Part II

Applications of Quantum Mechanics

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Paper 1, Section II

35D Applications of Quantum Mechanics

(a) A beam of particles of mass m and energy E, moving in one dimension, scatters off a potential barrier $V(x)$ which is localised near the origin $x = 0$ and is reflection invariant, $V(x) = V(-x)$ for all x. With reference to the asymptotic form of the wave function as $x \to \pm\infty$, define the corresponding *reflection* and *transmission coefficients*, denoted r and t respectively, and write down the *S-matrix* $\mathcal{S}$.

For the case $V(x) = V_0\,\delta(x)$, where $\delta(x)$ denotes the Dirac δ-function, determine r and t as functions of the energy E, and show explicitly that $\mathcal{S}$ is a unitary matrix.

(b) A particle of mass m and energy E moves in one dimension subject to a potential $\tilde{V}(x)$ obeying $\tilde{V}(x+a) = \tilde{V}(x)$ for all x. Define the corresponding *Floquet matrix* $\mathcal{M}$. Explain briefly how the Floquet matrix determines the resulting energy spectrum of continuous bands separated by forbidden regions. [You may state without proof any results from the course you might need.]

Determine $\mathcal{M}$ as a function of E for the case $\tilde{V}(x) = V_0 \sum_{n=-\infty}^{+\infty} \delta(x - na)$. Find algebraic equations which determine all the edges of the allowed energy bands. For each edge express $\exp(-ika)$ at the edge in terms of r and t. Here $r = r(E)$ and $t = t(E)$ are the reflection and transmission coefficients determined in part (a), and $E = \hbar^2 k^2/2m$ with $k > 0$.

Paper 2, Section II

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Consider a quantum system with Hamiltonian $\hat{H}$ having a discrete spectrum with a unique groundstate $|\psi_0\rangle$ of energy E_0. For any state $|\psi\rangle$, define the *Rayleigh-Ritz quotient*, $R[\psi]$, and show that it attains its minimum value when $|\psi\rangle = |\psi_0\rangle$.

A particle of mass m moves in one dimension subject to the potential,

$$V(x) \quad = \quad \frac{\hbar^2}{2m}\left(x^6 - 3x^2 + 2\right).$$

Show that the system has an energy eigenstate with (unnormalised) wavefunction,

$$\tilde{\psi}(x) := \exp(-\beta x^n),$$

for a value of β, a positive integer value of n and an energy each of which you should determine.

Estimate the groundstate energy of this system using the variational principle with a Gaussian trial wavefunction of the form

$$\psi_\alpha(x) \quad := \quad \exp\left(-\frac{\alpha}{2}x^2\right)$$

with parameter $\alpha > 0$. Show that the best estimate of the ground-state energy is obtained for the unique value

$$\alpha = \alpha_* = \sqrt{\frac{(p+\sqrt{q})}{2}},$$

where p and q are integers that you should determine. Give the corresponding approximate ground-state energy, E_0^*, in terms of α_*. You should not attempt to evaluate this function numerically. [*Hint: You may use without proof the following definite integral,*

$$\int_{-\infty}^{\infty} x^{2n} \exp\left(-\alpha x^2\right)\, dx \quad = \quad \frac{(2n)!}{n!(4\alpha)^n}\sqrt{\frac{\pi}{\alpha}}. \quad]$$

Is your result consistent with the hypothesis that the exact eigenstate $\tilde{\psi}(x)$ found above is the true groundstate? Explain your reasoning carefully.

Paper 3, Section II

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Let Λ be a Bravais lattice in three dimensions with primitive vectors $\mathbf{a}_1$, $\mathbf{a}_2$, $\mathbf{a}_3$. Define the *reciprocal lattice* Λ^* and show that it is a Bravais lattice.

An incident particle of mass m and wavevector $\mathbf{k}$ scatters off a crystal which consists of identical atoms located at the vertices of a finite subset $\mathcal{S}$ of the lattice Λ,

$$\mathcal{S} \quad = \quad \{\mathbf{l} = l_1\mathbf{a}_1 + l_2\mathbf{a}_2 + l_3\mathbf{a}_3 : l_i \in \mathbb{Z},\ -L_i/2 \leqslant l_i \leqslant +L_i/2 \ \text{ for } \ i = 1,2,3\},$$

where L_1, L_2 and L_3 are positive even integers. After scattering the particle has wavevector $\mathbf{k}'$ with $|\mathbf{k}| = |\mathbf{k}'| = k$ and the scattering angle θ, with $0 \leqslant \theta \leqslant \pi$, is defined by $\mathbf{k}\cdot\mathbf{k}' = k^2\cos\theta$. Show that the resulting scattering amplitude is proportional to

$$\Delta\left(\mathbf{k}-\mathbf{k}'\right) \quad := \quad \sum_{\mathbf{l}\in\mathcal{S}} \exp\left(i(\mathbf{k}-\mathbf{k}')\cdot\mathbf{l}\right) .$$

For L_1, L_2, $L_3 \gg 1$, show that this quantity is strongly peaked for wavevectors $\mathbf{k}$ and $\mathbf{k}'$ obeying $\mathbf{k}-\mathbf{k}' = \mathbf{q}$ for some $\mathbf{q}\in\Lambda^*$.

Consider the case where Λ is a body centered cubic lattice with primitive vectors

$$\mathbf{a}_1 = \frac{a}{2}\left(\mathbf{e}_x + \mathbf{e}_y + \mathbf{e}_z\right), \qquad \mathbf{a}_2 = \frac{a}{2}\left(\mathbf{e}_x - \mathbf{e}_y + \mathbf{e}_z\right), \qquad \mathbf{a}_3 = a\,\mathbf{e}_z\,,$$

where $a > 0$ and $\mathbf{e}_x$, $\mathbf{e}_y$ and $\mathbf{e}_z$ are, respectively, unit vectors in the x-, y- and z-directions. For scattering at fixed energy $E = \hbar^2k^2/2m$ with $ka \gg 1$, find the smallest non-zero value of the scattering angle θ for which the scattering amplitude has a strong peak (i.e. a peak such as you found in the previous part of the question).

Paper 4, Section II

34D Applications of Quantum Mechanics

(a) A scalar particle of mass m and charge e is moving in three dimensions in a background electromagnetic field with vector potential $\mathbf{A}(\mathbf{x}, t)$ and zero scalar potential. The Hamiltonian is given as

$$\hat{H} \;=\; \frac{1}{2m}\left(-i\hbar\nabla + e\mathbf{A}\right)\cdot\left(-i\hbar\nabla + e\mathbf{A}\right) .$$

Specialise to the case of a constant, homogeneous magnetic field $\mathbf{B} = \nabla\times\mathbf{A} = (0,0,B)$ in the z-direction. Suppose further that the x and y coordinates of the particle are constrained to lie in a rectangular region R of the x-y plane with sides of length R_x and R_y, and that the particle has vanishing momentum in the z-direction. By solving the Schrödinger equation in a suitable gauge with periodic boundary conditions in the x- and y-directions, find the energy levels of the system and give the degeneracy of each level. [You may use without proof any results about the spectrum of the quantum harmonic oscillator you may need, and you may assume that R_x and R_y are large compared to other length scales in the problem.]

(b) An electron is a particle of mass m, charge e and spin $1/2$. It is described by a two-component wave function $\vec{\Psi} \in \mathbb{C}^2$ with energy eigenstates obeying a matrix Schrödinger equation

$$\hat{\mathbb{H}}\,\vec{\Psi} \;=\; E\vec{\Psi}\,,$$

where

$$\hat{\mathbb{H}} \;=\; \hat{H}\,\mathbb{I}_2 \;+\; \frac{e\hbar}{2m}\,\mathbf{B}\cdot\boldsymbol{\sigma}\,,$$

where $\hat{H}$ is the Hamiltonian for the spinless particle given above, $\mathbb{I}_2$ is the (2×2)-unit matrix and $\boldsymbol{\sigma} = (\sigma_1, \sigma_2, \sigma_3)$ is a three-component vector whose entries are the Pauli matrices σ_i, for $i = 1, 2, 3$.

Find the energy levels of a single electron in a constant, homogeneous magnetic field $\mathbf{B} = (0,0,B)$ under the same conditions as in part (a). Give the degeneracy of each energy level.

Now consider N non-interacting electrons occupying these energy levels. Find the ground-state energy $E_{\rm gs}$ of the system as a function of N, identifying any thresholds which occur. Sketch the graph of $E_{\rm gs}$ against N. [*Hint: Recall that electrons are identical fermionic particles obeying the Pauli exclusion principle.*]

Paper 1, Section II
35D Applications of Quantum Mechanics

A particle of mass m and energy $E = \hbar^2 k^2/2m$, moving in one dimension, is incident on a localised potential barrier.

(a) Define *reflection* and *transmission coefficients*, r and t, for a right-moving particle incident from $x = -\infty$. Define corresponding coefficients r' and t' for a left-moving particle incident from $x = +\infty$. Prove that the S-matrix

$$\mathcal{S} \quad = \quad \begin{pmatrix} t' & r \\ r' & t \end{pmatrix}$$

is unitary. [You may use without proof the conservation of the probability current.]

(b) Explain what is meant by the *parity* of a wavefunction. Under what circumstances do energy eigenstates of the system described above have definite parity?

(c) Consider the potential barrier

$$V(x) = \begin{cases} V_0 & \text{for } |x| < a/2 \\ 0 & \text{for } |x| > a/2, \end{cases}$$

where $V_0 > 0$. Find an even parity wavefunction satisfying the Schrödinger equation for a particle of energy $E = \hbar^2 k^2/2m$ with $E < V_0$. Hence compute $r + t$.

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A particle of mass m moves in one dimension in the periodic potential

$$V(x) = \sum_{n \in \mathbb{Z}} V_n \exp\left(\frac{2\pi i n x}{a}\right),$$

where $V_{-n} = (V_n)^*$. Treating the Hamiltonian $\hat{H} = \hat{H}_0 + V(x)$ as a small perturbation of the free Hamiltonian $\hat{H}_0$, show that the energy spectrum consists of continuous bands separated by gaps of width $2|V_n|$ that occur for each positive integer n.

What is meant by the *dispersion relation* of the particle? Determine an explicit form of the dispersion relation near each band gap.

Work out the locations and widths of the gaps in the energy spectrum for the potential

$$V(x) = \frac{8}{3} V_0 \cos^4\left(\frac{2\pi x}{a}\right).$$

Sketch the dispersion relation of a particle moving in this potential.

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34D Applications of Quantum Mechanics

A two-dimensional Bravais lattice Λ has primitive basis vectors $\{\mathbf{a}_1, \mathbf{a}_2\}$, where

$$\mathbf{a}_1 = \hat{\mathbf{x}} \,, \qquad \mathbf{a}_2 = -\frac{1}{2}\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}\hat{\mathbf{y}} \,,$$

and $\{\hat{\mathbf{x}}, \hat{\mathbf{y}}\}$ is the standard Cartesian basis. Express a general primitive basis $\{\mathbf{a}'_1, \mathbf{a}'_2\}$ for Λ in terms of $\{\mathbf{a}_1, \mathbf{a}_2\}$.

Find the lattice Λ^* which is dual to Λ, giving a basis of primitive vectors dual to $\{\mathbf{a}_1, \mathbf{a}_2\}$. Sketch the region of the lattice Λ^* containing the origin, indicating all those points which are nearest neighbours of the origin. Determine the *Wigner-Seitz unit cell* of Λ^* as polygonal region of the plane, giving the coordinates of all vertices of this polygon. Determine the area of this unit cell.

A particle of mass m moves in a potential $V(\mathbf{x})$ which is invariant under shifts by vectors in Λ,

$$V(\mathbf{x} + \mathbf{l}) = V(\mathbf{x}) \qquad \forall\ \mathbf{l} \in \Lambda \,.$$

Define the n^{th} *Brillouin zone* of this system and briefly describe its physical significance. Draw a sketch showing the first and second Brillouin zones.

Paper 4, Section II
34D Applications of Quantum Mechanics

A particle of mass m and charge e moves in a constant homogeneous magnetic field $\mathbf{B} = \nabla \times \mathbf{A}$ with vector potential

$$\mathbf{A}(\mathbf{x}) = \frac{B}{2}\,(-y, x, 0)\,,$$

where $\mathbf{x} = (x, y, z)$ are Cartesian coordinates on $\mathbb{R}^3$.

(a) Write down the Hamiltonian $\hat{H}$ for the particle as a differential operator in Cartesian coordinates. Find a corresponding expression for $\hat{H}$ in cylindrical polar coordinates (r, θ, z), where $x = r\cos\theta$ and $y = r\sin\theta$.

[*You may use without proof the relations*

$$\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} = \frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial}{\partial r}\right) + \frac{1}{r^2}\frac{\partial^2}{\partial \theta^2} \qquad \text{and} \qquad x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x} = \frac{\partial}{\partial \theta}\,. \quad]$$

(b) Consider wavefunctions of the form

$$\psi_{k_z,n}\,(r, \theta, z) = \exp(ik_z z)\,\exp(in\theta)\,\phi_n(r)\,.$$

What is the physical interpretation of the quantum numbers $k_z \in \mathbb{R}$ and $n \in \mathbb{Z}$? For $n \geqslant 0$, show that $\psi_{k_z,n}$ is an eigenstate of $\hat{H}$ provided that

$$\phi_n(r) = r^\alpha \exp\left(-\beta\frac{r^2}{2}\right),$$

where α and β are (possibly n-dependent) constants which you should determine. Find the corresponding energy eigenvalue E.

(c) By noting that $\phi_n(r)$ is sharply peaked at a particular value of r, work out the total degeneracy of this energy level when the particle is confined to lie inside a large circle of radius R. Determine the number of states per unit area.

Paper 1, Section II

35B Applications of Quantum Mechanics

(a) Discuss the variational principle that allows one to derive an upper bound on the energy E_0 of the ground state for a particle in one dimension subject to a potential $V(x)$.

If $V(x) = V(-x)$, how could you adapt the variational principle to derive an upper bound on the energy E_1 of the first excited state?

(b) Consider a particle of mass $2m = \hbar^2$ (in certain units) subject to a potential

$$V(x) = -V_0 e^{-x^2} \quad \text{with} \quad V_0 > 0\,.$$

(i) Using the trial wavefunction

$$\psi(x) = e^{-\frac{1}{2}x^2 a}\,,$$

with $a > 0$, derive the upper bound $E_0 \leqslant E(a)$, where

$$E(a) = \frac{1}{2}a - V_0 \frac{\sqrt{a}}{\sqrt{1+a}}\,.$$

(ii) Find the zero of $E(a)$ in $a > 0$ and show that any extremum must obey

$$(1+a)^3 = \frac{V_0^2}{a}\,.$$

(iii) By sketching $E(a)$ or otherwise, deduce that there must always be a minimum in $a > 0$. Hence deduce the existence of a bound state.

(iv) Working perturbatively in $0 < V_0 \ll 1$, show that

$$-V_0 < E_0 \leqslant -\frac{1}{2}V_0^2 + \mathcal{O}(V_0^3)\,.$$

[*Hint: You may use that* $\displaystyle\int_{-\infty}^{\infty} e^{-bx^2}dx = \sqrt{\frac{\pi}{b}}$ *for* $b > 0$.]

Paper 2, Section II

36B Applications of Quantum Mechanics

(a) The s-wave solution ψ_0 for the scattering problem of a particle of mass m and momentum $\hbar k$ has the asymptotic form

$$\psi_0(r) \sim \frac{A}{r}\left[\sin(kr) + g(k)\cos(kr)\right].$$

Define the *phase shift* δ_0 and verify that $\tan\delta_0 = g(k)$.

(b) Define the *scattering amplitude* f. For a spherically symmetric potential of finite range, starting from $\sigma_T = \int |f|^2 d\Omega$, derive the expression

$$\sigma_T = \frac{4\pi}{k^2}\sum_{l=0}^{\infty}(2l+1)\sin^2\delta_l$$

giving the cross-section σ_T in terms of the phase shifts δ_l of the partial waves.

(c) For $g(k) = -k/K$ with $K > 0$, show that a bound state exists and compute its energy. Neglecting the contributions from partial waves with $l > 0$, show that

$$\sigma_T \approx \frac{4\pi}{K^2 + k^2}.$$

(d) For $g(k) = \gamma/(K_0 - k)$ with $K_0 > 0$, $\gamma > 0$ compute the s-wave contribution to σ_T. Working to leading order in $\gamma \ll K_0$, show that σ_T has a local maximum at $k = K_0$. Interpret this fact in terms of a resonance and compute its energy and decay width.

Paper 3, Section II

34B Applications of Quantum Mechanics

(a) In three dimensions, define a *Bravais lattice* Λ and its *reciprocal lattice* Λ^*.

A particle is subject to a potential $V(\mathbf{x})$ with $V(\mathbf{x}) = V(\mathbf{x}+\mathbf{r})$ for $\mathbf{x} \in \mathbb{R}^3$ and $\mathbf{r} \in \Lambda$. State and prove Bloch's theorem and specify how the Brillouin zone is related to the reciprocal lattice.

(b) A body-centred cubic lattice Λ_{BCC} consists of the union of the points of a cubic lattice Λ_1 and all the points Λ_2 at the centre of each cube:

$$\begin{aligned}
\Lambda_{BCC} &\equiv \Lambda_1 \cup \Lambda_2\,, \\
\Lambda_1 &\equiv \left\{ \mathbf{r} \in \mathbb{R}^3 : \mathbf{r} = n_1 \hat{\mathbf{i}} + n_2 \hat{\mathbf{j}} + n_3 \hat{\mathbf{k}}\,,\ \text{with } n_{1,2,3} \in \mathbb{Z} \right\}\,, \\
\Lambda_2 &\equiv \left\{ \mathbf{r} \in \mathbb{R}^3 : \mathbf{r} = \tfrac{1}{2}\big(\hat{\mathbf{i}} + \hat{\mathbf{j}} + \hat{\mathbf{k}}\big) + \mathbf{r}',\ \text{with } \mathbf{r}' \in \Lambda_1 \right\}\,,
\end{aligned}$$

where $\hat{\mathbf{i}}$, $\hat{\mathbf{j}}$ and $\hat{\mathbf{k}}$ are unit vectors parallel to the Cartesian coordinates in $\mathbb{R}^3$. Show that Λ_{BCC} is a Bravais lattice and determine the primitive vectors $\mathbf{a}_1$, $\mathbf{a}_2$ and $\mathbf{a}_3$.

Find the reciprocal lattice Λ^*_{BCC}. Briefly explain what sort of lattice it is.

$\Big[$*Hint: The matrix* $M = \frac{1}{2}\begin{pmatrix} -1 & 1 & 1 \\ 1 & -1 & 1 \\ 1 & 1 & -1 \end{pmatrix}$ *has inverse* $M^{-1} = \begin{pmatrix} 0 & 1 & 1 \\ 1 & 0 & 1 \\ 1 & 1 & 0 \end{pmatrix}$. $\Big]$

Paper 4, Section II
34B Applications of Quantum Mechanics

(a) Consider the nearly free electron model in one dimension with mass m and periodic potential $V(x) = \lambda U(x)$ with $0 < \lambda \ll 1$ and

$$U(x) = \sum_{l=-\infty}^{\infty} U_l \exp\left(\frac{2\pi i}{a} lx\right) .$$

Ignoring degeneracies, the energy spectrum of Bloch states with wavenumber k is

$$E(k) = E_0(k) + \lambda\langle k|U|k\rangle + \lambda^2 \sum_{k'\neq k} \frac{\langle k|U|k'\rangle\langle k'|U|k\rangle}{E_0(k) - E_0(k')} + \mathcal{O}(\lambda^3) ,$$

where $\{|k\rangle\}$ are normalized eigenstates of the free Hamiltonian with wavenumber k. What is E_0 in this formula?

If we impose periodic boundary conditions on the wavefunctions, $\psi(x) = \psi(x + L)$ with $L = Na$ and N a positive integer, what are the allowed values of k and k'? Determine $\langle k|U|k'\rangle$ for these allowed values.

(b) State when the above expression for $E(k)$ ceases to be a good approximation and explain why. Quoting any result you need from degenerate perturbation theory, calculate to $\mathcal{O}(\lambda)$ the location and width of the band gaps.

(c) Determine the allowed energy bands for each of the potentials

$$\text{(i)} \quad V(x) = 2\lambda \cos\left(\frac{2\pi x}{a}\right) ,$$

$$\text{(ii)} \quad V(x) = \lambda a \sum_{n=-\infty}^{\infty} \delta(x - na) .$$

(d) Briefly discuss a macroscopic physical consequence of the existence of energy bands.

Paper 1, Section II

35C Applications of Quantum Mechanics

Consider the quantum mechanical scattering of a particle of mass m in one dimension off a parity-symmetric potential, $V(x) = V(-x)$. State the constraints imposed by parity, unitarity and their combination on the components of the S-matrix in the parity basis,

$$S = \begin{pmatrix} S_{++} & S_{+-} \\ S_{-+} & S_{--} \end{pmatrix} .$$

For the specific potential

$$V = \hbar^2 \frac{U_0}{2m} \left[\delta_D(x+a) + \delta_D(x-a) \right] ,$$

show that

$$S_{--} = e^{-i2ka} \left[\frac{(2k - iU_0)e^{ika} + iU_0 e^{-ika}}{(2k + iU_0)e^{-ika} - iU_0 e^{ika}} \right] .$$

For $U_0 < 0$, derive the condition for the existence of an odd-parity bound state. For $U_0 > 0$ and to leading order in $U_0 a \gg 1$, show that an odd-parity resonance exists and discuss how it evolves in time.

Paper 2, Section II

35C Applications of Quantum Mechanics

a) Consider a particle moving in one dimension subject to a periodic potential, $V(x) = V(x+a)$. Define the *Brillouin zone*. State and prove Bloch's theorem.

b) Consider now the following periodic potential

$$V = V_0 \left(\cos(x) - \cos(2x) \right) ,$$

with positive constant V_0.

i) For very small V_0, use the nearly-free electron model to compute explicitly the lowest-energy band gap to leading order in degenerate perturbation theory.

ii) For very large V_0, the electron is localised very close to a minimum of the potential. Estimate the two lowest energies for such localised eigenstates and use the tight-binding model to estimate the lowest-energy band gap.

Paper 3, Section II

34C Applications of Quantum Mechanics

(a) For the quantum scattering of a beam of particles in three dimensions off a spherically symmetric potential $V(r)$ that vanishes at large r, discuss the boundary conditions satisfied by the wavefunction ψ and define the scattering amplitude $f(\theta)$. Assuming the asymptotic form

$$\psi = \sum_{l=0}^{\infty} \frac{2l+1}{2ik} \left[(-1)^{l+1} \frac{e^{-ikr}}{r} + (1+2if_l) \frac{e^{ikr}}{r} \right] P_l(\cos\theta)\,,$$

state the constraints on f_l imposed by the unitarity of the S-matrix and define the *phase shifts* δ_l.

(b) For $V_0 > 0$, consider the specific potential

$$V(r) = \begin{cases} \infty\,, & r \leqslant a\,, \\ -V_0\,, & a < r \leqslant 2a\,, \\ 0\,, & r > 2a\,. \end{cases}$$

(i) Show that the s-wave phase shift δ_0 obeys

$$\tan(\delta_0) = \frac{k\cos(2ka) - \kappa\cot(\kappa a)\sin(2ka)}{k\sin(2ka) + \kappa\cot(\kappa a)\cos(2ka)}\,,$$

where $\kappa^2 = k^2 + 2mV_0/\hbar^2$.

(ii) Compute the scattering length a_s and find for which values of κ it diverges. Discuss briefly the physical interpretation of the divergences. [*Hint: you may find this trigonometric identity useful*

$$\tan(A+B) = \frac{\tan A + \tan B}{1 - \tan A \tan B}\,. \quad]$$

Paper 4, Section II

34C Applications of Quantum Mechanics

(a) For a particle of charge q moving in an electromagnetic field with vector potential $\boldsymbol{A}$ and scalar potential ϕ, write down the classical Hamiltonian and the equations of motion.

(b) Consider the vector and scalar potentials

$$\boldsymbol{A} = \frac{B}{2}(-y, x, 0)\,, \qquad \phi = 0\,.$$

(i) Solve the equations of motion. Define and compute the *cyclotron frequency* ω_B.

(ii) Write down the quantum Hamiltonian of the system in terms of the angular momentum operator

$$L_z = xp_y - yp_x\,.$$

Show that the states

$$\psi(x,y) = f(x+iy)e^{-(x^2+y^2)qB/4\hbar}\,, \qquad (\dagger)$$

for any function f, are energy eigenstates and compute their energy. Define Landau levels and discuss this result in relation to them.

(iii) Show that for $f(w) = w^M$, the wavefunctions in $(\dagger)$ are eigenstates of angular momentum and compute the corresponding eigenvalue. These wavefunctions peak in a ring around the origin. Estimate its radius. Using these two facts or otherwise, estimate the degeneracy of Landau levels.

Paper 4, Section II

33B Applications of Quantum Mechanics

(a) A classical beam of particles scatters off a spherically symmetric potential $V(r)$. Draw a diagram to illustrate the differential cross-section $d\sigma/d\Omega$, and use this to derive an expression for $d\sigma/d\Omega$ in terms of the impact parameter b and the scattering angle θ.

A quantum beam of particles of mass m and momentum $p = \hbar k$ is incident along the z-axis and scatters off a spherically symmetric potential $V(r)$. Write down the asymptotic form of the wavefunction ψ in terms of the scattering amplitude $f(\theta)$. By considering the probability current $\mathbf{J} = -i(\hbar/2m)\,(\psi^\star \nabla\psi - (\nabla\psi^\star)\psi)$, derive an expression for the differential cross-section $d\sigma/d\Omega$ in terms of $f(\theta)$.

(b) The solution $\psi(\mathbf{r})$ of the radial Schrödinger equation for a particle of mass m and wave number k moving in a spherically symmetric potential $V(r)$ has the asymptotic form

$$\psi(\mathbf{r}) \quad \sim \quad \sum_{l=0}^{\infty} \left[A_l(k) \frac{\sin\left(kr - \frac{l\pi}{2}\right)}{kr} \; - \; B_l(k) \frac{\cos\left(kr - \frac{l\pi}{2}\right)}{kr} \right] P_l\left(\cos\theta\right) \,,$$

valid for $kr \gg 1$, where $A_l(k)$ and $B_l(k)$ are constants and P_l denotes the l'th Legendre polynomial. Define the S-matrix element S_l and the corresponding phase shift δ_l for the partial wave of angular momentum l, in terms of $A_l(k)$ and $B_l(k)$. Define also the scattering length a_s for the potential V.

Outside some core region, $r > r_0$, the Schrödinger equation for some such potential is solved by the s-wave (i.e. $l = 0$) wavefunction $\psi(\mathbf{r}) = \psi(r)$ with,

$$\psi(r) = \frac{e^{-ikr}}{r} + \frac{k + i\lambda \tanh(\lambda r)}{k - i\lambda} \frac{e^{ikr}}{r}$$

where $\lambda > 0$ is a constant. Extract the S-matrix element S_0, the phase shift δ_0 and the scattering length a_s. Deduce that the potential $V(r)$ has a bound state of zero angular momentum and compute its energy. Give the form of the (un-normalised) bound state wavefunction in the region $r > r_0$.

Paper 3, Section II

34B Applications of Quantum Mechanics

A Hamiltonian H is invariant under the discrete translational symmetry of a Bravais lattice Λ. This means that there exists a unitary translation operator $T_{\mathbf{r}}$ such that $[H, T_{\mathbf{r}}] = 0$ for all $\mathbf{r} \in \Lambda$. State and prove *Bloch's theorem* for H.

Consider the two-dimensional Bravais lattice Λ defined by the basis vectors

$$\mathbf{a}_1 = \frac{a}{2}(\sqrt{3}, 1)\,, \quad \mathbf{a}_2 = \frac{a}{2}(\sqrt{3}, -1)\,.$$

Find basis vectors $\mathbf{b_1}$ and $\mathbf{b}_2$ for the reciprocal lattice. Sketch the Brillouin zone. Explain why the Brillouin zone has only two physically distinct corners. Show that the positions of these corners may be taken to be $\mathbf{K} = \frac{1}{3}(2\mathbf{b}_1 + \mathbf{b}_2)$ and $\mathbf{K}' = \frac{1}{3}(\mathbf{b}_1 + 2\mathbf{b}_2)$.

The dynamics of a single electron moving on the lattice Λ is described by a tight-binding model with Hamiltonian

$$H = \sum_{\mathbf{r}\in\Lambda} \Big[E_0|\mathbf{r}\rangle\langle\mathbf{r}| - \lambda\Big(|\mathbf{r}\rangle\langle\mathbf{r}+\mathbf{a}_1| + |\mathbf{r}\rangle\langle\mathbf{r}+\mathbf{a}_2| + |\mathbf{r}+\mathbf{a}_1\rangle\langle\mathbf{r}| + |\mathbf{r}+\mathbf{a}_2\rangle\langle\mathbf{r}|\Big)\Big]\,,$$

where E_0 and λ are real parameters. What is the energy spectrum as a function of the wave vector $\mathbf{k}$ in the Brillouin zone? How does the energy vary along the boundary of the Brillouin zone between $\mathbf{K}$ and $\mathbf{K}'$? What is the width of the band?

In a real material, each site of the lattice Λ contains an atom with a certain valency. Explain how the conducting properties of the material depend on the valency.

Suppose now that there is a second band, with minimum $E = E_0 + \Delta$. For what values of Δ and the valency is the material an insulator?

Paper 2, Section II

34B Applications of Quantum Mechanics

Give an account of the variational principle for establishing an upper bound on the ground state energy of a Hamiltonian H.

A particle of mass m moves in one dimension and experiences the potential $V = A|x|^n$ with n an integer. Use a variational argument to prove the *virial theorem*,

$$2\langle T\rangle_0 = n\langle V\rangle_0$$

where $\langle\cdot\rangle_0$ denotes the expectation value in the true ground state. Deduce that there is no normalisable ground state for $n \leqslant -3$.

For the case $n = 1$, use the ansatz $\psi(x) \propto e^{-\alpha^2 x^2}$ to find an estimate for the energy of the ground state.

Paper 1, Section II

34B Applications of Quantum Mechanics

A particle of mass m and charge q moving in a uniform magnetic field $\mathbf{B} = \nabla \times \mathbf{A} = (0, 0, B)$ and electric field $\mathbf{E} = -\nabla\phi$ is described by the Hamiltonian

$$H = \frac{1}{2m} |\mathbf{p} - q\mathbf{A}|^2 + q\phi \,,$$

where $\mathbf{p}$ is the canonical momentum.

[In the following you may use without proof any results concerning the spectrum of the harmonic oscillator as long as they are stated clearly.]

(a) Let $\mathbf{E} = \mathbf{0}$. Choose a gauge which preserves translational symmetry in the y-direction. Determine the spectrum of the system, restricted to states with $p_z = 0$. The system is further restricted to lie in a rectangle of area $A = L_x L_y$, with sides of length L_x and L_y parallel to the x- and y-axes respectively. Assuming periodic boundary conditions in the y-direction, estimate the degeneracy of each Landau level.

(b) Consider the introduction of an additional electric field $\mathbf{E} = (\mathcal{E}, 0, 0)$. Choosing a suitable gauge (with the same choice of vector potential $\mathbf{A}$ as in part (a)), write down the resulting Hamiltonian. Find the energy spectrum for a particle on $\mathbb{R}^3$ again restricted to states with $p_z = 0$.

Define the *group velocity* of the electron and show that its y-component is given by $v_y = -\mathcal{E}/B$.

When the system is further restricted to a rectangle of area A as above, show that the previous degeneracy of the Landau levels is lifted and determine the resulting energy gap ΔE between the ground-state and the first excited state.

Paper 1, Section II

34A Applications of Quantum Mechanics

A particle of mass m moves in one dimension in a periodic potential $V(x)$ satisfying $V(x+a) = V(x)$. Define the *Floquet matrix* F. Show that $\det F = 1$ and explain why $\operatorname{Tr} F$ is real. Show that allowed bands occur for energies such that $(\operatorname{Tr} F)^2 < 4$. Consider the potential

$$V(x) = -\frac{\hbar^2 \lambda}{m} \sum_{n=-\infty}^{+\infty} \delta(x - na).$$

For states of negative energy, construct the Floquet matrix with respect to the basis of states $e^{\pm \mu x}$. Derive an inequality for the values of μ in an allowed energy band.

For states of positive energy, construct the Floquet matrix with respect to the basis of states $e^{\pm ikx}$. Derive an inequality for the values of k in an allowed energy band.

Show that the state with zero energy lies in a forbidden region for $\lambda a > 2$.

Paper 4, Section II

34A Applications of Quantum Mechanics

Define a *Bravais lattice* Λ in three dimensions. Define the *reciprocal lattice* $\Lambda^\star$. Define the *Brillouin zone*.

An FCC lattice has a basis of primitive vectors given by

$$\mathbf{a}_1 = \frac{a}{2}(\mathbf{e}_2 + \mathbf{e}_3)\ , \quad \mathbf{a}_2 = \frac{a}{2}(\mathbf{e}_1 + \mathbf{e}_3)\ , \quad \mathbf{a}_3 = \frac{a}{2}(\mathbf{e}_1 + \mathbf{e}_2),$$

where $\mathbf{e}_i$ is an orthonormal basis of $\mathbb{R}^3$. Find a basis of reciprocal lattice vectors. What is the volume of the Brillouin zone?

The asymptotic wavefunction for a particle, of wavevector $\mathbf{k}$, scattering off a potential $V(\mathbf{r})$ is

$$\psi(\mathbf{r}) \sim e^{i\mathbf{k}\cdot\mathbf{r}} + f_{\mathrm{V}}(\mathbf{k};\mathbf{k}')\frac{e^{ikr}}{r}\ ,$$

where $\mathbf{k}' = k\hat{\mathbf{r}}$ and $f_{\mathrm{V}}(\mathbf{k};\mathbf{k}')$ is the scattering amplitude. Give a formula for the *Born approximation* to the scattering amplitude.

Scattering of a particle off a single atom is modelled by a potential $V(\mathbf{r}) = V_0\delta(r-d)$ with δ-function support on a spherical shell, $r = |\mathbf{r}| = d$ centred at the origin. Calculate the Born approximation to the scattering amplitude, denoting the resulting expression as $\tilde{f}_{\mathrm{V}}(\mathbf{k};\mathbf{k}')$.

Scattering of a particle off a crystal consisting of atoms located at the vertices of a lattice Λ is modelled by a potential

$$V_\Lambda = \sum_{\mathbf{R}\in\Lambda} V(\mathbf{r}-\mathbf{R}),$$

where $V(\mathbf{r}) = V_0\delta(r-d)$ as above. Calculate the Born approximation to the scattering amplitude giving your answer in terms of your approximate expression $\tilde{f}_{\mathrm{V}}$ for scattering off a single atom. Show that the resulting amplitude vanishes unless the momentum transfer $\mathbf{q} = \mathbf{k} - \mathbf{k}'$ lies in the reciprocal lattice $\Lambda^\star$.

For the particular FCC lattice considered above, show that, when $k = |\mathbf{k}| > 2\pi/a$, scattering occurs for two values of the scattering angle, θ_1 and θ_2, related by

$$\frac{\sin\left(\frac{\theta_1}{2}\right)}{\sin\left(\frac{\theta_2}{2}\right)} = \frac{2}{\sqrt{3}}\,.$$

Paper 3, Section II

35A Applications of Quantum Mechanics

A beam of particles of mass m and momentum $p = \hbar k$ is incident along the z-axis. The beam scatters off a spherically symmetric potential $V(r)$. Write down the asymptotic form of the wavefunction in terms of the scattering amplitude $f(\theta)$.

The incoming plane wave and the scattering amplitude can be expanded in partial waves as,

$$e^{ikr\cos\theta} \sim \frac{1}{2ikr}\sum_{l=0}^{\infty}(2l+1)\left(e^{ikr} - (-1)^l e^{-ikr}\right) P_l(\cos\theta)$$

$$f(\theta) = \sum_{l=0}^{\infty}\frac{2l+1}{k} f_l \, P_l(\cos\theta)$$

where P_l are Legendre polynomials. Define the *S-matrix*. Assuming that the S-matrix is unitary, explain why we can write

$$f_l = e^{i\delta_l}\sin\delta_l$$

for some real phase shifts δ_l. Obtain an expression for the total cross-section σ_T in terms of the phase shifts δ_l.

[*Hint: You may use the orthogonality of Legendre polynomials:*

$$\int_{-1}^{+1} dw \; P_l(w)P_{l'}(w) = \frac{2}{2l+1}\delta_{ll'} \; . \quad]$$

Consider the repulsive, spherical potential

$$V(r) = \begin{cases} +V_0 & r < a \\ 0 & r > a \end{cases}$$

where $V_0 = \hbar^2\gamma^2/2m$. By considering the s-wave solution to the Schrödinger equation, show that

$$\frac{\tan(ka + \delta_0)}{ka} = \frac{\tanh(\sqrt{\gamma^2 - k^2}a)}{\sqrt{\gamma^2 - k^2}a} \; .$$

For low momenta, $ka \ll 1$, compute the s-wave contribution to the total cross-section. Comment on the physical interpretation of your result in the limit $\gamma a \to \infty$.

Paper 2, Section II

35A Applications of Quantum Mechanics

Consider a one-dimensional chain of $2N \gg 1$ atoms, each of mass m. Impose periodic boundary conditions. The forces between neighbouring atoms are modelled as springs, with alternating spring constants λ and $\alpha\lambda$. In equilibrium, the separation between the atoms is a.

Denote the position of the n^{th} atom as $x_n(t)$. Let $u_n(t) = x_n(t) - na$ be the displacement from equilibrium. Write down the equations of motion of the system.

Show that the longitudinal modes of vibration are labelled by a wavenumber k that is restricted to lie in a Brillouin zone. Find the frequency spectrum. What is the frequency gap at the edge of the Brillouin zone? Show that the gap vanishes when $\alpha = 1$. Determine approximations for the frequencies near the centre of the Brillouin zone. Plot the frequency spectrum. What is the speed of sound in this system?

Paper 1, Section II

33C Applications of Quantum Mechanics

A one-dimensional lattice has N sites with lattice spacing a. In the tight-binding approximation, the Hamiltonian describing a single electron is given by

$$H = E_0 \sum_n |n\rangle\langle n| - J \sum_n \Big(|n\rangle\langle n+1| + |n+1\rangle\langle n| \Big) ,$$

where $|n\rangle$ is the normalised state of the electron localised on the n^{th} lattice site. Using periodic boundary conditions $|N+1\rangle \equiv |1\rangle$, solve for the spectrum of this Hamiltonian to derive the dispersion relation

$$E(k) = E_0 - 2J\cos(ka) .$$

Define the *Brillouin zone*. Determine the number of states in the Brillouin zone.

Calculate the velocity v and effective mass $m^\star$ of the particle. For which values of k is the effective mass negative?

In the semi-classical approximation, derive an expression for the time-dependence of the position of the electron in a constant electric field.

Describe how the concepts of *metals* and *insulators* arise in the model above.

Paper 2, Section II

33C Applications of Quantum Mechanics

Give an account of the variational method for establishing an upper bound on the ground-state energy of a Hamiltonian H with a discrete spectrum $H|n\rangle = E_n|n\rangle$, where $E_n \leqslant E_{n+1}$, $n = 0, 1, 2 \ldots$.

A particle of mass m moves in the three-dimensional potential

$$V(r) = -\frac{Ae^{-\mu r}}{r},$$

where $A, \mu > 0$ are constants and r is the distance to the origin. Using the normalised variational wavefunction

$$\psi(r) = \sqrt{\frac{\alpha^3}{\pi}}e^{-\alpha r},$$

show that the expected energy is given by

$$E(\alpha) = \frac{\hbar^2\alpha^2}{2m} - \frac{4A\alpha^3}{(\mu + 2\alpha)^2}.$$

Explain why there is necessarily a bound state when $\mu < Am/\hbar^2$. What can you say about the existence of a bound state when $\mu \geqslant Am/\hbar^2$?

[*Hint: The Laplacian in spherical polar coordinates is*

$$\nabla^2 = \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) + \frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) + \frac{1}{r^2\sin^2\theta}\frac{\partial^2}{\partial\phi^2}. \quad]$$

Paper 3, Section II

33C Applications of Quantum Mechanics

A particle of mass m and charge q moving in a uniform magnetic field $\mathbf{B} = \boldsymbol{\nabla} \times \mathbf{A} = (0,0,B)$ is described by the Hamiltonian

$$H = \frac{1}{2m}(\mathbf{p} - q\mathbf{A})^2$$

where $\mathbf{p}$ is the canonical momentum, which obeys $[x_i, p_j] = i\hbar\delta_{ij}$. The *mechanical momentum* is defined as $\boldsymbol{\pi} = \mathbf{p} - q\mathbf{A}$. Show that

$$[\pi_x, \pi_y] = iq\hbar B\,.$$

Define

$$a = \frac{1}{\sqrt{2q\hbar B}}(\pi_x + i\pi_y) \quad \text{and} \quad a^\dagger = \frac{1}{\sqrt{2q\hbar B}}(\pi_x - i\pi_y)\,.$$

Derive the commutation relation obeyed by a and $a^\dagger$. Write the Hamiltonian in terms of a and $a^\dagger$ and hence solve for the spectrum.

In symmetric gauge, states in the lowest Landau level with $k_z = 0$ have wavefunctions

$$\psi(x,y) = (x+iy)^M \, e^{-qBr^2/4\hbar}$$

where $r^2 = x^2 + y^2$ and M is a positive integer. By considering the profiles of these wavefunctions, estimate how many lowest Landau level states can fit in a disc of radius R.

Paper 4, Section II

33C Applications of Quantum Mechanics

(a) In one dimension, a particle of mass m is scattered by a potential $V(x)$ where $V(x) \to 0$ as $|x| \to \infty$. For wavenumber $k > 0$, the incoming ($\mathcal{I}$) and outgoing ($\mathcal{O}$) asymptotic plane wave states with positive ($+$) and negative ($-$) parity are given by

$$\mathcal{I}_+(x) = e^{-ik|x|}\,, \qquad \mathcal{I}_-(x) = \mathrm{sign}(x)\, e^{-ik|x|}\,,$$
$$\mathcal{O}_+(x) = e^{+ik|x|}\,, \qquad \mathcal{O}_-(x) = -\mathrm{sign}(x)\, e^{+ik|x|}\,.$$

(i) Explain how this basis may be used to define the *S-matrix*,

$$\mathcal{S}^P = \begin{pmatrix} S_{++} & S_{+-} \\ S_{-+} & S_{--} \end{pmatrix}.$$

(ii) For what choice of potential would you expect $S_{+-} = S_{-+} = 0$? Why?

(b) The potential $V(x)$ is given by

$$V(x) = V_0\Big[\delta(x-a) + \delta(x+a)\Big]$$

with V_0 a constant.

(i) Show that

$$S_{--}(k) = e^{-2ika}\left[\frac{(2k - iU_0)e^{ika} + iU_0 e^{-ika}}{(2k + iU_0)e^{-ika} - iU_0 e^{ika}}\right],$$

where $U_0 = 2mV_0/\hbar^2$. Verify that $|S_{--}|^2 = 1$. Explain the physical meaning of this result.

(ii) For $V_0 < 0$, by considering the poles or zeros of $S_{--}(k)$, show that there exists one bound state of negative parity if $aU_0 < -1$.

(iii) For $V_0 > 0$ and $aU_0 \gg 1$, show that $S_{--}(k)$ has a pole at

$$ka = \pi + \alpha - i\gamma\,,$$

where α and γ are real and

$$\alpha = -\frac{\pi}{aU_0} + O\left(\frac{1}{(aU_0)^2}\right) \quad \text{and} \quad \gamma = \left(\frac{\pi}{aU_0}\right)^2 + O\left(\frac{1}{(aU_0)^3}\right).$$

Explain the physical significance of this result.

Paper 1, Section II

32A Applications of Quantum Mechanics

A particle in one dimension of mass m and energy $E = \hbar^2 k^2/2m$ ($k > 0$) is incident from $x = -\infty$ on a potential $V(x)$ with $V(x) \to 0$ as $x \to -\infty$ and $V(x) = \infty$ for $x > 0$. The relevant solution of the time-independent Schrödinger equation has the asymptotic form

$$\psi(x) \sim \exp(ikx) + r(k)\exp(-ikx), \qquad x \to -\infty.$$

Explain briefly why a pole in the reflection amplitude $r(k)$ at $k = i\kappa$ with $\kappa > 0$ corresponds to the existence of a stable bound state in this potential. Indicate why a pole in $r(k)$ just below the real k-axis, at $k = k_0 - i\rho$ with $k_0 \gg \rho > 0$, corresponds to a quasi-stable bound state. Find an approximate expression for the lifetime τ of such a quasi-stable state.

Now suppose that

$$V(x) = \begin{cases} (\hbar^2 U/2m)\,\delta(x+a) & \text{for } x < 0 \\ \infty & \text{for } x > 0 \end{cases}$$

where $U > 0$ and $a > 0$ are constants. Compute the reflection amplitude $r(k)$ in this case and deduce that there are quasi-stable bound states if U is large. Give expressions for the wavefunctions and energies of these states and compute their lifetimes, working to leading non-vanishing order in $1/U$ for each expression.

[You may assume $\psi = 0$ for $x \geqslant 0$ and $\lim_{\epsilon\to 0+}\{\,\psi'(-a+\epsilon) - \psi'(-a-\epsilon)\,\} = U\,\psi(-a)$.]

Paper 3, Section II

32A Applications of Quantum Mechanics

(a) A spinless charged particle moves in an electromagnetic field defined by vector and scalar potentials $\mathbf{A}(\mathbf{x},t)$ and $\phi(\mathbf{x},t)$. The wavefunction $\psi(\mathbf{x},t)$ for the particle satisfies the time-dependent Schrödinger equation with Hamiltonian

$$\hat{H}_0 \;=\; \frac{1}{2m}\left(-i\hbar\boldsymbol{\nabla} + e\mathbf{A}\right)\cdot\left(-i\hbar\boldsymbol{\nabla} + e\mathbf{A}\right) \;-\; e\phi\;.$$

Consider a gauge transformation

$$\mathbf{A} \to \tilde{\mathbf{A}} \;=\; \mathbf{A} + \boldsymbol{\nabla} f\,, \qquad \phi \to \tilde{\phi} \;=\; \phi - \frac{\partial f}{\partial t}\,, \qquad \psi \to \tilde{\psi} \;=\; \exp\Big(-\frac{ief}{\hbar}\Big)\,\psi\,,$$

for some function $f(\mathbf{x},t)$. Define *covariant derivatives* with respect to space and time, and show that $\tilde{\psi}$ satisfies the Schrödinger equation with potentials $\tilde{\mathbf{A}}$ and $\tilde{\phi}$.

(b) Suppose that in part (a) the magnetic field has the form $\mathbf{B} = \boldsymbol{\nabla}\times\mathbf{A} = (0,0,B)$, where B is a constant, and that $\phi = 0$. Find a suitable $\mathbf{A}$ with $A_y = A_z = 0$ and determine the energy levels of the Hamiltonian $\hat{H}_0$ when the z-component of the momentum of the particle is zero. Suppose in addition that the particle is constrained to lie in a rectangular region of area $\mathcal{A}$ in the (x,y)-plane. By imposing periodic boundary conditions in the x-direction, estimate the degeneracy of each energy level. [You may use without proof results for a quantum harmonic oscillator, provided they are clearly stated.]

(c) An electron is a charged particle of spin $\frac{1}{2}$ with a two-component wavefunction $\boldsymbol{\psi}(\mathbf{x},t)$ governed by the Hamiltonian

$$\hat{H} \;=\; \hat{H}_0\,\mathbb{I}_2 \,+\, \frac{e\hbar}{2m}\,\mathbf{B}\cdot\boldsymbol{\sigma}$$

where $\mathbb{I}_2$ is the $2{\times}2$ unit matrix and $\boldsymbol{\sigma} = (\sigma_1,\sigma_2,\sigma_3)$ denotes the Pauli matrices. Find the energy levels for an electron in the constant magnetic field defined in part (b), assuming as before that the z-component of the momentum of the particle is zero.

Consider N such electrons confined to the rectangular region defined in part (b). Ignoring interactions between the electrons, show that the ground state energy of this system vanishes for N less than some integer $N_{\max}$ which you should determine. Find the ground state energy for $N = (2p+1)N_{\max}$, where p is a positive integer.

Paper 4, Section II

32A Applications of Quantum Mechanics

Let $\Lambda \subset \mathbb{R}^2$ be a Bravais lattice. Define the dual lattice Λ^* and show that

$$V(\mathbf{x}) = \sum_{\mathbf{q}\in\Lambda^*} V_{\mathbf{q}} \exp(i\mathbf{q}\cdot\mathbf{x})$$

obeys $V(\mathbf{x}+\boldsymbol{l}) = V(\mathbf{x})$ for all $\boldsymbol{l} \in \Lambda$, where $V_{\mathbf{q}}$ are constants. Suppose $V(\mathbf{x})$ is the potential for a particle of mass m moving in a two-dimensional crystal that contains a very large number of lattice sites of Λ and occupies an area $\mathcal{A}$. Adopting periodic boundary conditions, plane-wave states $|\,\mathbf{k}\,\rangle$ can be chosen such that

$$\langle\,\mathbf{x}\,|\,\mathbf{k}\,\rangle = \frac{1}{\mathcal{A}^{1/2}} \exp(i\mathbf{k}\cdot\mathbf{x}) \qquad \text{and} \qquad \langle\,\mathbf{k}\,|\,\mathbf{k}'\,\rangle = \delta_{\mathbf{k}\mathbf{k}'}\,.$$

The allowed wavevectors $\mathbf{k}$ are closely spaced and include all vectors in Λ^*. Find an expression for the matrix element $\langle\,\mathbf{k}\,|\,V(\mathbf{x})\,|\,\mathbf{k}'\,\rangle$ in terms of the coefficients $V_{\mathbf{q}}$. [You need not discuss additional details of the boundary conditions.]

Now suppose that $V(\mathbf{x}) = \lambda\, U(\mathbf{x})$, where $\lambda \ll 1$ is a dimensionless constant. Find the energy $E(\mathbf{k})$ for a particle with wavevector $\mathbf{k}$ to order λ^2 in non-degenerate perturbation theory. Show that this expansion in λ breaks down on the Bragg lines in $\mathbf{k}$-space defined by the condition

$$\mathbf{k}\cdot\mathbf{q} = \frac{1}{2}|\mathbf{q}|^2 \qquad \text{for} \qquad \mathbf{q} \in \Lambda^*\,,$$

and explain briefly, without additional calculations, the significance of this for energy levels in the crystal.

Consider the particular case in which Λ has primitive vectors

$$\mathbf{a}_1 = 2\pi\Big(\mathbf{i} + \frac{1}{\sqrt{3}}\mathbf{j}\Big)\,, \qquad \mathbf{a}_2 = 2\pi\,\frac{2}{\sqrt{3}}\,\mathbf{j}\,,$$

where $\mathbf{i}$ and $\mathbf{j}$ are orthogonal unit vectors. Determine the polygonal region in $\mathbf{k}$-space corresponding to the lowest allowed energy band.

Paper 2, Section II

33A Applications of Quantum Mechanics

A particle of mass m moves in three dimensions subject to a potential $V(\mathbf{r})$ localised near the origin. The wavefunction for a scattering process with incident particle of wavevector $\mathbf{k}$ is denoted $\psi(\mathbf{k}, \mathbf{r})$. With reference to the asymptotic form of ψ, define the scattering amplitude $f(\mathbf{k}, \mathbf{k}')$, where $\mathbf{k}'$ is the wavevector of the outgoing particle with $|\mathbf{k}'| = |\mathbf{k}| = k$.

By recasting the Schrödinger equation for $\psi(\mathbf{k}, \mathbf{r})$ as an integral equation, show that

$$f(\mathbf{k}, \mathbf{k}') \;=\; -\frac{m}{2\pi\hbar^2} \int d^3\mathbf{r}' \exp(-i\mathbf{k}' \cdot \mathbf{r}')\, V(\mathbf{r}')\, \psi(\mathbf{k}, \mathbf{r}') \;.$$

[You may assume that

$$\mathcal{G}(k; \mathbf{r}) \;=\; -\frac{1}{4\pi|\mathbf{r}|} \exp(\, ik|\mathbf{r}|\,)$$

is the Green's function for $\nabla^2 + k^2$ which obeys the appropriate boundary conditions for a scattering solution.]

Now suppose $V(\mathbf{r}) = \lambda\, U(\mathbf{r})$, where $\lambda \ll 1$ is a dimensionless constant. Determine the first two non-zero terms in the expansion of $f(\mathbf{k}, \mathbf{k}')$ in powers of λ, giving each term explicitly as an integral over one or more position variables $\mathbf{r}$, $\mathbf{r}'$, ...

Evaluate the contribution to $f(\mathbf{k}, \mathbf{k}')$ of order λ in the case $U(\mathbf{r}) = \delta(\,|\mathbf{r}| - a\,)$, expressing the answer as a function of a, k and the scattering angle θ (defined so that $\mathbf{k} \cdot \mathbf{k}' = k^2 \cos\theta$).

Paper 4, Section II

31A Applications of Quantum Mechanics

Let Λ be a Bravais lattice with basis vectors $\mathbf{a}_1$, $\mathbf{a}_2$, $\mathbf{a}_3$. Define the reciprocal lattice Λ^* and write down basis vectors $\mathbf{b}_1$, $\mathbf{b}_2$, $\mathbf{b}_3$ for Λ^* in terms of the basis for Λ.

A finite crystal consists of identical atoms at sites of Λ given by

$$\boldsymbol{\ell} = n_1\mathbf{a}_1 + n_2\mathbf{a}_2 + n_3\mathbf{a}_3 \qquad \text{with} \qquad 0 \leqslant n_i < N_i \ .$$

A particle of mass m scatters off the crystal; its wavevector is $\mathbf{k}$ before scattering and $\mathbf{k}'$ after scattering, with $|\mathbf{k}| = |\mathbf{k}'|$. Show that the scattering amplitude in the Born approximation has the form

$$-\frac{m}{2\pi\hbar^2}\,\Delta(\mathbf{q})\,\tilde{U}(\mathbf{q}) \ , \qquad \mathbf{q} = \mathbf{k}' - \mathbf{k} \ ,$$

where $U(\mathbf{x})$ is the potential due to a single atom at the origin and $\Delta(\mathbf{q})$ depends on the crystal structure. [You may assume that in the Born approximation the amplitude for scattering off a potential $V(\mathbf{x})$ is $-(m/2\pi\hbar^2)\,\tilde{V}(\mathbf{q})$ where tilde denotes the Fourier transform.]

Derive an expression for $|\,\Delta(\mathbf{q})\,|$ that is valid when $e^{-i\mathbf{q}\cdot\mathbf{a}_i} \neq 1$. Show also that when $\mathbf{q}$ is a reciprocal lattice vector $|\,\Delta(\mathbf{q})\,|$ is equal to the total number of atoms in the crystal. Comment briefly on the significance of these results.

Now suppose that Λ is a face-centred-cubic lattice:

$$\mathbf{a}_1 = \frac{a}{2}(\hat{\mathbf{y}} + \hat{\mathbf{z}}) \ , \quad \mathbf{a}_2 = \frac{a}{2}(\hat{\mathbf{z}} + \hat{\mathbf{x}}) \ , \quad \mathbf{a}_3 = \frac{a}{2}(\hat{\mathbf{x}} + \hat{\mathbf{y}})$$

where a is a constant. Show that for a particle incident with $|\mathbf{k}| > 2\pi/a$, enhanced scattering is possible for at least two values of the scattering angle, θ_1 and θ_2, related by

$$\frac{\sin(\theta_1/2)}{\sin(\theta_2/2)} = \frac{\sqrt{3}}{2} \ .$$

Paper 2, Section II

32A Applications of Quantum Mechanics

A beam of particles of mass m and energy $\hbar^2 k^2/2m$ is incident on a target at the origin described by a spherically symmetric potential $V(r)$. Assuming the potential decays rapidly as $r \to \infty$, write down the asymptotic form of the wavefunction, defining the scattering amplitude $f(\theta)$.

Consider a free particle with energy $\hbar^2 k^2/2m$. State, without proof, the general axisymmetric solution of the Schrödinger equation for $r > 0$ in terms of spherical Bessel and Neumann functions j_ℓ and n_ℓ, and Legendre polynomials P_ℓ ($\ell = 0, 1, 2, \ldots$). Hence define the partial wave phase shifts δ_ℓ for scattering from a potential $V(r)$ and derive the partial wave expansion for $f(\theta)$ in terms of phase shifts.

Now suppose

$$V(r) = \begin{cases} \hbar^2\gamma^2/2m & r < a \\ 0 & r > a \end{cases}$$

with $\gamma > k$. Show that the S-wave phase shift δ_0 obeys

$$\frac{\tanh(\kappa a)}{\kappa a} = \frac{\tan(ka + \delta_0)}{ka}$$

where $\kappa^2 = \gamma^2 - k^2$. Deduce that for an S-wave solution

$$f \to \frac{\tanh \gamma a - \gamma a}{\gamma} \qquad \text{as} \qquad k \to 0\,.$$

[You may assume : $\quad \exp(ikr\cos\theta) = \sum_{\ell=0}^{\infty} (2\ell+1)\, i^\ell\, j_\ell(kr)\, P_\ell(\cos\theta)$

and $\quad j_\ell(\rho) \sim \frac{1}{\rho}\sin(\rho - \ell\pi/2)\,, \quad n_\ell(\rho) \sim -\frac{1}{\rho}\cos(\rho - \ell\pi/2) \quad$ as $\quad \rho \to \infty$.]

Paper 1, Section II

32A Applications of Quantum Mechanics

Define the Rayleigh–Ritz quotient $R[\psi]$ for a normalisable state $|\psi\rangle$ of a quantum system with Hamiltonian H. Given that the spectrum of H is discrete and that there is a unique ground state of energy E_0, show that $R[\psi] \geqslant E_0$ and that equality holds if and only if $|\psi\rangle$ is the ground state.

A simple harmonic oscillator (SHO) is a particle of mass m moving in one dimension subject to the potential

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

Estimate the ground state energy E_0 of the SHO by using the ground state wavefunction for a particle in an infinite potential well of width a, centred on the origin (the potential is $U(x) = 0$ for $|x| < a/2$ and $U(x) = \infty$ for $|x| > a/2$). Take a as the variational parameter.

Perform a similar estimate for the energy E_1 of the first excited state of the SHO by using the first excited state of the infinite potential well as a trial wavefunction.

Is the estimate for E_1 necessarily an upper bound? Justify your answer.

$$\left[\text{You may use :} \quad \int_{-\pi/2}^{\pi/2} y^2 \cos^2 y \, dy \ = \ \frac{\pi}{4}\left(\frac{\pi^2}{6} - 1\right) \quad \text{and} \quad \int_{-\pi}^{\pi} y^2 \sin^2 y \, dy \ = \ \pi\left(\frac{\pi^2}{3} - \frac{1}{2}\right) . \ \right]$$

Paper 3, Section II

32A Applications of Quantum Mechanics

A particle of mass m and energy $E = -\hbar^2\kappa^2/2m < 0$ moves in one dimension subject to a periodic potential

$$V(x) = -\frac{\hbar^2\lambda}{m}\sum_{\ell=-\infty}^{\infty}\delta\left(x-\ell a\right) \qquad \text{with} \qquad \lambda > 0\,.$$

Determine the corresponding Floquet matrix $\mathcal{M}$. [You may assume without proof that for the Schrödinger equation with potential $\alpha\,\delta(x)$ the wavefunction $\psi(x)$ is continuous at $x = 0$ and satisfies $\psi'(0+) - \psi'(0-) = (2m\alpha/\hbar^2)\,\psi(0)$.]

Explain briefly, with reference to Bloch's theorem, how restrictions on the energy of a Bloch state can be derived from $\mathcal{M}$. Deduce that for the potential $V(x)$ above, κ is confined to a range whose boundary values are determined by

$$\tanh\left(\frac{\kappa a}{2}\right) = \frac{\kappa}{\lambda} \qquad \text{and} \qquad \coth\left(\frac{\kappa a}{2}\right) = \frac{\kappa}{\lambda}\,.$$

Sketch the left-hand and right-hand sides of each of these equations as functions of $y = \kappa a/2$. Hence show that there is exactly one allowed band of negative energies with either (i) $E_- \leqslant E < 0$ or (ii) $E_- \leqslant E \leqslant E_+ < 0$ and determine the values of λa for which each of these cases arise. [You should not attempt to evaluate the constants $E_\pm$.]

Comment briefly on the limit $a \to \infty$ with λ fixed.

Paper 4, Section II

33A Applications of Quantum Mechanics

Let Λ be a Bravais lattice in three dimensions. Define the *reciprocal lattice* Λ^*.

State and prove *Bloch's theorem* for a particle moving in a potential $V(\mathbf{x})$ obeying

$$V(\mathbf{x}+\boldsymbol{\ell}) = V(\mathbf{x}) \qquad \forall\, \boldsymbol{\ell} \in \Lambda,\ \mathbf{x} \in \mathbb{R}^3 .$$

Explain what is meant by a *Brillouin zone* for this potential and how it is related to the reciprocal lattice.

A simple cubic lattice Λ_1 is given by the set of points

$$\Lambda_1 \quad = \quad \left\{ \boldsymbol{\ell} \in \mathbb{R}^3 : \boldsymbol{\ell} = n_1 \hat{\mathbf{i}} + n_2 \hat{\mathbf{j}} + n_3 \hat{\mathbf{k}} ,\ n_1, n_2, n_3 \in \mathbb{Z} \right\} ,$$

where $\hat{\mathbf{i}}$, $\hat{\mathbf{j}}$ and $\hat{\mathbf{k}}$ are unit vectors parallel to the Cartesian coordinate axes in $\mathbb{R}^3$. A body-centred cubic (BCC) lattice Λ_{BCC} is obtained by adding to Λ_1 the points at the centre of each cube, i.e. all points of the form

$$\boldsymbol{\ell} + \frac{1}{2}\left(\hat{\mathbf{i}} + \hat{\mathbf{j}} + \hat{\mathbf{k}}\right) , \qquad \boldsymbol{\ell} \in \Lambda_1 .$$

Show that Λ_{BCC} is Bravais with primitive vectors

$$\begin{aligned} \mathbf{a}_1 &= \frac{1}{2}\left(\hat{\mathbf{j}} + \hat{\mathbf{k}} - \hat{\mathbf{i}}\right) , \\ \mathbf{a}_2 &= \frac{1}{2}\left(\hat{\mathbf{k}} + \hat{\mathbf{i}} - \hat{\mathbf{j}}\right) , \\ \mathbf{a}_3 &= \frac{1}{2}\left(\hat{\mathbf{i}} + \hat{\mathbf{j}} - \hat{\mathbf{k}}\right) . \end{aligned}$$

Find the reciprocal lattice Λ^*_{BCC}. Hence find a consistent choice for the first Brillouin zone of a potential $V(\mathbf{x})$ obeying

$$V(\mathbf{x}+\boldsymbol{\ell}) \quad = \quad V(\mathbf{x}) \qquad \forall\, \boldsymbol{\ell} \in \Lambda_{BCC},\ \mathbf{x} \in \mathbb{R}^3 .$$

[*Hint: The matrix* $M = \dfrac{1}{2}\begin{pmatrix} -1 & 1 & 1 \\ 1 & -1 & 1 \\ 1 & 1 & -1 \end{pmatrix}$ *has inverse* $M^{-1} = \begin{pmatrix} 0 & 1 & 1 \\ 1 & 0 & 1 \\ 1 & 1 & 0 \end{pmatrix}$.]

Paper 3, Section II

34A Applications of Quantum Mechanics

In the *nearly-free electron model* a particle of mass m moves in one dimension in a periodic potential of the form $V(x) = \lambda U(x)$, where $\lambda \ll 1$ is a dimensionless coupling and $U(x)$ has a Fourier series

$$U(x) = \sum_{l=-\infty}^{+\infty} U_l \exp\left(\frac{2\pi i}{a} lx\right),$$

with coefficients obeying $U_{-l} = U_l^*$ for all l.

Ignoring any degeneracies in the spectrum, the exact energy $E(k)$ of a Bloch state with wavenumber k can be expanded in powers of λ as

$$E(k) = E_0(k) + \lambda\langle k|U|k\rangle + \lambda^2 \sum_{k'\neq k} \frac{\langle k|U|k'\rangle\langle k'|U|k\rangle}{E_0(k) - E_0(k')} + O(\lambda^3), \tag{1}$$

where $|k\rangle$ is a normalised eigenstate of the free Hamiltonian $\hat{H}_0 = \hat{p}^2/2m$ with momentum $p = \hbar k$ and energy $E_0(k) = \hbar^2 k^2/2m$.

Working on a finite interval of length $L = Na$, where N is a positive integer, we impose periodic boundary conditions on the wavefunction:

$$\psi(x + Na) = \psi(x).$$

What are the allowed values of the wavenumbers k and k' which appear in (1)? For these values evaluate the matrix element $\langle k|U|k'\rangle$.

For what values of k and k' does (1) cease to be a good approximation? Explain your answer. Quoting any results you need from degenerate perturbation theory, calculate to $O(\lambda)$ the location and width of the gaps between allowed energy bands for the periodic potential $V(x)$, in terms of the Fourier coefficients U_l.

Hence work out the allowed energy bands for the following potentials:

$$\text{(i)} \qquad V(x) = 2\lambda \cos\left(\frac{2\pi x}{a}\right),$$

$$\text{(ii)} \qquad V(x) = \lambda a \sum_{n=-\infty}^{+\infty} \delta(x - na).$$

Paper 2, Section II

34A Applications of Quantum Mechanics

(a) A classical particle of mass m scatters on a central potential $V(r)$ with energy E, impact parameter b, and scattering angle θ. Define the corresponding *differential cross-section.*

For particle trajectories in the Coulomb potential,

$$V_C(r) = \frac{e^2}{4\pi\epsilon_0 r}\,,$$

the impact parameter is given by

$$b = \frac{e^2}{8\pi\epsilon_0 E}\cot\left(\frac{\theta}{2}\right).$$

Find the differential cross-section as a function of E and θ.

(b) A quantum particle of mass m and energy $E = \hbar^2 k^2/2m$ scatters in a localised potential $V(\mathbf{r})$. With reference to the asymptotic form of the wavefunction at large $|\mathbf{r}|$, define the *scattering amplitude* $f(\mathbf{k}, \mathbf{k}')$ as a function of the incident and outgoing wavevectors $\mathbf{k}$ and $\mathbf{k}'$ (where $|\mathbf{k}| = |\mathbf{k}'| = k$). Define the differential cross-section for this process and express it in terms of $f(\mathbf{k}, \mathbf{k}')$.

Now consider a potential of the form $V(\mathbf{r}) = \lambda U(\mathbf{r})$, where $\lambda \ll 1$ is a dimensionless coupling and U does not depend on λ. You may assume that the Schrödinger equation for the wavefunction $\psi(\mathbf{k};\mathbf{r})$ of a scattering state with incident wavevector $\mathbf{k}$ may be written as the integral equation

$$\psi(\mathbf{k};\mathbf{r}) = \exp\left(i\mathbf{k}\cdot\mathbf{r}\right) \;+\; \frac{2m\lambda}{\hbar^2}\int d^3r'\,\mathcal{G}_0^{(+)}\left(k;\mathbf{r}-\mathbf{r}'\right)\,U(\mathbf{r}')\,\psi(\mathbf{k};\mathbf{r}')\,,$$

where

$$\mathcal{G}_0^{(+)}(k;\mathbf{r}) = -\frac{1}{4\pi}\frac{\exp\left(ik|\mathbf{r}|\right)}{|\mathbf{r}|}\,.$$

Show that the corresponding scattering amplitude is given by

$$f(\mathbf{k},\mathbf{k}') = -\frac{m\lambda}{2\pi\hbar^2}\int d^3r'\,\exp\left(-i\mathbf{k}'\cdot\mathbf{r}'\right)\,U(\mathbf{r}')\,\psi(\mathbf{k};\mathbf{r}')\,.$$

By expanding the wavefunction in powers of λ and keeping only the leading term, calculate the leading-order contribution to the differential cross-section, and evaluate it for the case of the Yukawa potential

$$V(\mathbf{r}) = \lambda\frac{\exp(-\mu r)}{r}\,.$$

By taking a suitable limit, obtain the differential cross-section for quantum scattering in the Coulomb potential $V_C(r)$ defined in Part (a) above, correct to leading order in an expansion in powers of the constant $\tilde{\alpha} = e^2/4\pi\epsilon_0$. Express your answer as a function of the particle energy E and scattering angle θ, and compare it to the corresponding classical cross-section calculated in Part (a).

Paper 1, Section II

34A Applications of Quantum Mechanics

A particle of mass m scatters on a localised potential well $V(x)$ in one dimension. With reference to the asymptotic behaviour of the wavefunction as $x \to \pm\infty$, define the *reflection* and *transmission amplitudes*, r and t, for a right-moving incident particle of wave number k. Define also the corresponding amplitudes, r' and t', for a left-moving incident particle of wave number k. Derive expressions for r' and t' in terms of r and t.

(a) Define the *S-matrix*, giving its elements in terms of r and t. Using the relation

$$|r|^2 + |t|^2 = 1$$

(which you need not derive), show that the S-matrix is unitary. How does the S-matrix simplify if the potential well satisfies $V(-x) = V(x)$?

(b) Consider the potential well

$$V(x) = -\frac{3\hbar^2}{m}\frac{1}{\cosh^2(x)}\,.$$

The corresponding Schrödinger equation has an exact solution

$$\psi_k(x) = \exp(ikx)\,\left[3\tanh^2(x) - 3ik\tanh(x) - (1+k^2)\right]\,,$$

with energy $E = \hbar^2k^2/2m$, for every real value of k. [You do not need to verify this.] Find the S-matrix for scattering on this potential. What special feature does the scattering have in this case?

(c) Explain the connection between singularities of the S-matrix and bound states of the potential well. By analytic continuation of the solution $\psi_k(x)$ to appropriate complex values of k, find the wavefunctions and energies of the bound states of the well. [You do not need to normalise the wavefunctions.]

Paper 4, Section II

33D Applications of Quantum Mechanics

Define the *Floquet matrix* for a particle moving in a periodic potential in one dimension and explain how it determines the allowed energy bands of the system.

A potential barrier in one dimension has the form

$$V(x) = \begin{cases} V_0(x)\,, & |x| < a/4\,, \\ 0\,, & |x| > a/4\,, \end{cases}$$

where $V_0(x)$ is a smooth, positive function of x. The reflection and transmission amplitudes for a particle of wavenumber $k > 0$, incident from the left, are $r(k)$ and $t(k)$ respectively. For a particle of wavenumber $-k$, incident from the right, the corresponding amplitudes are $r'(k)$ and $t'(k) = t(k)$. In the following, for brevity, we will suppress the k-dependence of these quantities.

Consider the periodic potential $\widetilde{V}$, defined by $\widetilde{V}(x) = V(x)$ for $|x| < a/2$ and by $\widetilde{V}(x + a) = \widetilde{V}(x)$ elsewhere. Write down two linearly independent solutions of the corresponding Schrödinger equation in the region $-3a/4 < x < -a/4$. Using the scattering data given above, extend these solutions to the region $a/4 < x < 3a/4$. Hence find the Floquet matrix of the system in terms of the amplitudes r, r' and t defined above.

Show that the edges of the allowed energy bands for this potential lie at $E = \hbar^2 k^2/2m$, where

$$ka \;=\; i \log\left(t \pm \sqrt{rr'}\right)\,.$$

Paper 3, Section II

34D Applications of Quantum Mechanics

Write down the classical Hamiltonian for a particle of mass m, electric charge $-e$ and momentum $\mathbf{p}$ moving in the background of an electromagnetic field with vector and scalar potentials $\mathbf{A}(\mathbf{x},t)$ and $\phi(\mathbf{x},t)$.

Consider the case of a constant uniform magnetic field, $\mathbf{B}=(0,0,B)$ and $\mathbf{E}=0$. Working in the gauge with $\mathbf{A}=(-By,0,0)$ and $\phi=0$, show that Hamilton's equations,

$$\dot{\mathbf{x}} = \frac{\partial H}{\partial \mathbf{p}}\,, \qquad \dot{\mathbf{p}} = -\frac{\partial H}{\partial \mathbf{x}}\,,$$

admit solutions corresponding to circular motion in the x-y plane with angular frequency $\omega_B = eB/m$.

Show that, in the same gauge, the coordinates $(x_0,y_0,0)$ of the centre of the circle are related to the instantaneous position $\mathbf{x}=(x,y,z)$ and momentum $\mathbf{p}=(p_x,p_y,p_z)$ of the particle by

$$x_0 = x - \frac{p_y}{eB}\,, \qquad y_0 = \frac{p_x}{eB}\,. \tag{1}$$

Write down the quantum Hamiltonian $\hat{H}$ for the system. In the case of a uniform constant magnetic field discussed above, find the allowed energy levels. Working in the gauge specified above, write down quantum operators corresponding to the classical quantities x_0 and y_0 defined in (1) above and show that they are conserved.

[In this question you may use without derivation any facts relating to the energy spectrum of the quantum harmonic oscillator provided they are stated clearly.]

Paper 2, Section II

34D Applications of Quantum Mechanics

(i) A particle of momentum $\hbar k$ and energy $E = \hbar^2 k^2/2m$ scatters off a spherically-symmetric target in three dimensions. Define the corresponding *scattering amplitude* f as a function of the scattering angle θ. Expand the scattering amplitude in partial waves of definite angular momentum l, and determine the coefficients of this expansion in terms of the phase shifts $\delta_l(k)$ appearing in the following asymptotic form of the wavefunction, valid at large distance from the target,

$$\psi(\mathbf{r}) \quad \sim \quad \sum_{l=0}^{\infty} \frac{2l+1}{2ik} \left[e^{2i\delta_l} \frac{e^{ikr}}{r} \; - \; (-1)^l \, \frac{e^{-ikr}}{r} \right] P_l(\cos\theta)\,.$$

Here, $r = |\mathbf{r}|$ is the distance from the target and P_l are the Legendre polynomials.

[You may use without derivation the following approximate relation between plane and spherical waves (valid asymptotically for large r):

$$\exp(ikz) \quad \sim \quad \sum_{l=0}^{\infty} (2l+1)\, i^l \, \frac{\sin\left(kr - \frac{1}{2} l\pi\right)}{kr} \, P_l(\cos\theta)\,.$$

]

(ii) Suppose that the potential energy takes the form $V(r) = \lambda\, U(r)$ where $\lambda \ll 1$ is a dimensionless coupling. By expanding the wavefunction in a power series in λ, derive the *Born Approximation* to the scattering amplitude in the form

$$f(\theta) \quad = \quad -\frac{2m\lambda}{\hbar^2} \int_0^{\infty} U(r)\, \frac{\sin qr}{q}\, r dr\,,$$

up to corrections of order λ^2, where $q = 2k\sin(\theta/2)$. [You may quote any results you need for the Green's function for the differential operator $\nabla^2 + k^2$ provided they are stated clearly.]

(iii) Derive the corresponding order λ contribution to the phase shift $\delta_l(k)$ of angular momentum l.

[You may use the orthogonality relations

$$\int_{-1}^{+1} P_l(w) P_m(w)\, dw \quad = \quad \frac{2}{(2l+1)}\, \delta_{lm}$$

and the integral formula

$$\int_0^1 P_l\left(1 - 2x^2\right) \sin(ax)\, dx \quad = \quad \frac{a}{2} \left[j_l\left(\frac{a}{2}\right)\right]^2\,,$$

where $j_l(z)$ is a spherical Bessel function.]

Paper 1, Section II

34D Applications of Quantum Mechanics

Consider a quantum system with Hamiltonian $\widehat{H}$ and energy levels

$$E_0 < E_1 < E_2 < \dots .$$

For any state $|\psi\rangle$ define the *Rayleigh–Ritz quotient* $R[\psi]$ and show the following:

(i) the ground state energy E_0 is the minimum value of $R[\psi]$;

(ii) all energy eigenstates are stationary points of $R[\psi]$ with respect to variations of $|\psi\rangle$.

Under what conditions can the value of $R[\psi_\alpha]$ for a trial wavefunction ψ_α (depending on some parameter α) be used as an estimate of the energy E_1 of the first excited state? Explain your answer.

For a suitably chosen trial wavefunction which is the product of a polynomial and a Gaussian, use the Rayleigh–Ritz quotient to estimate E_1 for a particle of mass m moving in a potential $V(x) = g|x|$, where g is a constant.

[You may use the integral formulae,

$$\begin{aligned}\int_0^\infty x^{2n} \exp\left(-px^2\right) dx &= \frac{(2n-1)!!}{2(2p)^n}\sqrt{\frac{\pi}{p}} \\ \int_0^\infty x^{2n+1} \exp\left(-px^2\right) dx &= \frac{n!}{2p^{n+1}}\end{aligned}$$

where n is a non-negative integer and p is a constant.]

Paper 4, Section II
33E Applications of Quantum Mechanics
Consider a one-dimensional crystal lattice of lattice spacing a with the n-th atom having position $r_n = na + x_n$ and momentum p_n, for $n = 0, 1, \ldots, N-1$. The atoms interact with their nearest neighbours with a harmonic force and the classical Hamiltonian is

$$H = \sum_n \frac{p_n^2}{2m} + \frac{1}{2}\lambda(x_n - x_{n-1})^2 ,$$

where we impose periodic boundary conditions: $x_N = x_0$. Show that the normal mode frequencies for the classical harmonic vibrations of the system are given by

$$\omega_l = 2\sqrt{\frac{\lambda}{m}} \left| \sin\left(\frac{k_l a}{2}\right) \right| ,$$

where $k_l = 2\pi l/Na$, with l integer and (for N even, which you may assume) $-N/2 < l \leqslant N/2$. What is the velocity of sound in this crystal?

Show how the system may be quantized to give the quantum operator

$$x_n(t) = X_0(t) + \sum_{l \neq 0} \sqrt{\frac{\hbar}{2Nm\omega_l}} \left[a_l e^{-i(\omega_l t - k_l na)} + a_l^\dagger e^{i(\omega_l t - k_l na)} \right] ,$$

where $a_l^\dagger$ and a_l are creation and annihilation operators, respectively, whose commutation relations should be stated. Briefly describe the spectrum of energy eigenstates for this system, stating the definition of the ground state $|0\rangle$ and giving the expression for the energy eigenvalue of any eigenstate.

The Debye–Waller factor $e^{-W(Q)}$ associated with Bragg scattering from this crystal is defined by the matrix element

$$e^{-W(Q)} = \langle 0 | e^{iQx_0(0)} | 0 \rangle .$$

In the case where $\langle 0 | X_0 | 0 \rangle = 0$, calculate $W(Q)$.

Paper 3, Section II

34E Applications of Quantum Mechanics

A simple model of a crystal consists of a 1D linear array of sites at positions $x = na$, for all integer n and separation a, each occupied by a similar atom. The potential due to the atom at the origin is $U(x)$, which is symmetric: $U(-x) = U(x)$. The Hamiltonian, H_0, for the atom at the n-th site in isolation has electron eigenfunction $\psi_n(x)$ with energy E_0. Write down H_0 and state the relationship between $\psi_n(x)$ and $\psi_0(x)$.

The Hamiltonian H for an electron moving in the crystal is $H = H_0 + V(x)$. Give an expression for $V(x)$.

In the tight-binding approximation for this model the ψ_n are assumed to be orthonormal, $(\psi_n, \psi_m) = \delta_{nm}$, and the only non-zero matrix elements of H_0 and V are

$$(\psi_n, H_0\psi_n) = E_0, \quad (\psi_n, V\psi_n) = \alpha, \quad (\psi_n, V\psi_{n\pm1}) = -A\,,$$

where $A > 0$. By considering the trial wavefunction $\Psi(x,t) = \sum_n c_n(t)\psi_n(x)$, show that the time-dependent Schrödinger equation governing the amplitudes $c_n(t)$ is

$$i\hbar\dot{c}_n = (E_0 + \alpha)c_n - A(c_{n+1} + c_{n-1})\,.$$

By examining a solution of the form

$$c_n = e^{i(kna - Et/\hbar)}\,,$$

show that E, the energy of the electron in the crystal, lies in a band given by

$$E = E_0 + \alpha - 2A\cos ka\,.$$

Using the fact that $\psi_0(x)$ is a parity eigenstate show that

$$(\psi_n, x\psi_n) = na\,.$$

The electron in this model is now subject to an electric field $\mathcal{E}$ in the direction of increasing x, so that $V(x)$ is replaced by $V(x) - e\mathcal{E}x$, where $-e$ is the charge on the electron. Assuming that $(\psi_n, x\psi_m) = 0,\ n \neq m$, write down the new form of the time-dependent Schrödinger equation for the probability amplitudes c_n. Verify that it has solutions of the form

$$c_n = \exp\left[-\frac{i}{\hbar}\int_0^t \epsilon(t')dt' + i\left(k + \frac{e\mathcal{E}t}{\hbar}\right)na\right]\,,$$

where

$$\epsilon(t) = E_0 + \alpha - 2A\cos\left[\left(k + \frac{e\mathcal{E}t}{\hbar}\right)a\right]\,.$$

Use this result to show that the dynamical behaviour of an electron near the bottom of an energy band is the same as that for a free particle in the presence of an electric field with an effective mass $m^* = \hbar^2/(2Aa^2)$.

Paper 2, Section II

34E Applications of Quantum Mechanics

A solution of the S-wave Schrödinger equation at large distances for a particle of mass m with momentum $\hbar k$ and energy $E = \hbar^2 k^2/2m$, has the form

$$\psi_0(\boldsymbol{r}) \;\sim\; \frac{A}{r}\left[\sin kr + g(k)\cos kr\right] \;.$$

Define the phase shift δ_0 and verify that $\tan\delta_0(k) = g(k)$.

Write down a formula for the cross-section σ, for a particle of momentum $\hbar k$ scattering on a radially symmetric potential of finite range, as a function of the phase shifts δ_l for the partial waves with quantum number l.

(i) Suppose that $g(k) = -k/K$ for $K > 0$. Show that there is a bound state of energy $E_B = -\hbar^2 K^2/2m$. Neglecting the contribution from partial waves with $l > 0$ show that the cross section is

$$\sigma \;=\; \frac{4\pi}{K^2 + k^2} \;.$$

(ii) Suppose now that $g(k) = \gamma/(K_0 - k)$ with $K_0 > 0$, $\gamma > 0$ and $\gamma \ll K_0$. Neglecting the contribution from partial waves with $l > 0$, derive an expression for the cross section σ, and show that it has a local maximum when $E \approx \hbar^2 K_0^2/2m$. Discuss the interpretation of this phenomenon in terms of resonant behaviour and derive an expression for the decay width of the resonant state.

Paper 1, Section II

34E Applications of Quantum Mechanics

Give an account of the variational principle for establishing an upper bound on the ground-state energy E_0 of a particle moving in a potential $V(x)$ in one dimension.

A particle of unit mass moves in the potential

$$V(x) = \begin{cases} \infty & x \leqslant 0 \\ \lambda x & x > 0 \end{cases},$$

with λ a positive constant. Explain why it is important that any trial wavefunction used to derive an upper bound on E_0 should be chosen to vanish for $x \leqslant 0$.

Use the trial wavefunction

$$\psi(x) = \begin{cases} 0 & x \leqslant 0 \\ xe^{-ax} & x > 0 \end{cases},$$

where a is a positive real parameter, to establish an upper bound $E_0 \leqslant E(a, \lambda)$ for the energy of the ground state, and hence derive the lowest upper bound on E_0 as a function of λ.

Explain why the variational method cannot be used in this case to derive an upper bound for the energy of the first excited state.

Paper 1, Section II

34E Applications of Quantum Mechanics

In one dimension a particle of mass m and momentum $\hbar k$, $k > 0$, is scattered by a potential $V(x)$ where $V(x) \to 0$ as $|x| \to \infty$. Incoming and outgoing plane waves of positive (+) and negative (−) parity are given, respectively, by

$$I_+(k,x) = e^{-ik|x|}\,, \qquad I_-(k,x) = \mathrm{sgn}(x)e^{-ik|x|}\,,$$
$$O_+(k,x) = e^{ik|x|}\,, \qquad O_-(k,x) = -\mathrm{sgn}(x)e^{ik|x|}\,.$$

The scattering solutions to the time-independent Schrödinger equation with positive and negative parity incoming waves are $\psi_+(x)$ and $\psi_-(x)$, respectively. State how the asymptotic behaviour of ψ_+ and ψ_- can be expressed in terms of I_+, I_-, O_+, O_- and the S-matrix denoted by

$$\boldsymbol{S} = \begin{pmatrix} S_{++} & S_{+-} \\ S_{-+} & S_{--} \end{pmatrix}\,.$$

In the case where $V(x) = V(-x)$ explain briefly why you expect $S_{+-} = S_{-+} = 0$.

The potential $V(x)$ is given by

$$V(x) = V_0[\delta(x-a) + \delta(x+a)]\,,$$

where V_0 is a constant. In this case, show that

$$S_{--}(k) = e^{-2ika}\left[\frac{(2k - iU_0)e^{ika} + iU_0e^{-ika}}{(2k + iU_0)e^{-ika} - iU_0e^{ika}}\right]\,,$$

where $U_0 = 2mV_0/\hbar^2$. Verify that $|S_{--}|^2 = 1$ and explain briefly the physical meaning of this result.

For $V_0 < 0$, by considering the poles or zeros of $S_{--}(k)$ show that there exists one bound state of negative parity in this potential if $U_0 a < -1$.

For $V_0 > 0$ and $U_0 a \gg 1$, show that $S_{--}(k)$ has a pole at

$$ka = \pi + \alpha - i\gamma$$

where, to leading order in $1/(U_0 a)$,

$$\alpha = -\frac{\pi}{U_0 a}\,, \qquad \gamma = \left(\frac{\pi}{U_0 a}\right)^2\,.$$

Explain briefy the physical meaning of this result, and why you expect that $\gamma > 0$.

Paper 2, Section II

34E Applications of Quantum Mechanics

A beam of particles of mass m and momentum $p = \hbar k$, incident along the z-axis, is scattered by a spherically symmetric potential $V(r)$, where $V(r) = 0$ for large r. State the boundary conditions on the wavefunction as $r \to \infty$ and hence define the scattering amplitude $f(\theta)$, where θ is the scattering angle.

Given that, for large r,

$$e^{ikr\cos\theta} = \frac{1}{2ikr}\sum_{l=0}^{\infty}(2l+1)\left(e^{ikr} - (-1)^l e^{-ikr}\right)P_l(\cos\theta)\,,$$

explain how the partial-wave expansion can be used to define the phase shifts $\delta_l(k)$ ($l = 0, 1, 2, \ldots$). Furthermore, given that $d\sigma/d\Omega = |f(\theta)|^2$, derive expressions for $f(\theta)$ and the total cross-section σ in terms of the δ_l.

In a particular case $V(r)$ is given by

$$V(r) = \begin{cases} \infty\,, & r < a\,, \\ -V_0\,, & a < r < 2a\,, \\ 0\,, & r > 2a\,, \end{cases}$$

where $V_0 > 0$. Show that the S-wave phase shift δ_0 satisfies

$$\tan(\delta_0) = \frac{k\cos(2ka) - \kappa\cot(\kappa a)\sin(2ka)}{k\sin(2ka) + \kappa\cot(\kappa a)\cos(2ka)}\,,$$

where $\kappa^2 = 2mV_0/\hbar^2 + k^2$.

Derive an expression for the scattering length a_s in terms of κ. Find the values of κ for which $|a_s|$ diverges and briefly explain their physical significance.

Paper 3, Section II

34E Applications of Quantum Mechanics

An electron of mass m moves in a D-dimensional periodic potential that satisfies the periodicity condition

$$V(\boldsymbol{r} + \boldsymbol{l}) = V(\boldsymbol{r}) \quad \forall\, \boldsymbol{l} \in \Lambda\,,$$

where Λ is a D-dimensional Bravais lattice. State Bloch's theorem for the energy eigenfunctions of the electron.

For a one-dimensional potential $V(x)$ such that $V(x+a) = V(x)$, give a full account of how the "nearly free electron model" leads to a band structure for the energy levels.

Explain briefly the idea of a Fermi surface and its rôle in explaining the existence of conductors and insulators.

Paper 4, Section II

33E Applications of Quantum Mechanics

A particle of charge $-e$ and mass m moves in a magnetic field $\boldsymbol{B}(\boldsymbol{x},t)$ and in an electric potential $\phi(\boldsymbol{x},t)$. The time-dependent Schrödinger equation for the particle's wavefunction $\Psi(\boldsymbol{x},t)$ is

$$i\hbar\left(\frac{\partial}{\partial t}-\frac{ie}{\hbar}\phi\right)\Psi=-\frac{\hbar^2}{2m}\left(\boldsymbol{\nabla}+\frac{ie}{\hbar}\boldsymbol{A}\right)^2\Psi\,,$$

where $\boldsymbol{A}$ is the vector potential with $\boldsymbol{B}=\boldsymbol{\nabla}\wedge\boldsymbol{A}$. Show that this equation is invariant under the gauge transformations

$$\begin{aligned}\boldsymbol{A}(\boldsymbol{x},t) &\rightarrow \boldsymbol{A}(\boldsymbol{x},t)+\boldsymbol{\nabla}f(\boldsymbol{x},t)\,,\\ \phi(\boldsymbol{x},t) &\rightarrow \phi(\boldsymbol{x},t)-\tfrac{\partial}{\partial t}f(\boldsymbol{x},t)\,,\end{aligned}$$

where f is an arbitrary function, together with a suitable transformation for Ψ which should be stated.

Assume now that $\partial\Psi/\partial z=0$, so that the particle motion is only in the x and y directions. Let $\boldsymbol{B}$ be the constant field $\boldsymbol{B}=(0,0,B)$ and let $\phi=0$. In the gauge where $\boldsymbol{A}=(-By,0,0)$ show that the stationary states are given by

$$\Psi_k(\boldsymbol{x},t)=\psi_k(\boldsymbol{x})e^{-iEt/\hbar}\,,$$

with

$$\psi_k(\boldsymbol{x})=e^{ikx}\chi_k(y)\,. \qquad (*)$$

Show that $\chi_k(y)$ is the wavefunction for a simple one-dimensional harmonic oscillator centred at position $y_0=\hbar k/eB$. Deduce that the stationary states lie in infinitely degenerate levels (Landau levels) labelled by the integer $n\geqslant 0$, with energy

$$E_n=(2n+1)\frac{\hbar eB}{2m}\,.$$

A uniform electric field $\mathcal{E}$ is applied in the y-direction so that $\phi=-\mathcal{E}y$. Show that the stationary states are given by $(*)$, where $\chi_k(y)$ is a harmonic oscillator wavefunction centred now at

$$y_0=\frac{1}{eB}\left(\hbar k-m\frac{\mathcal{E}}{B}\right)\,.$$

Show also that the eigen-energies are given by

$$E_{n,k}=(2n+1)\frac{\hbar eB}{2m}+e\mathcal{E}y_0+\frac{m\mathcal{E}^2}{2B^2}\,.$$

Why does this mean that the Landau energy levels are no longer degenerate in two dimensions?

Paper 1, Section II

34B Applications of Quantum Mechanics

Give an account of the variational principle for establishing an upper bound on the ground-state energy, E_0, of a particle moving in a potential $V(x)$ in one dimension.

Explain how an upper bound on the energy of the first excited state can be found in the case that $V(x)$ is a symmetric function.

A particle of mass $2m = \hbar^2$ moves in the potential

$$V(x) = -V_0\, e^{-x^2}, \qquad V_0 > 0\,.$$

Use the trial wavefunction

$$\psi(x) = e^{-\frac{1}{2}ax^2},$$

where a is a positive real parameter, to establish the upper bound $E_0 \leqslant E(a)$ for the energy of the ground state, where

$$E(a) = \frac{1}{2}a - V_0 \frac{\sqrt{a}}{\sqrt{1+a}}\,.$$

Show that, for $a > 0$, $E(a)$ has one zero and find its position.

Show that the turning points of $E(a)$ are given by

$$(1+a)^3 = \frac{V_0^2}{a}\,,$$

and deduce that there is one turning point in $a > 0$ for all $V_0 > 0$.

Sketch $E(a)$ for $a > 0$ and hence deduce that $V(x)$ has at least one bound state for all $V_0 > 0$.

For $0 < V_0 \ll 1$ show that

$$-V_0 < E_0 \leqslant \epsilon(V_0)\,,$$

where $\epsilon(V_0) = -\frac{1}{2}V_0^{\,2} + \mathrm{O}(V_0^{\,4})$.

[You may use the result that $\int_{-\infty}^{\infty} e^{-bx^2}\,dx = \sqrt{\frac{\pi}{b}}$ for $b > 0$.]

Paper 2, Section II

34B Applications of Quantum Mechanics

A beam of particles of mass m and momentum $p = \hbar k$ is incident along the z-axis. Write down the asymptotic form of the wave function which describes scattering under the influence of a spherically symmetric potential $V(r)$ and which defines the scattering amplitude $f(\theta)$.

Given that, for large r,

$$e^{ikr\cos\theta} \sim \frac{1}{2ikr}\sum_{l=0}^{\infty}(2l+1)\left(e^{ikr} - (-1)^l\, e^{-ikr}\right) P_l(\cos\theta)\,,$$

show how to derive the partial-wave expansion of the scattering amplitude in the form

$$f(\theta) = \frac{1}{k}\sum_{l=0}^{\infty}(2l+1)\, e^{i\delta_l}\sin\delta_l\, P_l(\cos\theta)\,.$$

Obtain an expression for the total cross-section, σ.

Let $V(r)$ have the form

$$V(r) = \begin{cases} -V_0\,, & r < a\,, \\ 0\,, & r > a\,, \end{cases}$$

where $V_0 = \dfrac{\hbar^2}{2m}\gamma^2$.

Show that the $l = 0$ phase-shift δ_0 satisfies

$$\frac{\tan(ka + \delta_0)}{ka} = \frac{\tan\kappa a}{\kappa a}\,,$$

where $\kappa^2 = k^2 + \gamma^2$.

Assume γ to be large compared with k so that κ may be approximated by γ. Show, using graphical methods or otherwise, that there are values for k for which $\delta_0(k) = n\pi$ for some integer n, which should not be calculated. Show that the smallest value, k_0, of k for which this condition holds certainly satisfies $k_0 < 3\pi/2a$.

Paper 3, Section II

34B Applications of Quantum Mechanics

State Bloch's theorem for a one dimensional lattice which is invariant under translations by a.

A simple model of a crystal consists of a one-dimensional linear array of identical sites with separation a. At the nth site the Hamiltonian, neglecting all other sites, is H_n and an electron may occupy either of two states, $\phi_n(x)$ and $\chi_n(x)$, where

$$H_n\,\phi_n(x) \;=\; E_0\,\phi_n(x)\,, \qquad\qquad H_n\,\chi_n(x) \;=\; E_1\,\chi_n(x)\,,$$

and ϕ_n and χ_n are orthonormal. How are $\phi_n(x)$ and $\chi_n(x)$ related to $\phi_0(x)$ and $\chi_0(x)$?

The full Hamiltonian is H and is invariant under translations by a. Write trial wavefunctions $\psi(x)$ for the eigenstates of this model appropriate to a tight binding approximation if the electron has probability amplitudes b_n and c_n to be in the states ϕ_n and χ_n respectively.

Assume that the only non-zero matrix elements in this model are, for all n,

$$(\phi_n, H_n\,\phi_n) \;=\; E_0\,, \qquad\qquad (\chi_n, H_n\,\chi_n) \;=\; E_1\,,$$

$$(\phi_n, V\phi_{n\pm1}) \;=\; (\chi_n, V\,\chi_{n\pm1}) \;=\; (\phi_n, V\,\chi_{n\pm1}) \;=\; (\chi_n, V\phi_{n\pm1}) \;=\; -A\,,$$

where $H = H_n + V$ and $A > 0$. Show that the time-dependent Schrödinger equation governing the amplitudes becomes

$$i\hbar\,\dot{b}_n \;=\; E_0\,b_n - A(b_{n+1} + b_{n-1} + c_{n+1} + c_{n-1})\,,$$

$$i\hbar\,\dot{c}_n \;=\; E_1\,c_n - A(c_{n+1} + c_{n-1} + b_{n+1} + b_{n-1})\,.$$

By examining solutions of the form

$$\begin{pmatrix} b_n \\ c_n \end{pmatrix} = \begin{pmatrix} B \\ C \end{pmatrix} e^{\,i(kna - Et/\hbar)}\,,$$

show that the allowed energies of the electron are two bands given by

$$E \;=\; \frac{1}{2}\,(E_0 + E_1 - 4\,A\cos ka) \pm \frac{1}{2}\,\sqrt{(E_0 - E_1)^2 + 16\,A^2\cos^2 ka}\,.$$

Define the *Brillouin zone* for this system and find the energies at the top and bottom of both bands. Hence, show that the energy gap between the bands is

$$\Delta E \;=\; -4\,A + \sqrt{(E_1 - E_0)^2 + 16\,A^2}\,.$$

Show that the wavefunctions $\psi(x)$ satisfy Bloch's theorem.

Describe briefly what are the crucial differences between insulators, conductors and semiconductors.

Paper 4, Section II

33B Applications of Quantum Mechanics

The scattering amplitude for electrons of momentum $\hbar\mathbf{k}$ incident on an atom located at the origin is $f(\hat{\mathbf{r}})$ where $\hat{\mathbf{r}} = \mathbf{r}/r$. Explain why, if the atom is displaced by a position vector $\mathbf{a}$, the asymptotic form of the scattering wave function becomes

$$\psi_{\mathbf{k}}(\mathbf{r}) \sim e^{i\mathbf{k}\cdot\mathbf{r}} + e^{i\mathbf{k}\cdot\mathbf{a}} \frac{e^{ikr'}}{r'} f(\hat{\mathbf{r}}') \sim e^{i\mathbf{k}\cdot\mathbf{r}} + e^{i(\mathbf{k}-\mathbf{k}')\cdot\mathbf{a}} \frac{e^{ikr}}{r} f(\hat{\mathbf{r}}),$$

where $\mathbf{r}' = \mathbf{r} - \mathbf{a}$, $r' = |\mathbf{r}'|$, $\hat{\mathbf{r}}' = \mathbf{r}'/r'$ and $k = |\mathbf{k}|$, $\mathbf{k}' = k\hat{\mathbf{r}}$. For electrons incident on N atoms in a regular Bravais crystal lattice show that the differential cross-section for scattering in the direction $\hat{\mathbf{r}}$ is

$$\frac{d\sigma}{d\Omega} = N\,|f(\hat{\mathbf{r}})|^2\,\Delta(\mathbf{k}-\mathbf{k}')\,.$$

Derive an explicit form for $\Delta(\mathbf{Q})$ and show that it is strongly peaked when $\mathbf{Q} \approx \mathbf{b}$ for $\mathbf{b}$ a reciprocal lattice vector.

State the Born approximation for $f(\hat{\mathbf{r}})$ when the scattering is due to a potential $V(\mathbf{r})$. Calculate the Born approximation for the case $V(\mathbf{r}) = -a\,\delta(\mathbf{r})$.

Electrons with de Broglie wavelength λ are incident on a target composed of many randomly oriented small crystals. They are found to be scattered strongly through an angle of $60°$. What is the likely distance between planes of atoms in the crystal responsible for the scattering?

Paper 1, Section II

34D Applications of Quantum Mechanics

Consider the scaled one-dimensional Schrödinger equation with a potential $V(x)$ such that there is a complete set of real, normalized bound states $\psi_n(x)$, $n = 0, 1, 2, \ldots$, with discrete energies $E_0 < E_1 < E_2 < \ldots$, satisfying

$$-\frac{d^2\psi_n}{dx^2} + V(x)\psi_n = E_n\psi_n.$$

Show that the quantity

$$\langle E\rangle = \int_{-\infty}^{\infty} \left(\left(\frac{d\psi}{dx}\right)^2 + V(x)\psi^2 \right) dx,$$

where $\psi(x)$ is a real, normalized trial function depending on one or more parameters α, can be used to estimate E_0, and show that $\langle E\rangle \geqslant E_0$.

Let the potential be $V(x) = |x|$. Using a suitable one-parameter family of either Gaussian or piecewise polynomial trial functions, find a good estimate for E_0 in this case.

How could you obtain a good estimate for E_1? [You should suggest suitable trial functions, but DO NOT carry out any further integration.]

Paper 2, Section II

34D Applications of Quantum Mechanics

A particle scatters quantum mechanically off a spherically symmetric potential $V(r)$. In the $l = 0$ sector, and assuming $\hbar^2/2m = 1$, the radial wavefunction $u(r)$ satisfies

$$-\frac{d^2u}{dr^2} + V(r)u = k^2 u,$$

and $u(0) = 0$. The asymptotic behaviour of u, for large r, is

$$u(r) \sim C\left(S(k)e^{ikr} - e^{-ikr}\right),$$

where C is a constant. Show that if $S(k)$ is analytically continued to complex k, then

$$S(k)S(-k) = 1 \quad \text{and} \quad S(k)^* S(k^*) = 1.$$

Deduce that for real k, $S(k) = e^{2i\delta_0(k)}$ for some real function $\delta_0(k)$, and that $\delta_0(k) = -\delta_0(-k)$.

For a certain potential,

$$S(k) = \frac{(k + i\lambda)(k + 3i\lambda)}{(k - i\lambda)(k - 3i\lambda)},$$

where λ is a real, positive constant. Evaluate the scattering length a and the total cross section $4\pi a^2$.

Briefly explain the significance of the zeros of $S(k)$.

Paper 3, Section II

34D Applications of Quantum Mechanics

An electron of charge $-e$ and mass m is subject to a magnetic field of the form $\mathbf{B} = (0, 0, B(y))$, where $B(y)$ is everywhere greater than some positive constant B_0. In a stationary state of energy E, the electron's wavefunction Ψ satisfies

$$-\frac{\hbar^2}{2m}\left(\boldsymbol{\nabla} + \frac{ie}{\hbar}\mathbf{A}\right)^2 \Psi + \frac{e\hbar}{2m}\mathbf{B}\cdot\boldsymbol{\sigma}\Psi = E\Psi, \qquad (*)$$

where $\mathbf{A}$ is the vector potential and σ_1, σ_2 and σ_3 are the Pauli matrices.

Assume that the electron is in a spin down state and has no momentum along the z-axis. Show that with a suitable choice of gauge, and after separating variables, equation $(*)$ can be reduced to

$$-\frac{d^2\chi}{dy^2} + (k + a(y))^2\chi - b(y)\chi = \epsilon\chi, \qquad (**)$$

where χ depends only on y, ϵ is a rescaled energy, and $b(y)$ a rescaled magnetic field strength. What is the relationship between $a(y)$ and $b(y)$?

Show that $(**)$ can be factorized in the form $M^\dagger M\chi = \epsilon\chi$ where

$$M = \frac{d}{dy} + W(y)$$

for some function $W(y)$, and deduce that ϵ is non-negative.

Show that zero energy states exist for all k and are therefore infinitely degenerate.

Paper 4, Section II

33D Applications of Quantum Mechanics

What are meant by Bloch states and the Brillouin zone for a quantum mechanical particle moving in a one-dimensional periodic potential?

Derive an approximate value for the lowest-lying energy gap for the Schrödinger equation

$$-\frac{d^2\psi}{dx^2} - V_0(\cos x + \cos 2x)\psi = E\psi$$

when V_0 is small and positive.

Estimate the width of this gap in the case that V_0 is large and positive.

1/II/33E **Applications of Quantum Mechanics**

A beam of particles each of mass m and energy $\hbar^2 k^2/(2m)$ scatters off an axisymmetric potential V. In the first Born approximation the scattering amplitude is

$$f(\theta) = -\frac{m}{2\pi\hbar^2} \int e^{-i(\mathbf{k}-\mathbf{k}_0)\cdot\mathbf{x}'} V(\mathbf{x}')\, d^3x', \qquad (*)$$

where $\mathbf{k}_0 = (0, 0, k)$ is the wave vector of the incident particles and $\mathbf{k} = (k\sin\theta, 0, k\cos\theta)$ is the wave vector of the outgoing particles at scattering angle θ (and $\phi = 0$). Let $\mathbf{q} = \mathbf{k} - \mathbf{k}_0$ and $q = |\mathbf{q}|$. Show that when the scattering potential V is spherically symmetric the expression $(*)$ simplifies to

$$f(\theta) = -\frac{2m}{\hbar^2 q} \int_0^\infty r' V(r') \sin(qr')\, dr',$$

and find the relation between q and θ.

Calculate this scattering amplitude for the potential $V(r) = V_0 e^{-r}$ where V_0 is a constant, and show that at high energies the particles emerge predominantly in a narrow cone around the forward beam direction. Estimate the angular width of the cone.

2/II/33E **Applications of Quantum Mechanics**

Consider a large, essentially two-dimensional, rectangular sample of conductor of area A, and containing $2N$ electrons of charge $-e$. Suppose a magnetic field of strength B is applied perpendicularly to the sample. Write down the Landau Hamiltonian for one of the electrons assuming that the electron interacts just with the magnetic field.

[You may ignore the interaction of the electron spin with the magnetic field.]

Find the allowed energy levels of the electron.

Find the total energy of the $2N$ electrons at absolute zero temperature as a function of B, assuming that B is in the range

$$\frac{\pi\hbar N}{eA} \leqslant B \leqslant \frac{2\pi\hbar N}{eA}.$$

Comment on the values of the total energy when B takes the values at the two ends of this range.

3/II/33E **Applications of Quantum Mechanics**

Consider the body-centred cuboidal lattice L with lattice points $(n_1 a, n_2 a, n_3 b)$ and $((n_1+\frac{1}{2})a, (n_2+\frac{1}{2})a, (n_3+\frac{1}{2})b)$, where a and b are positive and n_1, n_2 and n_3 take all possible integer values. Find the reciprocal lattice $\widetilde{L}$ and describe its geometrical form. Calculate the volumes of the unit cells of the lattices L and $\widetilde{L}$.

Find the reciprocal lattice vector associated with the lattice planes parallel to the plane containing the points $(0,0,b)$, $(0,a,b)$, $(\frac{1}{2}a, \frac{1}{2}a, \frac{1}{2}b)$, $(a,0,0)$ and $(a,a,0)$. Deduce the allowed Bragg scattering angles of X-rays off these planes, assuming that $b=\frac{4}{3}a$ and that the X-rays have wavelength $\lambda = \frac{1}{2}a$.

4/II/33E **Applications of Quantum Mechanics**

Explain why the allowed energies of electrons in a three-dimensional crystal lie in energy bands. What quantum numbers can be used to classify the electron energy eigenstates?

Describe the effect on the energy level structure of adding a small density of impurity atoms randomly to the crystal.

1/II/33A Applications of Quantum Mechanics

In a certain spherically symmetric potential, the radial wavefunction for particle scattering in the $l = 0$ sector (S-wave), for wavenumber k and $r \gg 0$, is

$$R(r,k) = \frac{A}{kr}\left(g(-k)e^{-ikr} - g(k)e^{ikr}\right)$$

where

$$g(k) = \frac{k + i\kappa}{k - i\alpha}$$

with κ and α real, positive constants. Scattering in sectors with $l \neq 0$ can be neglected. Deduce the formula for the S-matrix in this case and show that it satisfies the expected symmetry and reality properties. Show that the phase shift is

$$\delta(k) = \tan^{-1}\frac{k(\kappa + \alpha)}{k^2 - \kappa\alpha}\ .$$

What is the scattering length for this potential?

From the form of the radial wavefunction, deduce the energies of the bound states, if any, in this system. If you were given only the S-matrix as a function of k, and no other information, would you reach the same conclusion? Are there any resonances here?

[*Hint: Recall that* $S(k) = e^{2i\delta(k)}$ *for real* k, *where* $\delta(k)$ *is the phase shift.*]

2/II/33A Applications of Quantum Mechanics

Describe the variational method for estimating the ground state energy of a quantum system. Prove that an error of order ϵ in the wavefunction leads to an error of order ϵ^2 in the energy.

Explain how the variational method can be generalized to give an estimate of the energy of the first excited state of a quantum system.

Using the variational method, estimate the energy of the first excited state of the anharmonic oscillator with Hamiltonian

$$H = -\frac{d^2}{dx^2} + x^2 + x^4\ .$$

How might you improve your estimate?

[*Hint: If* $I_{2n} = \int_{-\infty}^{\infty} x^{2n}\, e^{-ax^2} dx$ *then*

$$I_0 = \sqrt{\frac{\pi}{a}},\quad I_2 = \sqrt{\frac{\pi}{a}}\,\frac{1}{2a},\quad I_4 = \sqrt{\frac{\pi}{a}}\,\frac{3}{4a^2},\quad I_6 = \sqrt{\frac{\pi}{a}}\,\frac{15}{8a^3}.\ ]$$

3/II/33A **Applications of Quantum Mechanics**

Consider the Hamiltonian

$$H = \mathbf{B}(t) \cdot \mathbf{S}$$

for a particle of spin $\frac{1}{2}$ fixed in space, in a rotating magnetic field, where

$$S_1 = \frac{\hbar}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad S_2 = \frac{\hbar}{2}\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad S_3 = \frac{\hbar}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

and

$$\mathbf{B}(t) = B(\sin\alpha\cos\omega t,\ \sin\alpha\sin\omega t,\ \cos\alpha)$$

with B, α and ω constant, and $B > 0$, $\omega > 0$.

There is an exact solution of the time-dependent Schrödinger equation for this Hamiltonian,

$$\chi(t) = \left(\cos\left(\tfrac{1}{2}\lambda t\right) - i\frac{B - \omega\cos\alpha}{\lambda}\sin\left(\tfrac{1}{2}\lambda t\right)\right) e^{-i\omega t/2}\,\chi_+ + i\left(\frac{\omega}{\lambda}\sin\alpha\sin\left(\tfrac{1}{2}\lambda t\right)\right) e^{i\omega t/2}\,\chi_-$$

where $\lambda \equiv (\omega^2 - 2\omega B\cos\alpha + B^2)^{1/2}$ and

$$\chi_+ = \begin{pmatrix} \cos\frac{\alpha}{2} \\ e^{i\omega t}\sin\frac{\alpha}{2} \end{pmatrix}, \quad \chi_- = \begin{pmatrix} e^{-i\omega t}\sin\frac{\alpha}{2} \\ -\cos\frac{\alpha}{2} \end{pmatrix}.$$

Show that, for $\omega \ll B$, this exact solution simplifies to a form consistent with the adiabatic approximation. Find the dynamic phase and the geometric phase in the adiabatic regime. What is the Berry phase for one complete cycle of $\mathbf{B}$?

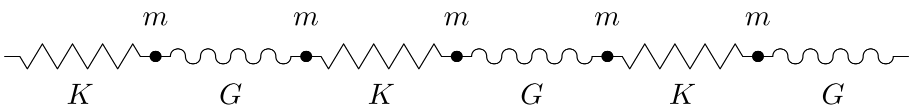
The Berry phase can be calculated as an integral of the form

$$\Gamma = i\oint \langle\psi|\nabla_{\mathbf{R}}\psi\rangle \cdot d\mathbf{R}\,.$$

Evaluate Γ for the adiabatic evolution described above.

4/II/33A **Applications of Quantum Mechanics**

Consider a 1-dimensional chain of $2N$ atoms of mass m (with N large and with periodic boundary conditions). The interactions between neighbouring atoms are modelled by springs with alternating spring constants K and G, with $K > G$.



In equilibrium, the separation of the atoms is a, the natural length of the springs.

Find the frequencies of the longitudinal modes of vibration for this system, and show that they are labelled by a wavenumber q that is restricted to a Brillouin zone. Identify the acoustic and optical bands of the vibration spectrum, and determine approximations for the frequencies near the centre of the Brillouin zone. What is the frequency gap between the acoustic and optical bands at the zone boundary?

Describe briefly the properties of the phonons in this system.

1/II/33A **Applications of Quantum Mechanics**

Consider a particle of mass m and momentum $\hbar k$ moving under the influence of a spherically symmetric potential $V(r)$ such that $V(r) = 0$ for $r \geqslant a$. Define the scattering amplitude $f(\theta)$ and the phase shift $\delta_\ell(k)$. Here θ is the scattering angle. How is $f(\theta)$ related to the differential cross section?

Obtain the partial-wave expansion

$$f(\theta) = \frac{1}{k}\sum_{\ell=0}^{\infty}(2\ell+1)\, e^{i\delta_\ell}\sin\delta_\ell\, P_\ell(\cos\theta)\,.$$

Let $R_\ell(r)$ be a solution of the radial Schrödinger equation, regular at $r = 0$, for energy $\hbar^2k^2/2m$ and angular momentum ℓ. Let

$$Q_\ell(k) = a\frac{R_\ell'(a)}{R_\ell(a)} - ka\frac{j_\ell'(ka)}{j_\ell(ka)}\,.$$

Obtain the relation

$$\tan\delta_\ell = \frac{Q_\ell(k) j_\ell^2(ka) ka}{Q_\ell(k) n_\ell(ka) j_\ell(ka) ka - 1}\,.$$

Suppose that

$$\tan\delta_\ell \approx \frac{\gamma}{k_0 - k}\,,$$

for some ℓ, with all other δ_ℓ small for $k \approx k_0$. What does this imply for the differential cross section when $k \approx k_0$?

[*For $V = 0$, the two independent solutions of the radial Schrödinger equation are $j_\ell(kr)$ and $n_\ell(kr)$ with*

$$j_\ell(\rho) \sim \frac{1}{\rho}\sin(\rho - \tfrac{1}{2}\ell\pi), \qquad n_\ell(\rho) \sim -\frac{1}{\rho}\cos(\rho - \tfrac{1}{2}\ell\pi) \quad \text{as} \quad \rho \to \infty\,,$$

$$e^{i\rho\cos\theta} = \sum_{\ell=0}^{\infty}(2\ell+1) i^\ell\, j_\ell(\rho)\, P_\ell(\cos\theta)\,.$$

Note that the Wronskian $\rho^2\big(j_\ell(\rho)\, n_\ell'(\rho) - j_\ell'(\rho)\, n_\ell(\rho)\big)$ is independent of ρ.]

2/II/33D **Applications of Quantum Mechanics**

State and prove Bloch's theorem for the electron wave functions for a periodic potential $V(\mathbf{r}) = V(\mathbf{r}+\mathbf{l})$ where $\mathbf{l} = \sum_i n_i\, \mathbf{a}_i$ is a lattice vector.

What is the reciprocal lattice? Explain why the Bloch wave-vector $\mathbf{k}$ is arbitrary up to $\mathbf{k} \to \mathbf{k}+\mathbf{g}$, where $\mathbf{g}$ is a reciprocal lattice vector.

Describe in outline why one can expect energy bands $E_n(\mathbf{k}) = E_n(\mathbf{k}+\mathbf{g})$. Explain how $\mathbf{k}$ may be restricted to a Brillouin zone B and show that the number of states in volume d^3k is

$$\frac{2}{(2\pi)^3}\, \mathrm{d}^3 k\,.$$

Assuming that the velocity of an electron in the energy band with Bloch wave-vector $\mathbf{k}$ is

$$\mathbf{v}(\mathbf{k}) = \frac{1}{\hbar}\frac{\partial}{\partial \mathbf{k}} E_n(\mathbf{k})\,,$$

show that the contribution to the electric current from a full energy band is zero. Given that $n(\mathbf{k}) = 1$ for each occupied energy level, show that the contribution to the current density is then

$$\mathbf{j} = -e\,\frac{2}{(2\pi)^3}\int_B \mathrm{d}^3 k\; n(\mathbf{k})\mathbf{v}(\mathbf{k})\,,$$

where $-e$ is the electron charge.

3/II/33A **Applications of Quantum Mechanics**

Consider a one-dimensional crystal of lattice space b, with atoms having positions x_s and momenta p_s, $s = 0, 1, 2, \ldots, N-1$, such that the classical Hamiltonian is

$$H = \sum_{s=0}^{N-1} \left(\frac{p_s^2}{2m} + \tfrac{1}{2} m\lambda^2 \big(x_{s+1} - x_s - b\big)^2 \right),$$

where we identify $x_N = x_0$. Show how this may be quantized to give the energy eigenstates consisting of a ground state $|0\rangle$ together with free phonons with energy $\hbar\omega(k_r)$ where $k_r = 2\pi r/Nb$ for suitable integers r. Obtain the following expression for the quantum operator x_s

$$x_s = s\,b + \left(\frac{\hbar}{2mN}\right)^{\frac{1}{2}} \sum_r \frac{1}{\sqrt{\omega(k_r)}} \left(a_r e^{ik_r sb} + a_r{}^{\dagger} e^{-ik_r sb}\right),$$

where $a_r, a_r{}^{\dagger}$ are annihilation and creation operators, respectively.

An interaction involves the matrix element

$$M = \sum_{s=0}^{N-1} \langle 0| e^{iqx_s} |0\rangle \,.$$

Calculate this and show that $|M|^2$ has its largest value when $q = 2\pi n/b$ for integer n. Disregard the case $\omega(k_r) = 0$.

[*You may use the relations*

$$\sum_{s=0}^{N-1} e^{ik_r sb} = \begin{cases} N\,, & r = Nb\,; \\ 0 & \textit{otherwise,} \end{cases}$$

and $e^{A+B} = e^A e^B e^{-\frac{1}{2}[A,B]}$ *if* $[A,B]$ *commutes with* A *and with* B.]

4/II/33D **Applications of Quantum Mechanics**

For the one-dimensional potential

$$V(x) = -\frac{\hbar^2\lambda}{m} \sum_n \delta(x - na)\,,$$

solve the Schrödinger equation for negative energy and obtain an equation that determines possible energy bands. Show that the results agree with the tight-binding model in appropriate limits.

$\left[\textit{It may be useful to note that } V(x) = -\dfrac{\hbar^2\lambda}{ma} \sum_n e^{2\pi inx/a}. \right]$

1/II/33B **Applications of Quantum Mechanics**

A beam of particles is incident on a central potential $V(r)$ $(r = |\mathbf{x}|)$ that vanishes for $r > R$. Define the differential cross-section $d\sigma/d\Omega$.

Given that each incoming particle has momentum $\hbar\mathbf{k}$, explain the relevance of solutions to the time-independent Schrödinger equation with the asymptotic form

$$\psi(\mathbf{x}) \sim e^{i\mathbf{k}\cdot\mathbf{x}} + f(\hat{\mathbf{x}})\,\frac{e^{ikr}}{r} \qquad (*)$$

as $r \to \infty$, where $k = |\mathbf{k}|$ and $\hat{\mathbf{x}} = \mathbf{x}/r$. Write down a formula that determines $d\sigma/d\Omega$ in this case.

Write down the time-independent Schrödinger equation for a particle of mass m and energy $E = \dfrac{\hbar^2 k^2}{2m}$ in a central potential $V(r)$, and show that it allows a solution of the form

$$\psi(\mathbf{x}) = e^{i\mathbf{k}\cdot\mathbf{x}} - \frac{m}{2\pi\hbar^2}\int d^3x'\,\frac{e^{ik|\mathbf{x}-\mathbf{x}'|}}{|\mathbf{x}-\mathbf{x}'|}\,V(r')\psi(\mathbf{x}')\;.$$

Show that this is consistent with $(*)$ and deduce an expression for $f(\hat{\mathbf{x}})$. Obtain the Born approximation for $f(\hat{\mathbf{x}})$, and show that $f(\hat{\mathbf{x}}) = F(k\hat{\mathbf{x}} - \mathbf{k})$, where

$$F(\mathbf{q}) = -\frac{m}{2\pi\hbar^2}\int d^3x\, e^{-i\mathbf{q}\cdot\mathbf{x}}\,V(r)\,.$$

Under what conditions is the Born approximation valid?

Obtain a formula for $f(\hat{\mathbf{x}})$ in terms of the scattering angle θ in the case that

$$V(r) = K\,\frac{e^{-\mu r}}{r}\,,$$

for constants K and μ. Hence show that $f(\hat{\mathbf{x}})$ is independent of $\hbar$ in the limit $\mu \to 0$, when expressed in terms of θ and the energy E.

[*You may assume that* $(\nabla^2 + k^2)\left(\dfrac{e^{ikr}}{r}\right) = -4\pi\delta^3(\mathbf{x})$.]

2/II/33B **Applications of Quantum Mechanics**

Describe briefly the variational approach to the determination of an approximate ground state energy E_0 of a Hamiltonian H.

Let $|\psi_1\rangle$ and $|\psi_2\rangle$ be two states, and consider the trial state

$$|\psi\rangle = a_1|\psi_1\rangle + a_2|\psi_2\rangle$$

for real constants a_1 and a_2. Given that

$$\begin{aligned} \langle\psi_1|\psi_1\rangle = \langle\psi_2|\psi_2\rangle = 1\,, \qquad \langle\psi_2|\psi_1\rangle = \langle\psi_1|\psi_2\rangle = s\,, \\ \langle\psi_1|H|\psi_1\rangle = \langle\psi_2|H|\psi_2\rangle = \mathcal{E}\,, \quad \langle\psi_2|H|\psi_1\rangle = \langle\psi_1|H|\psi_2\rangle = \epsilon\,, \end{aligned} \tag{$*$}$$

and that $\epsilon < s\mathcal{E}$, obtain an upper bound on E_0 in terms of $\mathcal{E}$, ϵ and s.

The normalized ground-state wavefunction of the Hamiltonian

$$H_1 = \frac{p^2}{2m} - K\delta(x)\,, \qquad K > 0,$$

is

$$\psi_1(x) = \sqrt{\lambda}\, e^{-\lambda|x|}\,, \qquad \lambda = \frac{mK}{\hbar^2}\,.$$

Verify that the ground state energy of H_1 is

$$E_B \equiv \langle\psi_1|H|\psi_1\rangle = -\frac{1}{2}K\lambda\,.$$

Now consider the Hamiltonian

$$H = \frac{p^2}{2m} - K\delta(x) - K\delta(x-R)\,,$$

and let $E_0(R)$ be its ground-state energy as a function of R. Assuming that

$$\psi_2(x) = \sqrt{\lambda}\, e^{-\lambda|x-R|}\,,$$

use $(*)$ to compute s, $\mathcal{E}$ and ϵ for ψ_1 and ψ_2 as given. Hence show that

$$E_0(R) \leqslant E_B\left[1 + 2\,\frac{e^{-\lambda R}\left(1+e^{-\lambda R}\right)}{1+(1+\lambda R)\,e^{-\lambda R}}\right].$$

Why should you expect this inequality to become an approximate equality for sufficiently large R? Describe briefly how this is relevant to molecular binding.

3/II/33B **Applications of Quantum Mechanics**

Let $\{\mathbf{l}\}$ be the set of lattice vectors of some lattice. Define the reciprocal lattice. What is meant by a Bravais lattice?

Let $\mathbf{i}$, $\mathbf{j}$, $\mathbf{k}$ be mutually orthogonal unit vectors. A crystal has identical atoms at positions given by the vectors

$$a\big[n_1\mathbf{i}+n_2\mathbf{j}+n_3\mathbf{k}\big]\,, \qquad a\big[(n_1+\tfrac{1}{2})\mathbf{i}+(n_2+\tfrac{1}{2})\mathbf{j}+n_3\mathbf{k}\big]\,,$$
$$a\big[(n_1+\tfrac{1}{2})\mathbf{i}+\mathbf{j}+(n_3+\tfrac{1}{2})\mathbf{k}\big]\,, \quad a\big[n_1\mathbf{i}+(n_2+\tfrac{1}{2})\mathbf{j}+(n_3+\tfrac{1}{2})\mathbf{k}\big]\,,$$

where (n_1, n_2, n_3) are arbitrary integers and a is a constant. Show that these vectors define a Bravais lattice with basis vectors

$$\mathbf{a}_1 = a\tfrac{1}{2}(\mathbf{j}+\mathbf{k})\,, \qquad \mathbf{a}_2 = a\tfrac{1}{2}(\mathbf{i}+\mathbf{k})\,, \qquad \mathbf{a}_3 = a\tfrac{1}{2}(\mathbf{i}+\mathbf{j})\,.$$

Verify that a basis for the reciprocal lattice is

$$\mathbf{b}_1 = \frac{2\pi}{a}(\mathbf{j}+\mathbf{k}-\mathbf{i})\,, \qquad \mathbf{b}_2 = \frac{2\pi}{a}(\mathbf{i}+\mathbf{k}-\mathbf{j})\,, \qquad \mathbf{b}_3 = \frac{2\pi}{a}(\mathbf{i}+\mathbf{j}-\mathbf{k})\,.$$

In Bragg scattering, an incoming plane wave of wave-vector $\mathbf{k}$ is scattered to an outgoing wave of wave-vector $\mathbf{k}'$. Explain why $\mathbf{k}' = \mathbf{k}+\mathbf{g}$ for some reciprocal lattice vector $\mathbf{g}$. Given that θ is the scattering angle, show that

$$\sin\frac{1}{2}\theta = \frac{|\mathbf{g}|}{2\,|\mathbf{k}|}\,.$$

For the above lattice, explain why you would expect scattering through angles θ_1 and θ_2 such that

$$\frac{\sin\frac{1}{2}\theta_1}{\sin\frac{1}{2}\theta_2} = \frac{\sqrt{3}}{2}\,.$$

4/II/33B **Applications of Quantum Mechanics**

A semiconductor has a valence energy band with energies $E \leqslant 0$ and density of states $g_v(E)$, and a conduction energy band with energies $E \geqslant E_g$ and density of states $g_c(E)$. Assume that $g_v(E) \sim A_v(-E)^{\frac{1}{2}}$ as $E \to 0$, and that $g_c(E) \sim A_c(E - E_g)^{\frac{1}{2}}$ as $E \to E_g$. At zero temperature all states in the valence band are occupied and the conduction band is empty. Let p be the number of holes in the valence band and n the number of electrons in the conduction band at temperature T. Under suitable approximations derive the result

$$pn = N_v N_c e^{-E_g/kT}$$

where

$$N_v = \tfrac{1}{2}\sqrt{\pi} A_v (kT)^{\frac{3}{2}}\,, \qquad N_c = \tfrac{1}{2}\sqrt{\pi} A_c (kT)^{\frac{3}{2}}\,.$$

Briefly describe how a semiconductor may conduct electricity but with a conductivity that is strongly temperature dependent.

Describe how doping of the semiconductor leads to $p \neq n$. A pn junction is formed between an n-type semiconductor, with N_d donor atoms, and a p-type semiconductor, with N_a acceptor atoms. Show that there is a potential difference $V_{np} = \Delta E/|e|$ across the junction, where e is the electron charge, and

$$\Delta E = E_g - kT \ln \frac{N_v N_c}{N_d N_a}\,.$$

Two semiconductors, one p-type and one n-type, are joined to make a closed circuit with two pn junctions. Explain why a current will flow around the circuit if the junctions are at different temperatures.

[*The Fermi–Dirac distribution function at temperature T and chemical potential μ is* $\dfrac{g(E)}{e^{(E-\mu)/kT} + 1}$, *where $g(E)$ is the number of states with energy E.*

Note that $\displaystyle\int_0^\infty x^{\frac{1}{2}} e^{-x}\, dx = \tfrac{1}{2}\sqrt{\pi}$.]