all have the form

$$E = mc^2\sqrt{1 + \frac{2\hbar\omega N}{mc^2}}.$$

Determine the degeneracy of the eigenstates with even $N$.

[2 marks]

**3.** a) Show that the angular momentum operator $\hat{L}_x$ is the generator of rotations about the $x$-axis for a spinless particle. Derive an expression in terms of $\hat{L}_x$ for the operator $\hat{U}_\beta$ representing a finite rotation of angle $\beta$ about the $x$-axis. Show that the operator $\hat{U}_\beta$ is unitary.

[8 marks]

Write down the corresponding $\hat{U}_\beta$ for a particle with spin, and explain any notation you use.

[2 marks]

b) Consider a relativistic spinless particle of mass $m$ interacting with a weak scalar potential $S(x) = g\delta(x)$, where $g$ is the strength of the potential. The time-independent Klein-Gordon equation can be written approximately as

$$-\hbar^2 c^2 \frac{d^2\psi(x)}{dx^2} + m^2c^4\psi(x) + 2mc^2 g\delta(x)\psi(x) = E^2\psi(x).$$

i) Show that the generic solutions for the wavefunction can be written as

$$\begin{aligned} \psi_-(x) &= A_- e^{-ikx} + B_- e^{ikx}, \quad x < 0, \\ \psi_+(x) &= A_+ e^{-ikx} + B_+ e^{ikx}, \quad x > 0, \end{aligned}$$

where $A_\pm$ and $B_\pm$ are constants. Express $k$ in terms of the energy $E$.

[2 marks]

ii) Write down the continuity boundary condition for the wave functions at $x = 0$. By integrating the Klein-Gordon equation across $x = 0$, show that the other boundary condition is given by

$$\lim_{\epsilon \to 0} \left[ -\hbar^2 c^2 \left( \left. \frac{d\psi_+(x)}{dx} \right|_{x=+\epsilon} - \left. \frac{d\psi_-(x)}{dx} \right|_{x=-\epsilon} \right) \right] + 2mc^2 g\psi_+(0) = 0.$$

[3 marks]

iii) Assume that the particle is incident from the negative $x$ direction with $E > mc^2$. Solve the resulting boundary conditions to find the transmission amplitude $B_+$ and the reflection amplitude $A_-$ in terms of $k$.

[5 marks]

iv) Now consider the case of the bound state. Assume that the energy satisfies $|E| < mc^2$, and let $k = i\kappa$ where $\kappa > 0$. Explain why $A_+ = B_- = 0$ in this case. Solve the boundary conditions and show that a bound state exists only if $g < 0$. Find the bound-state energy $E$ in terms of $g$. Determine its nonrelativistic limit.

[5 marks]

**END OF EXAMINATION PAPER**

**One hour thirty minutes**

A list of Constants is enclosed

**UNIVERSITY OF MANCHESTER**

Fundamentals of Solid State Physics

4 June 2019, 2:00 – 3:30

Answer **ALL** parts of question 1 and **TWO** other questions

---

Electronic calculators may be used, provided that they cannot store text.

---

The numbers are given as a guide to the relative weights of the different parts of each question.

1.

a) Using a molecular orbital energy level diagram, explain why the bond length of the $H_2^+$ molecular ion is larger than that of the $H_2$ molecule. State whether you expect the bond length for the three-electron species $H_2^-$ to be smaller or larger than that for $H_2$. Briefly justify your answer.

[5 marks]

b) The density of free electrons $n$ in a metal is given by

$$n = \int_0^\infty g(\varepsilon) f(\varepsilon, T)\,\mathrm{d}\varepsilon,$$

where $g(\varepsilon)$ is the density of states function and $f(\varepsilon, T)$ is the Fermi-Dirac occupation function.

Explain why this expression can be written as

$$n = \int_0^{\varepsilon_\mathrm{F}} g(\varepsilon)\,\mathrm{d}\varepsilon,$$

where $\varepsilon_\mathrm{F}$ is the Fermi energy. Hence show that

$$n = A{\varepsilon_\mathrm{F}}^{3/2},$$

where $A$ is a constant.

[5 marks]

c) Use the Drude model to derive an expression for the electrical conductivity of a metal, defining the terms you use.

[5 marks]

d) Sketch the dispersion relation $\varepsilon(k)$ for a nearly free electron interacting with a one-dimensional lattice, over the range $-\frac{2\pi}{a} \leq k \leq +\frac{2\pi}{a}$, where $a$ is the spacing of the atoms.

[5 marks]

e) Using a diagram, show the experimental arrangement used in a Hall-effect measurement. By considering the forces on electrons in a current-carrying conductor, show that the Hall coefficient $R_\mathrm{H}$ is given by

$$R_\mathrm{H} = -\frac{1}{ne},$$

where $n$ is the electron density and $e$ is the electronic charge.

[5 marks]

P.T.O.

2.

a) Briefly describe each of the following, including its origin and its influence on the bonding of solids. In each case give one specific example, and discuss how it affects the interatomic distance in a solid:

(i) covalent bonding;

(ii) dipole-dipole interaction.

[6 marks]

b) Describe the two-dimensional primitive unit cell of graphene. State the type of lattice formed and the basis. Draw one unit cell.

[4 marks]

c) Three-dimensional graphite is made up of sheets of the two-dimensional material described in part b). X-ray diffraction is used to measure the distance between adjacent rows of carbon atoms in the layers, and the distance between the two-dimensional sheets.

(i) Draw diagrams to show how a single-crystal sample of graphite must be orientated with respect to the incident and scattered beams in order to make each of these measurements.

[2 marks]

(ii) The wavelength of the X-rays is 1.54 Å, and peaks are found at scattering angles of 42.4° and 26.6° in first order. Calculate the nearest-neighbour distance in the sheet, and the distance between the sheets.

[4 marks]

(iii) State the effects that give rise to the binding in the sheets, and to the binding between the sheets in graphite.

[2 marks]

d) Briefly describe how the Tight-Binding Model may be used to model the electronic structure of graphene close to the Fermi energy. Draw an *E-k* diagram of the band dispersion at the K-point of the Brillouin zone, indicate the band filling, and mark the position of the Dirac point. Indicate the position of the Fermi energy for the three cases of perfect undoped graphene, *n*-type doping and *p*-type doping.

[7 marks]

P.T.O.

3.

a) Define the terms 'intrinsic semiconductor' and 'extrinsic semiconductor'.

[2 marks]

b) The electron density $n$ in the conduction band of an *intrinsic* semiconductor can be written as

$$n = N_C e^{\frac{-(E_C-\varepsilon_F)}{k_B T}},$$

where $N_C$ is the effective density of states in the conduction band, and all other symbols have their conventional meaning.

Calculate $n$ at a temperature of 300 K for GaN, given that the band gap is 3.2 eV and the value of $N_C$ is 4 x $10^{25}$ $m^{-3}$.

[3 marks]

c) Sketch a graph showing a typical variation of log($n$) where $n$ is the free electron concentration for an $n$-type semiconductor as a function of the inverse of the absolute temperature. Indicate three important ranges on your graph and explain why the different ranges exist.

[6 marks]

d) Extrinsic $n$-type doping can be achieved in GaN by substituting silicon (Si) atoms onto Ga lattice sites. Draw a schematic energy level diagram to illustrate the band structure at $T$ = 0 K of GaN doped with Si atoms. Mark on your diagram the positions of the conduction and valence band edges and the Fermi energy.

[5 marks]

e) The dopant ionisation energy in Si-doped GaN is 20 meV. Assuming the semiconductor is in the impurity range, estimate the carrier density due to the dopant atoms at 300 K. You may use the value of $N_C$ given in part b). Compare your answer with your answer to part b), and give a physical interpretation.

[5 marks]

f) Comment on the suitability of GaN in the following applications:

(i) as a transistor;

[2 marks]

(ii) as a light-emitting diode.

[2 marks]

P.T.O.

4.

a) Sketch a graph of the measured molar heat capacity at constant volume, $C_V$, *versus* absolute temperature for copper, which has an Einstein temperature of 276 K.

[3 marks]

b) State the law of equipartition of energy. Using this and the first law of thermodynamics show for a monovalent solid that $C_V$ is equal to $3R$ where $R$ is the universal gas constant.

[6 marks]

c) Describe the Einstein model of specific heat, and explain why it predicts that $C_V$ should depend on temperature as opposed to the prediction based on the equipartition of energy. In your answer briefly discuss the relevance of the Einstein temperature.

[6 marks]

d) Using the Einstein model, calculate the energy difference between the allowed vibrational states in copper.

[2 marks]

e) Using the classical free electron model, estimate the contribution to the molar specific heat provided by *free electrons* in a metal.

[3 marks]

f) Explain qualitatively why, taking into account the quantum nature of the free electrons in a metal, your prediction in part e) is not reflected in your graph in part a) for $T \sim 300$ K.

[5 marks]

**END OF EXAMINATION PAPER**

**ONE HOUR THIRTY MINUTES**

A list of constants is enclosed.

**UNIVERSITY OF MANCHESTER**

Introduction to Quantum Mechanics

24 January 2019, 9.45 a.m. - 11.15 a.m.

Answer **ALL** parts of question 1 and **TWO** other questions

---

Electronic calculators may be used, provided that they cannot store text.

---

The numbers are given as a guide to the relative weights of the different parts of each question.

**1.** a) A particle of mass $m$ moves in two dimensions in a potential $\widehat{V}$. Write down the time-dependent Schrödinger equation (TDSE) for the particle's wavefunction $\Psi(\mathbf{r}, t)$. Assume that $\widehat{V}$ is time independent, substitute the stationary wavefunction with energy $E$,

$$\Psi(\mathbf{r}, t) = \psi(\mathbf{r}) \exp\left(-iEt/\hbar\right),$$

to obtain the time-independent Schrödinger equation for the spatial wavefunction $\psi(\mathbf{r})$.

[4 marks]

Given that $\Psi_1(\mathbf{r}, t) = \psi_1(\mathbf{r}) \exp\left(-iE_1 t/\hbar\right)$ and $\Psi_2(\mathbf{r}, t) = \psi_2(\mathbf{r}) \exp\left(-iE_2 t/\hbar\right)$ are two solutions of the TDSE of the particle where $\psi_1$ and $\psi_2$ are real, show that their linear combination,

$$\Phi = \frac{1}{\sqrt{2}} \left(\Psi_1 + \Psi_2\right),$$

is also a solution. Show also that the probability density $|\Phi|^2$ is an oscillatory function of time and find the period in terms of the energies $E_1$ and $E_2$.

[5 marks]

b) A particle is moving in two-dimensions. Show that the function

$$\psi(\mathbf{r}) = Ae^{i\mathbf{k}\cdot\mathbf{r}},$$

where $A$ is a constant and $\mathbf{k}$ is a constant wavevector, is an eigenfunction of the momentum operator $\hat{\mathbf{p}}$. Find the eigenvalue.

[2 marks]

The particle is in a state described by a wavefunction

$$\psi(x, y) = \frac{2}{a} \sin\frac{\pi x}{a} \sin\frac{2\pi y}{a},$$

where $a$ is a constant. What are the possible values of a measurement of the particle's momentum vector? What are the corresponding probabilities?

[4 marks]

c) In the usual notation the quantum numbers of hydrogen are $(n, l, m_l, m_s)$. Briefly state their meanings and give their allowed values.

[3 marks]

Explain what is meant by the parity of an electron state. For a given wavefunction $\psi_{n,l,m_l,m_s}$ of hydrogen, what is its parity?

[2 marks]

d) Write down the ground-state electronic configurations of oxygen ($Z = 8$) and selenium ($Z = 34$). Determine the total $S$, $L$ and $J$ of the ground state of oxygen and write down the corresponding spectroscopic term symbol.

[5 marks]

**2.** a) A strong magnetic field of magnitude $B$ is applied to a hydrogen atom in the $2p$ state. The magnetic interaction operator $\hat{V}_{\mathrm{mag}}$ is given, in the usual notation, as

$$\hat{V}_{\mathrm{mag}} = \frac{e}{2m_e}\left(\hat{\mathbf{L}} + 2\hat{\mathbf{S}}\right) \cdot \mathbf{B}.$$

Determine the energy splitting due to the magnetic field and sketch the energy levels with appropriate quantum numbers.

[6 marks]

b) The Hamiltonian of a one-dimensional simple harmonic oscillator (SHO) of mass $m$ and angular frequency $\omega$ is written as

$$\hat{H} = \frac{\hat{p}_x^2}{2m} + \frac{1}{2}m\omega^2\hat{x}^2.$$

i) The operators $\hat{a}$ and $\hat{a}^\dagger$ are defined as

$$\hat{a} = \frac{1}{\sqrt{2}}\left(\frac{\hat{x}}{x_0} + \frac{ix_0\hat{p}_x}{\hbar}\right), \quad \hat{a}^\dagger = \frac{1}{\sqrt{2}}\left(\frac{\hat{x}}{x_0} - \frac{ix_0\hat{p}_x}{\hbar}\right),$$

with $x_0 = \sqrt{\hbar/m\omega}$. Show that $[\hat{a}, \hat{a}^\dagger] = 1$. Also show that $\hat{H}$ can be expressed as

$$\hat{H} = \left(\hat{a}^\dagger\hat{a} + \frac{1}{2}\right)\hbar\omega.$$

[5 marks]

ii) Show that the ground-state wavefunction,

$$\psi_0(x) = A\exp\left(-\frac{x^2}{2x_0^2}\right)$$

with constant $A$, satisfies $\hat{a}\psi_0(x) = 0$. Hence find the ground-state energy $E_0$.

[4 marks]

iii) The oscillator carries a charge $q$. The recurrence relation of the eigenfunctions of the SHO is

$$x\psi_n(x) = A_n\psi_{n+1}(x) + B_n\psi_{n-1}(x), \quad n \geq 1$$

where $A_n$ and $B_n$ are coefficients independent of $x$. Use this recurrence relation to find the selection rule for an electric dipole transition for the oscillator.

[5 marks]

c) Consider a two-dimensional quantum SHO of angular frequency $\omega$. Write down the full set of its energy eigenvalues. Find the first three energy levels and their corresponding degeneracy.

[5 marks]

**3.** a) i) Write down the quantum operators for the angular momentum components, $\hat{L}_x, \hat{L}_y$ and $\hat{L}_z$, in terms of $\hat{x}, \hat{y}, \hat{z}$ and $\hat{p}_x, \hat{p}_y, \hat{p}_z$.

[3 marks]

ii) Show that in spherical coordinates $(r, \theta, \phi)$, $\hat{L}_z$ can be expressed as $\hat{L}_z = -i\hbar\partial/\partial\phi$.

[3 marks]

iii) Given the angular momentum squared operator in spherical coordinates,

$$\hat{L}^2 = -\hbar^2\left(\frac{\partial^2}{\partial\theta^2} + \cot\theta\frac{\partial}{\partial\theta} + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\right),$$

show that

$$\psi(\theta, \phi) = A\sin\theta\, e^{-i\phi}$$

with constant $A$, is an eigenfunction of both $\hat{L}_z$ and $\hat{L}^2$ and find the corresponding eigenvalues.

[5 marks]

b) The following wavefunctions are energy eigenfunctions of the hydrogen atom:

$$\begin{aligned}
\psi_1(r, \theta, \phi) &= A_1 e^{-r/a_0}, \\
\psi_2(r, \theta, \phi) &= \frac{1}{\sqrt{32\pi a_0^3}}\left(2 - \frac{r}{a_0}\right)e^{-r/2a_0}, \\
\psi_3(r, \theta, \phi) &= A_3\left(\frac{r}{a_0}\right)^2 e^{-r/3a_0}\sin^2\theta\, e^{-2i\phi},
\end{aligned}$$

where $A_1$ and $A_3$ are normalization constants and $a_0$ is the Bohr radius.

i) Determine the normalization constant $A_1$.

[3 marks]

ii) Consider the approximation that, over the small volume of the nucleus, the wavefunction $\psi_2$ is constant and equal to its value at $r = 0$. Estimate the probability that an electron in state $\psi_2$ would be found within the nucleus, which has a radius of 1 fm.

[5 marks]

iii) Show that $\psi_1$ and $\psi_3$ are orthogonal.

[2 marks]

iv) Write down the formula for the hydrogen energy levels in terms of the principle quantum number $n$. Calculate the wavelength of the emitted photon when the hydrogen atom makes a transition from $\psi_3$ to $\psi_1$. Comment on the likelihood of this transition.

[4 marks]

**4.** a) Give the definition of an Hermitian operator in one dimension. Show that the eigenvalues of an Hermitian operator are real.

[5 marks]

b) The ground-state electronic configuration of a helium atom is $(1s)^2$.

i) Write down the corresponding wavefunction in terms of the $1s$ orbital $\psi_{1s}$ and spin-1/2 wavefunctions $\chi_{\pm}$. Discuss the symmetry of the wavefunction.

[6 marks]

ii) Ignoring the Coulomb repulsion between the electrons, estimate the ground-state energy of helium in units of eV. By comparing your result with the observed value of $-79$ eV, estimate the Coulomb repulsion energy of the two electrons in the ground state and comment on your result.

[4 marks]

c) The spin-orbit coupling operator $\hat{V}_{\mathrm{SO}}$ for a hydrogen atom is given by

$$\hat{V}_{\mathrm{SO}} = f(r)\hat{\mathbf{S}} \cdot \hat{\mathbf{L}}$$

with the function $f(r)$ defined as

$$f(r) = \frac{\alpha\hbar}{2m_e^2 c} \cdot \frac{1}{r^3},$$

where $\alpha = 1/137$ and all other symbols have their usual meaning.

i) The hydrogen atom is in the $2p$ state. Determine the possible values of the total angular momentum quantum number $j$. Hence determine the eigenvalues of the operator $\hat{\mathbf{S}} \cdot \hat{\mathbf{L}}$.

[6 marks]

ii) Estimate the spin-orbit energy splitting between the states with these $j$ values. You may use the result that the expectation value for the $2p$ state of hydrogen is

$$\left\langle \frac{1}{r^3} \right\rangle = \frac{1}{(3a_0)^3},$$

where $a_0$ is the Bohr radius.

[4 marks]

**END OF EXAMINATION PAPER**

ONE HOUR THIRTY MINUTES

A list of constants is enclosed.

UNIVERSITY OF MANCHESTER

Advanced Quantum Mechanics

29th May 2018, 09.45 a.m. - 11.15 a.m.

Answer any TWO questions

---

Electronic calculators may be used, provided that they cannot store text.

---

The numbers are given as a guide to the relative weights of the different parts of each question.

You may assume the following formulae in any question *if proof is not explicitly requested*:

**Special integrals**

$$\int_{-\infty}^{\infty} x^{2n} e^{-ax^2} dx = \frac{1\cdot 3\cdot 5\cdots(2n-1)}{(2a)^n}\sqrt{\frac{\pi}{a}}, \qquad \int_0^{\infty} x^n e^{-ax} dx = \frac{n!}{a^{n+1}}, \quad a > 0.$$

**4-vectors**

Use notation $x^\mu = (x^0, \mathbf{x})$ for 4-position and $p^\mu = (E/c, \mathbf{p})$ for 4-momentum. In electromagnetism $A^\mu = (\Phi/c, \mathbf{A})$ for 4-potential.

**Klein-Gordon equation** in scalar $S$ and vector $(V_0/c, \mathbf{V})$ potential field

$$\left[(\hat{\mathbf{p}} - \mathbf{V})^2 c^2 + (mc^2 + S)^2\right]\Psi = (i\hbar\partial_t - V_0)^2\Psi.$$

**Dirac equation** in scalar $S$ and vector $(V_0/c, \mathbf{V})$ potential field

$$\left[\boldsymbol{\alpha}\cdot(\hat{\mathbf{p}} - \mathbf{V})c + \beta(mc^2 + S)\right]\Psi = (i\hbar\partial_t - V_0)\Psi.$$

**Standard spinor solutions** to the free massive Dirac equation

$$u^{(s)}(E, \mathbf{p}) = \sqrt{E + mc^2}\begin{pmatrix} \phi^s \\ \frac{c\boldsymbol{\sigma}\cdot\mathbf{p}}{E+mc^2}\phi^s \end{pmatrix}, \quad \phi^1 = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \text{ and } \phi^2 = \begin{pmatrix} 0 \\ 1 \end{pmatrix};$$

$$v^{(s)}(-|E|, -\mathbf{p},) = \sqrt{|E| + mc^2}\begin{pmatrix} \frac{c\boldsymbol{\sigma}\cdot\mathbf{p}}{|E|+mc^2}\chi^s \\ \chi^s \end{pmatrix}, \quad \chi^1 = \begin{pmatrix} 0 \\ 1 \end{pmatrix} \text{ and } \chi^2 = \begin{pmatrix} -1 \\ 0 \end{pmatrix}.$$

**Standard matrices**

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

$$\alpha_i = \begin{pmatrix} 0 & \sigma_i \\ \sigma_i & 0 \end{pmatrix}, \quad \beta = \begin{pmatrix} I_2 & 0 \\ 0 & -I_2 \end{pmatrix}, \quad \Sigma_i = \begin{pmatrix} \sigma_i & 0 \\ 0 & \sigma_i \end{pmatrix};$$

$$\gamma_0 = \begin{pmatrix} I_2 & 0 \\ 0 & -I_2 \end{pmatrix}, \quad \gamma_1 = \begin{pmatrix} 0 & \sigma_x \\ -\sigma_x & 0 \end{pmatrix}, \quad \gamma_2 = \begin{pmatrix} 0 & \sigma_y \\ -\sigma_y & 0 \end{pmatrix}, \quad \gamma_3 = \begin{pmatrix} 0 & \sigma_z \\ -\sigma_z & 0 \end{pmatrix}.$$

**Space-time metric** We use the metric $\eta_{\mu\nu} = \text{diag}(1, -1, -, 1, -1)$.

**Laplacian operator** in terms of angular momentum operator $\hat{\mathbf{L}}$

$$\nabla^2 = \frac{1}{r}\frac{\partial^2}{\partial r^2}r - \frac{\hat{\mathbf{L}}^2}{\hbar^2 r^2}.$$

**Solution to Dirac equation** in spherical vector potential $(V_0(r)/c, \mathbf{0})$

$$\psi^\kappa_{jm}(\mathbf{r}) = \begin{pmatrix} f^\kappa_j(r)\mathcal{Y}^\kappa_{jm}(\theta,\phi) \\ ig^\kappa_j(r)\mathcal{Y}^{-\kappa}_{jm}(\theta,\phi) \end{pmatrix} \quad \text{with } F = rf \text{ and } G = rg,$$

$$\hbar c\left[\frac{d}{dr} - \frac{\kappa}{r}\right]G^\kappa_j(r) = -\left(E - V_0(r) - mc^2\right)F^\kappa_j(r),$$

$$\hbar c\left[\frac{d}{dr} + \frac{\kappa}{r}\right]F^\kappa_j(r) = \left(E - V_0(r) + mc^2\right)G^\kappa_j(r).$$

1. a) Consider a free relativistic spin-1/2 particle of mass $m$.

i) Write down the proper definition for the probability current density of the particle and show that it satisfies the continuity equation.

[5 marks]

ii) Show that the orbital angular momentum $\hat{\mathbf{L}} = \mathbf{r} \times \hat{\mathbf{p}}$ is not a constant of motion and that

$$[\hat{H}, \hat{\mathbf{L}}] = -i\hbar c\boldsymbol{\alpha} \times \hat{\mathbf{p}}.$$

[4 marks]

iii) Write down the total angular momentum operator of the particle and show that it is a constant of motion.

[7 marks]

iv) Write down the wave function of the particle in a state with definite momentum and spin. For a massless particle, define a helicity basis and express the wave function in terms of the helicity basis.

[4 marks]

b) Write down the Dirac Hamiltonian of an electron in a uniform magnetic field $B$ in the $z$ direction. Derive the Hamiltonian in the non-relativistic limit and find the $g$ factor of the intrinsic spin of the electron.

[5 marks]

**2.** a) Consider the weak Zeeman effects for transitions ${}^1\mathrm{D}_2 \rightarrow {}^1\mathrm{P}_1$ in helium. The Landé $g$ factor is defined as

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

Determine the $g$ factor for the energy levels, and draw a level diagram accurately showing the weak Zeeman shifts. In the diagram mark all the transitions consistent with electric dipole selection rules. State how the spectral line ${}^1\mathrm{D}_2 \rightarrow {}^1\mathrm{P}_1$ changes due to the weak Zeeman effects.

[4 marks]

b) Find the generator of rotations about the $z$-axis for a spinless particle. Hence, derive the operator $\hat{U}_\alpha$ representing a finite rotation of angle $\alpha$ about the $z$-axis. Show that $\hat{U}_\alpha$ is unitary.

[9 marks]

c) Consider a spinless non-relativistic particle of charge $q$ and mass $m$.

i) Write down the electromagnetic gauge transformation for the scalar and vector potentials $\Phi$ and $\mathbf{A}$ in terms of a differentiable function $\lambda(\mathbf{r}, t)$.

[2 marks]

ii) The particle is placed in a laser field which is modeled by a homogeneous oscillating electric field in the $z$ direction, $E_z = E_0 \cos \omega t$. In two different gauges, the electric field may be considered as arising purely from a scalar potential $\Phi$, or purely from a vector potential $\mathbf{A}$. Write down the corresponding potentials, and find a function $\lambda(\mathbf{r}, t)$ which transforms from the first to the second. Write down the Hamiltonian of the particle for each case. Given that $\psi_1(\mathbf{r}, t)$ is a solution in the first case, show that

$$\psi_2(\mathbf{r}, t) = \exp(iq\lambda/\hbar)\, \psi_1(\mathbf{r}, t),$$

is a solution in the second case.

[10 marks]

**3.** a) A hydrogen atom in its ground state $\psi_{100}$ is subject to a uniform electric field in the $z$ direction,

$$E(t) = \begin{cases} 0, & t \le 0, \\ E_0 e^{-t/\tau}, & t > 0, \end{cases}$$

where $E_0$ and $\tau (> 0)$ are constants.

i) Find, at time $t\,(> 0)$, the probability $P(t)$ that the hydrogen atom ends up in the excited state $\psi_{210}$ using the first-order approximation. You may use the following wave functions of hydrogen,

$$\psi_{100}(r) = \frac{1}{\sqrt{\pi a_0^3}} e^{-r/a_0}, \quad \psi_{210}(\mathbf{r}) = \frac{r}{\sqrt{32\pi a_0^5}} e^{-r/2a_0} \cos\theta,$$

where $a_0$ is the Bohr radius.

[8 marks]

ii) Find the small $t$ behavior of $P(t)$. Determine the limit $P(\infty)$ and discuss the conditions for its validity.

[4 marks]

b) A spinless particle of charge $e$ is bounded by an infinite electrostatic spherical potential well of radius $R$,

$$e\Phi(r) = \begin{cases} 0, & r \le R, \\ \infty, & r > R. \end{cases}$$

i) Write down the time-independent Klein-Gordon equation for the eigenstates of the particle.

[2 marks]

ii) By considering an eigenstate of total angular momentum with quantum number $l$, find the eigenvalue equation for the radial part of the wave function of the particle.

[4 marks]

iii) Using suitable boundary conditions, find the normalized ground-state wave function and the ground-state energy of the particle. Discuss the non-relativistic limit for the ground-state energy.

[7 marks]

**END OF EXAMINATION PAPER**

**<u>One hour thirty minutes</u>**

<u>A list of Constants is enclosed</u>

**UNIVERSITY OF MANCHESTER**

Fundamentals of Solid State Physics

5th June 2018

2.00 p.m. – 3.30 p.m.

Answer **<u>ALL</u>** parts of question 1 and **<u>TWO</u>** other questions

---

Electronic calculators may be used, provided that they cannot store text.

---

The numbers are given as a guide to the relative weights of the different parts of each question.

P.T.O.

1.

a) Two electrons in a He atom occupy different single-particle wavefunctions $\psi_\alpha(\underline{r}_1)$ and $\psi_\beta(\underline{r}_2)$. Write down symmetric and antisymmetric two-particle wavefunctions. For a system of two interacting electrons, state which two-particle wavefunction gives rise to the lower energy state, and briefly justify your answer.

[5 marks]

b) A magnetic field of 20 T is applied to a lithium atom with electron configuration $(1s)^2(2s)^1$. What is the energy splitting between adjacent states in the presence of the field? How would you expect your answer to change for a helium atom with electron configuration $(1s)^2$?

[5 marks]

c) Briefly explain the process by which NaCl absorbs light of frequency 1.14 x $10^{13}$ Hz and calculate the interatomic force constant for the bond between the sodium and chlorine ions.
(Atomic mass of Na = 23 u; atomic mass of Cl = 35.5 u.)

[5 marks]

d) Using the free electron model of a metal, and given that the density of states per unit volume is $g(\varepsilon) = \dfrac{\sqrt{2m^3\varepsilon}}{\pi^2\hbar^3}$, show that the Fermi energy $\varepsilon_F$ is proportional to $n^{2/3}$ where $n$ is the electron density.

[5 marks]

e) Sketch graphs of the resistivity *vs.* absolute temperature for two samples of the same metal with different impurity contents, and indicate the important features.

[5 marks]

P.T.O.

2.

a) Describe the sequence of steps in a Hartree calculation of the states of a multi-electron atom.

[6 marks]

b) What is meant by a self-consistent potential?

[2 marks]

c) Hartree theory assumes that the potential arising from the other electrons is central. Why is that assumption justified for filled sub-shells?

[2 marks]

d) State Hund's Rules which prescribe the angular momentum quantum numbers $S, L$ and $J$ in the ground state of a partly full sub-shell, and give brief physical arguments to make the first two rules plausible. What is the effect which gives rise to the third rule?

[6 marks]

e) A $Cr^{3+}$ ion has three 3d electrons. What are $S, L$ and $J$ in the ground state of this ion? Write your answer in spectroscopic notation.

[4 marks]

f) Magnetic anisotropy arises for magnetic ions in solids as a result of the orbital angular momentum interacting with neighbouring atoms. $Yb^{3+}$ ions have thirteen 4f electrons, and $Lu^{3+}$ ions have fourteen 4f electrons. Would you expect greater magnetic anisotropy from materials containing $Yb^{3+}$ or $Lu^{3+}$ ions? Explain your answer.

[5 marks]

3.

a)

i. Sketch a graph of the confining potential for an independent oscillator in Einstein's model of specific heat and indicate the allowed energies in terms of the frequency of the oscillator.

[3 marks]

ii. In the context of the energy states described above, define the Einstein temperature.

[3 marks]

iii. Sketch a graph of the measured molar heat capacity at constant volume ($C_V$) versus $T$ for diamond, which has an Einstein temperature of 1325 K.

[3 marks]

b) Using the Einstein model for specific heat show that

$$C_V = 3R\frac{\theta_E^2 \exp\left(\frac{\theta_E}{T}\right)}{T^2\left[\exp\left(\frac{\theta_E}{T}\right) - 1\right]^2} ,$$

where $R$ is the universal gas constant, $\theta_E$ is the Einstein temperature and $T$ is the absolute temperature. State any simplifying assumptions.
You may take the occupation function for phonons to be

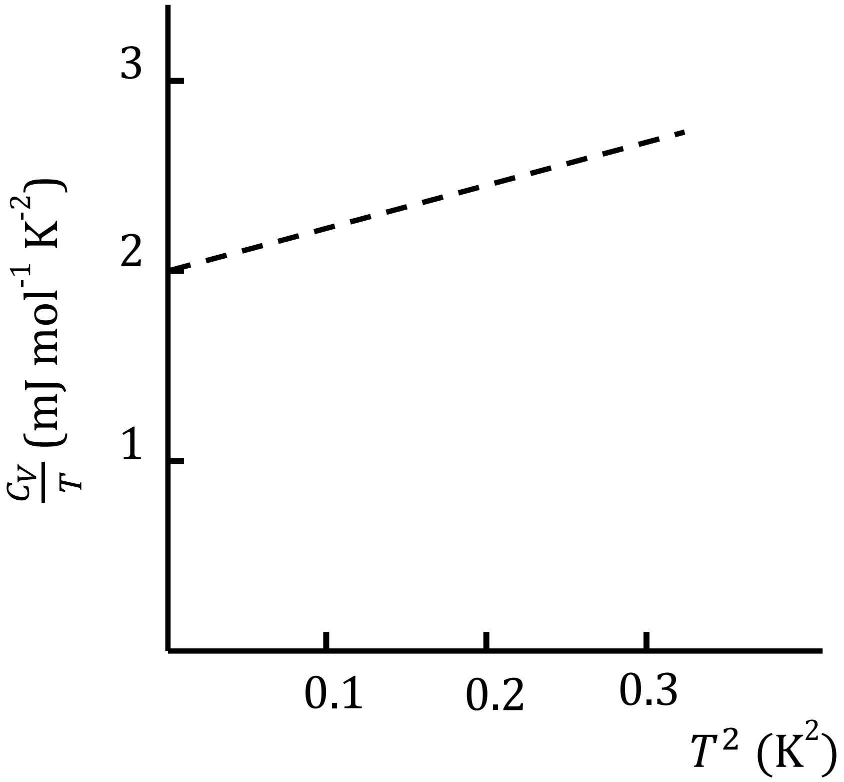
$$f(\varepsilon, T) = \frac{1}{\exp\left[\frac{\varepsilon}{k_B T}\right] - 1} .$$

[8 marks]

c) Compare the expression for $C_V$ in part b) with your sketch of the experimental finding in part a) iii, both in the low and high temperature limits.

[3 marks]

d) Shown overleaf is a plot of experimental data for the metal potassium.




The contribution to the molar heat capacity of the free electrons in a metal is given by

$$\frac{\pi^2}{2} R \frac{T}{T_F} \ ,$$

where $T_F$ is the Fermi temperature.
Using data from the graph calculate the Fermi temperature for electrons in potassium.

[5 marks]

P.T.O.

4.

a) Briefly describe the main characteristics of the bonding in silicon.

[3 marks]

b) Silicon has a fcc lattice and a basis of two Si atoms. The (200) Bragg reflection in first order is observed for an X-ray wavelength of 1.54 Å at a scattering angle (2θ) of 33.0°. Calculate the density of silicon. (Atomic mass of Si = 28 u.)

[7 marks]

c) The electron density, $n$, in a semiconductor is given by

$$n = 2\left(\frac{2\pi m_e^* k_B T}{h^2}\right)^{\frac{3}{2}} \exp\left(\frac{\varepsilon_F - E_C}{k_B T}\right),$$

where $m_e$* is the electron effective mass, $\varepsilon_F$ is the Fermi energy and $E_C$ is the energy of the conduction band edge.
Assuming that the effective masses of electrons in the conduction band and of holes in the valence band of Si are equal, calculate the hole density in the valence band of intrinsic Si at 1000 K.
(The band gap of Si is 1.1 eV, and $m_e^* = 1.06\, m_e$.)

[5 marks]

d) Extrinsic doping can be achieved in Si by substituting phosphorus (P) atoms onto Si lattice sites. Draw a schematic energy level diagram to illustrate the band structure at $T$ = 0 K of Si doped with P atoms. Mark on your diagram the positions of the conduction and valence band edges and the Fermi energy.

[5 marks]

e) The dopant ionisation energy in P-doped Si is 25 meV. Assuming the semiconductor is in the impurity range, estimate the carrier density due to the dopant atoms at 300 K. Comment on your answer in comparison with your answer to part c).

[5 marks]

**END OF EXAMINATION PAPER**

**ONE HOUR THIRTY MINUTES**

A list of constants is enclosed.

**UNIVERSITY OF MANCHESTER**

Introduction to Quantum Mechanics

26 January 2018, 09:45 - 11:15

Answer **ALL** parts of question 1 and **TWO** other questions

---

Electronic calculators may be used, provided that they cannot store text.

---

The numbers are given as a guide to the relative weights of the different parts of each question.

1. a) A particle of mass $m$ is moving in three dimensions in a potential $\hat{V}(x, y, z)$. Write down the time-independent Schrödinger equation for the particle in Cartesian coordinates and explain any notation you have used.

[4 marks]

b) The normalized wavefunction of a particle moving in one dimension is $\Psi$. Write down the definition of the expectation value of a physical operator $\hat{A}$ associated with a measurement of the particle. Briefly explain the physical meaning of this value.

[4 marks]

c) Calculate the kinetic energy in eV of a nonrelativistic electron which has a de Broglie wavelength of $8.67 \times 10^{-10}$ m.

[3 marks]

d) Write down the definition of the commutator $[\hat{A}, \hat{B}]$. Briefly describe the physical meanings of (i) $[\hat{A}, \hat{B}] = 0$ and (ii) $[\hat{A}, \hat{B}] \neq 0$. Give an example from quantum mechanics for each case without demonstration.

[5 marks]

e) The wavefunction of a particle moving in the $xy$ plane has the form $\psi(x, y) = xf(r)$, where $r = \sqrt{x^2 + y^2}$.

i) Write down in polar coordinates the definition of the operator for the $z$-component of angular momentum, $\hat{L}_z$. Show that $\psi(x, y)$ is not an eigenfunction of $\hat{L}_z$.

ii) What are the possible values of a measurement of $L_z$ of the particle?

[5 marks]

f) A magnetic rotor has a moment of inertia $I$ and is placed in a uniform magnetic field along the $z$ direction of strength $B$. The Hamiltonian of the rotor is given by

$$\hat{H} = \frac{\hat{L}^2}{2I} + \alpha B \hat{L}_z,$$

where $\alpha$ is a constant, and $\hat{L}^2$ and $\hat{L}_z$ are angular momentum operators in the usual notation. Write down the energy levels of the magnetic rotor.

[4 marks]

**2.** An electron is confined by a one-dimensional infinite square well potential to a region $0 < x < L$. Inside the well the potential is zero.

a) Write down the Hamiltonian $\hat{H}$ of the electron. Show that the wavefunctions,

$$\psi_n(x) = \begin{cases} \sqrt{\frac{2}{L}} \sin \frac{n\pi x}{L}, & 0 < x < L \\ 0, & \text{elsewhere} \end{cases},$$

where $n = 1, 2, 3, \cdots$, are normalized and are eigenfunctions of $\hat{H}$. Determine the corresponding eigenvalues $E_n$.

[6 marks]

b) Calculate the ground-state energy in eV of the electron when $L = 1$ Å and determine the wavelength in Å of the photon emitted by the electron when it makes a transition from the first excited state to the ground state.

[4 marks]

c) At time $t = 0$, the electron is in the state with the normalized wavefunction

$$\psi(x) = \frac{1}{\sqrt{2}} \left[\psi_1(x) + \psi_2(x)\right].$$

i) Write down the electron's wavefunction $\Psi(x, t)$ at time $t > 0$.

[2 marks]

ii) Determine the energy uncertainty $\Delta E$ in the state $\Psi(x, t)$.

[4 marks]

iii) Show that the probability density $|\Psi(x, t)|^2$ is an oscillatory function in time and find the period $\tau$. Show that the following uncertainty relation holds

$$\tau \Delta E > \frac{\hbar}{2}.$$

Calculate the maximum probability of finding the electron in the region $0 < x < L/2$. You may find the following identity useful:

$$2 \sin A \sin B = \cos(A - B) - \cos(A + B).$$

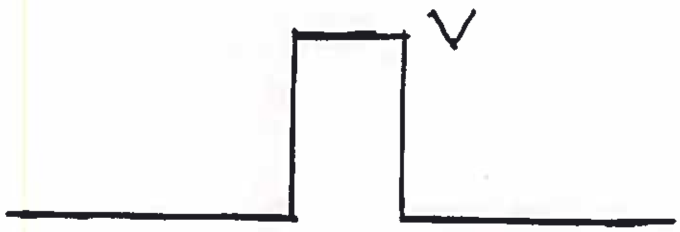
[6 marks]

iv) In one measurement, the electron's energy is found to be $E_1$. What are the possible values of a subsequent measurement of the electron's momentum?

[3 marks]

**3.** a) A particle of kinetic energy $E$ is moving in one dimension towards a rectangular potential barrier of height $V$ $(> E)$. The barrier is illustrated in the following figure. Sketch a possible energy eigenfunction of the particle.

[4 marks]




b) Consider a one-dimensional quantum simple harmonic oscillator (SHO) of angular frequency $\omega$. Sketch its ground-state and first excited-state wavefunctions. Write down the full set of its energy eigenvalues. Calculate the value of the zero-point energy in eV of the oscillator if $\omega = 2.5 \times 10^{14}$ **rad** s$^{-1}$.

[8 marks]

c) Consider a three-dimensional quantum SHO of angular frequency $\omega$. Write down the full set of its energy eigenvalues. Find the first three energy levels and their corresponding degeneracy.

[7 marks]

d) Consider a one-dimensional quantum harmonic oscillator with Hamiltonian given by:

$$\hat{H} = \frac{\hat{p}^2}{2m} + V,$$

where $V$ corresponds to an elastic spring which is extendable but incompressible. The potential of this spring is given by:

$$V(x) = \begin{cases} m\omega^2 x^2/2, & \text{if } x > 0, \\ \infty, & \text{if } x \leq 0. \end{cases}$$

Write down the full set of energy eigenvalues of this oscillator and sketch the eigenfunction of the ground state. Find the first excitation energy (i.e., the difference between the energies of the ground state and first-excited state). Briefly state the reasoning behind your results.

[6 marks]

**4.** a) Consider the following wavefunctions of a hydrogen atom

$$\begin{aligned}
\psi_A(r,\theta,\phi) &= Ae^{-r/a_0}, \\
\psi_B(r,\theta,\phi) &= B\left(1-\frac{r}{2a_0}\right)e^{-r/2a_0}, \\
\psi_C(r,\theta,\phi) &= C\left(\frac{r}{a_0}\right)e^{-r/2a_0}\sin\theta\, e^{-i\phi},
\end{aligned}$$

where $A, B, C$ and $a_0$ are constants.

i) Sketch the position probability density as a function of radial distance from the nucleus, $r$, for the electron described by the wavefunction $\psi_B$.

[4 marks]

ii) Show that $\psi_B$ and $\psi_C$ are orthogonal.

[3 marks]

iii) State the values of the hydrogen quantum numbers $(n, l, m)$ corresponding to each of the wavefunctions $\psi_A$, $\psi_B$ and $\psi_C$.

[3 marks]

iv) Find the wavelength of the emitted photon when the hydrogen atom makes a transition from $\psi_B$ to $\psi_A$. What is the corresponding wavelength in the case of a helium ion, $He^+$?

[6 marks]

b) i) Write down the quantum operators for the angular momentum components, $\hat{L}_x, \hat{L}_y$ and $\hat{L}_z$, in terms of $\hat{x}$ and $\hat{p}_x$, etc.

[4 marks]

ii) Given the following commutation relation,

$$[\hat{L}_z,\, \hat{L}^+] = \hbar\hat{L}^+,$$

where $\hat{L}^+ = \hat{L}_x + i\hat{L}_y$, show that the wavefunction

$$\psi = \hat{L}^+\psi_C(r,\theta,\phi)$$

is an eigenfunction of $\hat{L}_z$ and find the corresponding eigenvalue, where $\psi_C$ is given in part (a).

[5 marks]

**END OF EXAMINATION PAPER**

**ONE HOUR THIRTY MINUTES**

A list of constants is enclosed.

# UNIVERSITY OF MANCHESTER

Advanced Quantum Mechanics

6th June 2017, 2.00 p.m. - 3.30 p.m.

Answer any **TWO** questions

---

Electronic calculators may be used, provided that they cannot store text.

---

The numbers are given as a guide to the relative weights of the different parts of each question.

You may assume the following formulae in any question *if proof is not explicitly requested*:

**Special integrals**

$$\int_{-\infty}^{\infty} x^{2n} e^{-ax^2} dx = \frac{1 \cdot 3 \cdot 5 \cdots (2n-1)}{(2a)^n} \sqrt{\frac{\pi}{a}}, \qquad \int_0^{\infty} x^n e^{-ax} dx = \frac{n!}{a^{n+1}}, \quad a > 0.$$

**4-vectors**
Use notation $x^\mu = (x^0, \mathbf{x})$ for 4-position and $p^\mu = (E/c, \mathbf{p})$ for 4-momentum. In electromagnetism $A^\mu = (\Phi/c, \mathbf{A})$ for 4-potential.

**Klein-Gordon equation** in scalar $S$ and vector $(V_0/c, \mathbf{V})$ potential field

$$\left[(\hat{\mathbf{p}} - \mathbf{V})^2 c^2 + (mc^2 + S)^2\right] \Psi = (i\hbar\partial_t - V_0)^2 \Psi.$$

**Dirac equation** in scalar $S$ and vector $(V_0/c, \mathbf{V})$ potential field

$$\left[\alpha \cdot (\hat{\mathbf{p}} - \mathbf{V})c + \beta(mc^2 + S)\right] \Psi = (i\hbar\partial_t - V_0)\Psi.$$

**Standard spinor solutions** to the free massive Dirac equation

$$u^{(s)}(E, \mathbf{p}) = \sqrt{E + mc^2} \begin{pmatrix} \phi^s \\ \frac{c\sigma\cdot\mathbf{p}}{(E+mc^2)}\phi^s \end{pmatrix}, \quad \phi^1 = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \text{ and } \phi^2 = \begin{pmatrix} 0 \\ 1 \end{pmatrix};$$

$$v^{(s)}(-|E|, -\mathbf{p},) = \sqrt{|E| + mc^2} \begin{pmatrix} \frac{c\sigma\cdot\mathbf{p}}{(|E|+mc^2)}\chi^s \\ \chi^s \end{pmatrix}, \quad \chi^1 = \begin{pmatrix} 0 \\ 1 \end{pmatrix} \text{ and } \chi^2 = \begin{pmatrix} -1 \\ 0 \end{pmatrix}.$$

**Standard matrices**

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

$$\alpha_i = \begin{pmatrix} 0 & \sigma_i \\ \sigma_i & 0 \end{pmatrix}, \quad \beta = \begin{pmatrix} I_2 & 0 \\ 0 & -I_2 \end{pmatrix}, \quad \Sigma_i = \begin{pmatrix} \sigma_i & 0 \\ 0 & \sigma_i \end{pmatrix};$$

$$\gamma_0 = \begin{pmatrix} I_2 & 0 \\ 0 & -I_2 \end{pmatrix}, \quad \gamma_1 = \begin{pmatrix} 0 & \sigma_x \\ -\sigma_x & 0 \end{pmatrix}, \quad \gamma_2 = \begin{pmatrix} 0 & \sigma_y \\ -\sigma_y & 0 \end{pmatrix}, \quad \gamma_3 = \begin{pmatrix} 0 & \sigma_z \\ -\sigma_z & 0 \end{pmatrix}.$$

**Space-time metric** We use the metric $\eta_{\mu\nu} = \mathrm{diag}(1, -1, -, 1, -1)$.

**Laplacian operator** in terms of angular momentum operator $\hat{\mathbf{L}}$

$$\nabla^2 = \frac{1}{r}\frac{\partial^2}{\partial r^2} r - \frac{\hat{\mathbf{L}}^2}{\hbar^2 r^2}.$$

**Solution to Dirac equation** in spherical vector potential $(V_0(r)/c, \mathbf{0})$

$$\psi^\kappa_{jm}(\mathbf{r}) = \begin{pmatrix} f^\kappa_j(r)\mathcal{Y}^\kappa_{jm}(\theta, \phi) \\ ig^\kappa_j(r)\mathcal{Y}^{-\kappa}_{jm}(\theta, \phi) \end{pmatrix} \quad \text{with } F = rf \text{ and } G = rg,$$

$$\hbar c\left[\frac{d}{dr} - \frac{\kappa}{r}\right] G^\kappa_j(r) = -\left(E - V_0(r) - mc^2\right) F^\kappa_j(r),$$

$$\hbar c\left[\frac{d}{dr} + \frac{\kappa}{r}\right] F^\kappa_j(r) = \left(E - V_0(r) + mc^2\right) G^\kappa_j(r).$$

**1.** a) Show that the Hamiltonian $\hat{H}$ is the generator for time translation. Derive an expression in terms of $\hat{H}$ for the operator $\hat{U}_{t_0}$ representing a finite time $t_0$ translation for a time-independent Hamiltonian. Briefly state the reason for the assumption that the Hamiltonian is time-independent in your derivation. Show that the operator $\hat{U}_{t_0}$ is unitary.

[10 marks]

b) i) Write down the $(4 \times 4)$ Dirac vector matrix $\mathbf{\Sigma}$ in terms of the $(2 \times 2)$ Pauli vector matrix and show that $\mathbf{\Sigma}^2 = 3$. Prove the identity for the angular momentum operator $\hat{\mathbf{L}}$, $(\mathbf{\Sigma} \cdot \hat{\mathbf{L}})^2 = \hat{\mathbf{L}}^2 - \hbar \mathbf{\Sigma} \cdot \hat{\mathbf{L}}$.

[6 marks]

ii) The operator $\hat{K}$ is defined as $\hat{K} = \beta(\mathbf{\Sigma} \cdot \hat{\mathbf{L}} + \hbar)$ and commutes with the Dirac Hamiltonian of hydrogen. Use the identity in (i) to show that $\hat{K}^2 = \hat{\mathbf{J}}^2 + \frac{1}{4}\hbar^2$, where $\hat{\mathbf{J}}$ is the total angular momentum operator. Hence find the eigenvalues of $\hat{K}$.

[6 marks]

iii) Briefly discuss the physical meaning of $\hat{K}$. Determine its eigenvalues for the Dirac hydrogen energy levels $1S_{1/2}$, $2P_{1/2}$, and $2P_{3/2}$.

[3 marks]

**2.** a) State the selection rules for electric dipole transitions in light atoms. Which of the following transitions in carbon or nitrogen are NOT electric dipole transitions? Give your reasons.

i) $(2s)^2(2p)^3$, ${}^4S_{3/2} \rightarrow (2s)^2(2p)^2(3d)$, ${}^4P_{5/2}$
ii) $(2s)^2(2p)^2(3s)$, ${}^4D_{3/2} \rightarrow (2s)^2(2p)^2(3d)$, ${}^4P_{5/2}$
iii) $(2s)^2(2p)(3d)^2$, ${}^4D_{3/2} \rightarrow (2s)^2(2p)^3$, ${}^4S_{3/2}$
iv) $(2s)^2(2p)(3d)$, ${}^3D_0 \rightarrow (2s)^2(2p)^2$, ${}^3P_0$
v) $(2s)^2(2p)(3s)$, ${}^1P_1 \rightarrow (2s)^2(2p)^2$, ${}^1S_0$

[6 marks]

b) i) Find the energy spectrum of a nonrelativistic electron moving along a cylindrical surface of radius $R$ without any external field. Find the energy spectrum of the same electron (with $g = 0$) after a homogeneous magnetic field is applied parallel to the axis, described by the azimuthal vector potential $A_\varphi = Br/2$ for $r \leq R$. At what values of $B$ is the spectrum the same as for the zero-field case?

[9 marks]

ii) Now consider a relativistic electron moving along a cylindrical surface of radius $R$ with a homogeneous magnetic field applied parallel to the axis described by the azimuthal vector potential $A_\varphi = Br/2$ for $r \leq R$ as part (i). Given the identity for this potential,

$$[\sigma \cdot (\hat{\mathbf{p}} + e\mathbf{A})]^2 = (\hat{\mathbf{p}} + e\mathbf{A})^2 + e\hbar\sigma_z B,$$

express the Dirac equation of this electron in terms of the upper components only and find the energy eigenvalues. Consider the nonrelativistic limit and determine the electron's anomalous Zeeman energy.

[10 marks]

**3.** a) Briefly describe the three elementary rotations in terms of Euler angles $(\alpha, \beta, \gamma)$ for a general orientation. Show that the corresponding transformation operator is

$$\hat{U}(\alpha, \beta, \gamma) = e^{-i\alpha\hat{L}_z/\hbar}e^{-i\beta\hat{L}_x/\hbar}e^{-i\gamma\hat{L}_z/\hbar}.$$

You may use the transformation operator $\hat{U}_\phi = \exp(-i\phi\hat{L}_i/\hbar)$ for a rotation around the $i$-axis by angle $\phi$.

[8 marks]

b) A one-dimensional harmonic oscillator of mass $m$ and angular frequency $\omega$ is subject to a small constant force $F$ during the time period $0 < t < \tau$. Assuming that the oscillator is initially in the ground state, find the probability, in the first-order approximation, that the oscillator is in its first excited state after a sufficient time $(t > \tau)$. The ground and first excited state wavefunctions of the oscillator are

$$\phi_0(x) = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} \exp\left(-\frac{m\omega x^2}{2\hbar}\right), \quad \phi_1(x) = \sqrt{\frac{2m\omega}{\hbar}}\, x\phi_0(x)$$

respectively. Determine the value of $\tau$ for the maximum transition probability.

[8 marks]

c) A $\pi^-$ meson is moving in the $xy$ plane in a perpendicular uniform magnetic field of magnitude $B$.

i) Show that such a magnetic field can be described by a vector potential $\mathbf{A} = (-yB, 0, 0)$.

ii) Derive the time-independent Klein-Gordon equation for the eigenfunctions of the meson. Obtain the meson's energy eigenvalues and eigenfunctions in terms of the known functions. Obtain the energy levels in the weak field limit.

iii) Show that the different vector potential $\mathbf{A} = (0, xB, 0)$ also describes the same magnetic field. Demonstrate the energy eigenvalues of the meson remain the same as obtained in part (ii).

[9 marks]

**END OF EXAMINATION PAPER**

**ONE HOUR THIRTY MINUTES**

A list of constants is enclosed

**UNIVERSITY OF MANCHESTER**

Fundamentals of Solid State Physics

31st May 2017

09:45 a.m. – 11:15 a.m.

Answer **ALL** parts of question 1 and **TWO** other questions.

---

Electronic calculators may be used, provided that they cannot store text.

---

The numbers are given as a guide to the relative weights of the different parts of each question.

P.T.O.

1.

a) A plutonium ($Pu^{3+}$) ion has five 5f electrons. What are the orbital, spin and total angular momenta in the ground state of the ion? Write the answer in spectroscopic notation.

[5 marks]

b) A magnetic field of 18 T is applied to a hydrogen atom in the ground state. What is the energy splitting between adjacent states in the presence of the field? How would you expect your answer to change for a ground state neon atom with electron configuration $(1s)^2(2p)^6$?

[5 marks]

c) Using a molecular orbital energy level diagram, explain why the bond length of the $H_2^+$ molecular ion is larger than that of the $H_2$ molecule. Do you expect the bond length for the three-electron species $H_2^-$ to be smaller or larger than that for $H_2$? Briefly justify your answer.

[5 marks]

d) Use the Drude model to derive an expression for the electrical conductivity of a metal, defining the terms you use.

[5 marks]

e) Sketch the dispersion relation $\varepsilon(k)$ for a nearly free electron interacting with a one-dimensional lattice, over the range $-\frac{2\pi}{a} \leq k \leq +\frac{2\pi}{a}$, where $a$ is the spacing of the atoms.

[5 marks]

P.T.O.

2.

a) Write down two spatial wavefunctions that represent two identical electrons in terms of one-electron wavefunctions. In each case say whether the wavefunction is symmetrical or antisymmetrical when the particles are exchanged.

[4 marks]

b) The combined spin eigenfunctions of the total spin for two electrons are:

$$\chi_{s1} = \chi_1^+ \chi_2^+,$$
$$\chi_{s2} = \frac{1}{\sqrt{2}}\left(\chi_1^+ \chi_2^- + \chi_1^- \chi_2^+\right),$$
$$\chi_{s3} = \chi_1^- \chi_2^-,$$
$$\chi_a = \frac{1}{\sqrt{2}}\left(\chi_1^+ \chi_2^- - \chi_1^- \chi_2^+\right).$$

The operators for the $z$-components of the individual spins have the following eigenstates, $\chi_1^+, \chi_1^-, \chi_2^+, \chi_2^-$:

$$\hat{S}_{1z}\chi_1^+ = \frac{\hbar}{2}\chi_1^+;\ \hat{S}_{1z}\chi_1^- = -\frac{\hbar}{2}\chi_1^-;\ \hat{S}_{2z}\chi_2^+ = \frac{\hbar}{2}\chi_2^+;\ \hat{S}_{2z}\chi_2^- = -\frac{\hbar}{2}\chi_2^-.$$

By applying the operator for the $z$-component of the total spin, $\hat{S}_z = \hat{S}_{1z} + \hat{S}_{2z}$, show that these eigenfunctions are also eigenfunctions of the $z$-component of the total spin, and calculate the $M_S$ quantum numbers for each combined spin eigenfunction.

[8 marks]

c)

The table below shows the energies of a number of energy eigenstates of a helium atom. In each case, one electron is in the $n = 1, \ell = 0$ state. The combined spin state, $n$ and $\ell$ for the other electron are shown below.

| Combined spin state | $n$ | $\ell$ | Energy / eV |
|---|---|---|---|
| singlet | 1 | 0 | -79.2 |
| triplet | 2 | 0 | -59.7 |
| singlet | 2 | 0 | -58.5 |
| triplet | 2 | 1 | -58.2 |
| singlet | 2 | 1 | -57.7 |

P.T.O.

Explain:

(i) why the ground state ( $n = 1$, $\ell = 0$ ) energy is not $-8E_R$;

[3 marks]

(ii) why there is no state which is a triplet with $n = 1$, $\ell = 0$ ;

[3 marks]

(iii) why the energy depends on $\ell$ ;

[3 marks]

(iv) why the energies depend on the overall spin symmetry, and why the singlet energies are higher than those of the corresponding triplets.

[4 marks]

P.T.O.

3.

a) Cubic gallium nitride (GaN) has a fcc lattice and a basis of one gallium atom (69.7 amu) and one nitrogen atom (14.0 amu). The (200) Bragg reflection in first order is observed for an X-ray wavelength of 1.54 Å at a scattering angle ($2\theta$) of 40.0°. Calculate the density of cubic gallium nitride.

[7 marks]

b) The electron density $n$ in the conduction band of an *intrinsic* semiconductor can be written as

$$n = N_C e^{\frac{-(E_C - \varepsilon_F)}{k_B T}},$$

where $N_C$ is the effective density of states in the conduction band, and all other symbols have their conventional meaning.

Calculate $n$ at a temperature of 300 K for GaN, given that the band gap is 3.2 eV and the value of $N_C$ is $4 \times 10^{25}$ m$^{-3}$.

[3 marks]

c) Sketch a graph showing a typical variation of $\log(n)$ where $n$ is the free electron concentration for an $n$-type semiconductor as a function of the inverse of the absolute temperature. Indicate three important ranges on your graph and explain why the different ranges exist.

[5 marks]

d) Extrinsic $n$-type doping can be achieved in GaN by substituting silicon (Si) atoms onto Ga lattice sites. Draw a schematic energy level diagram to illustrate the band structure at $T = 0$ K of GaN doped with Si atoms. Mark on your diagram the positions of the conduction and valence band edges and the Fermi energy.

[5 marks]

e) The dopant ionisation energy in Si-doped GaN is 20 meV. Assuming the semiconductor is in the impurity range, estimate the carrier density due to the dopant atoms at 300 K. You may use the value of $N_C$ given in part (b). Comment on your answer in comparison with your answer to part (b).

[5 marks]

P.T.O.

4.

a) Sketch the form of a typical experimental plot of the molar heat capacity for a monatomic solid at constant volume, $C_v$, versus absolute temperature, measured from near absolute zero to room temperature.

[2 marks]

b) State the law of equipartition of energy. Using the first law of thermodynamics show for a monovalent solid that $C_v$ is equal to $3R$ where $R$ is the universal gas constant.

[7 marks]

c) Describe the Einstein model of specific heat, and explain why it predicts that $C_v$ should depend on temperature as opposed to the prediction based on the equipartition of energy. In your answer briefly discuss the relevance of the Einstein temperature.

[7 marks]

d) The Einstein temperature of diamond (atomic mass = 12 amu) is 1300 K and that of lead (atomic mass = 207 amu) is 60 K. Calculate the ratio of the spring constants of the C – C and Pb – Pb bonds. Illustrate on a diagram the relative values of the ground state vibrational energies of the C and Pb atoms, together with the confining potentials for both C and Pb.

[4 marks]

e) Briefly describe the shortcomings of the Einstein model, and explain how the Debye model rectifies them.

[5 marks]

**END OF EXAMINATION PAPER**

**ONE HOUR THIRTY MINUTES**

A list of constants is enclosed.

**UNIVERSITY OF MANCHESTER**

Introduction to Quantum Mechanics

25 January 2017, 9.45 a.m. - 11.15 a.m.

Answer **ALL** parts of question 1 and **TWO** other questions

---

Electronic calculators may be used, provided that they cannot store text.

---

The numbers are given as a guide to the relative weights of the different parts of each question.

**1.** a) A particle of mass $m$ is moving in one dimension in a potential $\widehat{V}$. Write down the time-dependent Schrödinger equation of the particle for its wavefunction $\Psi(x,t)$.

[3 marks]

If $\widehat{V}$ is time independent, by substituting the stationary wavefunction with energy $E$,

$$\Psi(x,t) = \psi(x)\exp\left(-iEt/\hbar\right),$$

obtain the time-independent Schrödinger equation for the spatial wavefunction $\psi(x)$.

[2 marks]

b) Electrons with 2 eV kinetic energy are passing through a narrow slit of 8 Å width. Are the wave properties of the electrons important? Give your reason.

[3 marks]

c) For a particle of mass $m$ moving in one dimension, write down the definition of the momentum operator $\hat{p}_x$ and derive the kinetic energy operator $\widehat{T}$.

[2 marks]

The particle is moving in a region of free space with a wavefunction

$$\psi(x) = A\cos kx,$$

where $A$ and $k$ are constants. Show that $\psi(x)$ is not an eigenfunction of $\hat{p}_x$ but is an eigenfunction of $\widehat{T}$. What are the possible outcomes of a measurement of the particle's momentum?

[5 marks]

d) In a scanning tunneling microscopic (STM) experiment, a metal tip is positioned about 3 Å from the sample surface. Use the wide-barrier approximation to estimate the probability for an electron with an energy deficit of 1.5 eV to tunnel through the vacuum gap.

[5 marks]

e) Specify the allowed values of the quantum numbers $(n, l, m_l, m_s)$ of a hydrogen atom. Briefly state their physical meanings. If the energy of a hydrogen atom in an external field depends on $(n, l)$ only, what is the degeneracy for each of the energy levels?

[5 marks]

**2.** A particle of mass $m$ is confined by a one-dimensional infinite square well potential to a region $-L/2 < x < L/2$, where inside the well the potential is zero.

a) Write down the Hamiltonian $\hat{H}$ of the particle. Show that the wavefunction

$$f(x) = \begin{cases} \sqrt{\frac{2}{L}} \cos \frac{\pi x}{L}, & -\frac{L}{2} < x < \frac{L}{2} \\ 0, & \text{elsewhere} \end{cases}$$

is normalized and is an eigenfunction of $\hat{H}$. Determine the eigenvalue $E$.

[5 marks]

b) Find the uncertainties of position $\Delta x$ and momentum $\Delta p$ of the particle described by the wavefunction $f(x)$. Verify that $\Delta x \Delta p \geq \hbar/2$. You may use the following integral

$$\int_{-L/2}^{L/2} x^2 \cos \frac{2\pi x}{L} dx = -\frac{L^3}{2\pi^2}.$$

[10 marks]

c) Write down another eigenfunction, $g(x)$, of $\hat{H}$ and the corresponding eigenvalue, $U$. Show that $g(x)$ satisfies the boundary conditions of the system.

[3 marks]

d) Assume that at time $t = 0$, the particle is in the state

$$\psi(x) = \frac{1}{\sqrt{2}} \left[ f(x) + g(x) \right].$$

Write down the particle wavefunction $\Psi(x, t)$ at time $t\,(> 0)$. Determine the probability of finding the particle in the interval $0 < x < L/2$. You may find the following identities useful:

$$2 \sin A \cos B = \sin(A + B) + \sin(A - B); \quad 2 \cos A \cos B = \cos(A + B) + \cos(A - B).$$

[7 marks]

**3.** a) A particle of energy $E$ is confined in one dimension to the region $x > 0$ with an impenetrable wall at $x = 0$. There is also a potential barrier of height $V$ $(> E)$ as illustrated in the following figure. Sketch a possible energy eigenfunction of the particle.

[5 marks]

b) The Hamiltonian of a one-dimensional harmonic oscillator of mass $m$ and angular frequency $\omega$ is written as

$$\hat{H} = \frac{\hat{p}_x^2}{2m} + \frac{1}{2}m\omega^2\hat{x}^2.$$

i) The operators $\hat{a}$ and $\hat{a}^\dagger$ are defined as

$$\hat{a} = \frac{1}{\sqrt{2}}\left(\frac{\hat{x}}{x_0} + \frac{ix_0\hat{p}_x}{\hbar}\right), \quad \hat{a}^\dagger = \frac{1}{\sqrt{2}}\left(\frac{\hat{x}}{x_0} - \frac{ix_0\hat{p}_x}{\hbar}\right),$$

with $x_0 = \sqrt{\hbar/m\omega}$. Show that

$$[\hat{a},\, \hat{a}^\dagger] = 1. \tag{1}$$

Show that $\hat{H}$ can be expressed as

$$\hat{H} = \left(\hat{a}^\dagger\hat{a} + \frac{1}{2}\right)\hbar\omega. \tag{2}$$

[5 marks]

ii) Show that the ground-state wavefunction,

$$\psi_0(x) = A\exp\left(-\frac{x^2}{2x_0^2}\right)$$

with constant $A$, satisfies $\hat{a}\psi_0(x) = 0$. Hence find the ground-state energy $E_0$.

[5 marks]

iii) Use Eqs. (1) and (2) to show that $\psi_1(x) = \hat{a}^\dagger\psi_0(x)$ describes an excited state and find the corresponding energy $E_1$.

[5 marks]

iv) In a hydrogen iodide (HI) molecule, the spring constant of the covalent bond has a value of 310 N m$^{-1}$. Estimate the energy interval $\Delta E = E_1 - E_0$ in eV, of the vibrational motion. (The atomic masses of hydrogen and iodine are 1 and 130 respectively.)

[5 marks]

**4.** a) Consider the following wavefunctions of a hydrogen atom

$$\psi_A(r,\theta,\phi) = A\left(1-\frac{r}{2a_0}\right)e^{-r/2a_0},$$
$$\psi_B(r,\theta,\phi) = B\left(\frac{r}{3a_0}\right)^2 e^{-r/3a_0}\sin^2\theta e^{i2\phi},$$

where $A, B$ and $a_0$ are constants.

i) Show that $\psi_A$ and $\psi_B$ are orthogonal to one another. State the values of the hydrogen quantum numbers $(n, l, m)$ for both $\psi_A$ and $\psi_B$.

[6 marks]

ii) Find the wavelength of the emitted (or absorbed) photon when the hydrogen atom makes a transition between these two states. What is the corresponding wavelength in the case of a lithium ion $Li^{2+}$?

[6 marks]

b) i) Write down the quantum operators for the angular momentum components, $\hat{L}_x, \hat{L}_y$ and $\hat{L}_z$, in terms of $\hat{x}$ and $\hat{p}_x$, etc.

[3 marks]

ii) Given the following commutation relation,

$$[\hat{L}_x,\, \hat{L}_y] = i\hbar\hat{L}_z,$$

use the cyclic rule to write down the other two commutation relations between the angular momentum component operators. Hence show that

$$[\hat{L}_z,\, \hat{L}^-] = -\hbar\hat{L}^-, \tag{3}$$

where $\hat{L}^- = \hat{L}_x - i\hat{L}_y$.

[5 marks]

iii) Use Eq. (3) to show that the wavefunction

$$\psi_C = \hat{L}^-\psi_B(r,\theta,\phi)$$

is also an eigenfunction of $\hat{L}_z$ and find the eigenvalue, where $\psi_B$ is given in Part (a).

[5 marks]

**END OF EXAMINATION PAPER**