UNIVERSITY OF LONDON
IMPERIAL COLLEGE OF SCIENCE, TECHNOLOGY AND MEDICINE

BSc/MSci EXAMINATION (MATHEMATICS) MAY – JUNE (2003)
2006

This paper is also taken for the relevant examination for the Associateship

M4A8 Quantum Mechanics II

DATE: 4 June 2006 TIME: 2-4pm

Credit will be given for all questions attempted, but extra credit will be given for complete or nearly complete answers.

Calculators may not be used.

1. A particle of mass m moving in a time-dependent potential, in one dimension, has a Hamiltonian of the form

$$\hat{H} = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + U(x,t)\ .$$

The potential is abruptly changed at time $t = 0$, so that

$$U(x,t) = \begin{cases} U_1(x), & \text{for} \quad t < 0 \\ U_2(x), & \text{for} \quad t > 0\ . \end{cases}$$

For $t < 0$ the particle is in the eigen-state $\psi_{1n}(x)$ of the initial Hamiltonian. Write down an expression for the probability that the particle is in the eigen-state $\psi_{2m}(x)$ of the final Hamiltonian for $t > 0$. In particular, write down the probability w that the particle remains in the ground state.

Determine the normalised ground-state wave-function for a particle in an attractive δ-potential $U(x) = -\lambda\delta(x)$, $\lambda > 0$. Using this, find the probability w for the case when $U_1(x) = -\lambda\delta(x)$ and $U_2(x) = -(\lambda/2)\delta(x-a)$, $a > 0$. Sketch the probability w as a function of the distance a. What is the probability w equal to when $a \to \infty$? Why?

Turn over...

2. The Hamiltonian for a particle of mass m, moving in the harmonic oscillator potential and subjected to an additional repulsive δ-potential, is of the form

$$\hat{H} = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + \frac{1}{2}m\omega_0^2 x^2 + \lambda\delta(x),$$

where $\lambda > 0$.

Show that, for odd n, the standard WKB quantisation rule,

$$2\int_{-a}^{a} p(x)dx = 2\pi\hbar(n + 1/2),$$

where $p(x)$ is the classical momentum and $\pm a$ are the turning points, remains unchanged in the presence of the δ-potential.

Show that, for even n, the quantisation rule is changed to

$$2\int_{-a}^{a} p(x)dx = 2\pi\hbar(n + \delta + 1/2),$$

where the energy dependent phase, $\delta = \delta(E)$, is to be determined from the discontinuity of $\psi'(x)$ at $x = 0$.

Calculate the phase integral for the harmonic potential and hence write down the modified quantisation condition as a transcendental equation for the energy levels $E_n(\lambda)$. Obtain the leading correction to $E_n(0)$ for small λ. Analyse $E_n(\lambda)$ for $\lambda \to \infty$. Do any degenerate levels occur? Why?

[Hint. Allow for the phase of the WKB wave-function to jump by $2\delta(E)$ across $x = 0$. Then add the extra phase to the total WKB phase.]

3. Two electrons (i.e. spin-1/2 particles obeying Fermi-Dirac statistics) interacting via the exchange interaction J are placed in a harmonic potential well:

$$\hat{H} = -\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial x_1^2} + \frac{\partial^2}{\partial x_2^2}\right) + \frac{1}{2}m\omega^2(x_1^2 + x_2^2) + J\hat{\vec{s}}_1\hat{\vec{s}}_2,$$

where J is the exchange interaction.

Determine all the eigenvalues of the Hamiltonian. Find the corresponding wave-functions in terms of products of the eigenstates of the individual oscillators $\psi_n(x_i)$ $(i = 1, 2)$ and the spin basis functions $|\pm>$, such that $\hat{s}^z_{1,2}|\pm>= \pm(\hbar/2)|\pm>$.

For $J = 0$ write down the ground-state energy and wave-function. Assume that the exchange is being changed from $J = 0$ towards negative values; at what value of $J = -J_0$ $(J_0 > 0)$ does the ground-state cease to be spin-singlet?

4. Let $\hat{x}$ and $\hat{p}$ be canonical coordinate and momentum operators with the commutation relation $[\hat{x}, \hat{p}] = i$ (in units such that $\hbar = 1$).

Use the annihilation and creation operators

$$\hat{a} = \frac{1}{\sqrt{2m\omega}}(m\omega\hat{x} + i\hat{p}), \quad \hat{a}^\dagger = \frac{1}{\sqrt{2m\omega}}(m\omega\hat{x} - i\hat{p})$$

to derive the second-quantised Hamiltonian for a harmonic oscillator with mass m and frequency ω.

An external non-linear perturbation

$$\hat{V} = \alpha\hat{x}^3$$

is applied to the oscillator.

Express $\hat{V}$ in terms of the annihilation and creation operators.

Using the fact that $\hat{a}|0\rangle = 0$ if $|0\rangle$ is the ground state and the commutation relation $[\hat{a}, \hat{a}^\dagger] = 1$, determine all the non-zero matrix elements of the perturbation, $V_{n,0} = \langle n|V|0\rangle$, between the ground-state and the excited states of the oscillator. (Note that $|n\rangle = (\hat{a}^\dagger)^n|0\rangle/\sqrt{n!}$, $\langle n|m\rangle = \delta_{n,m}$.)

Hence obtain the first-order and the second-order corrections to the ground-state energy.

5. Electrons hop between neighbouring sites of a two-dimensional square lattice, the hopping integral being $-t$. The lattice sites are at positions $a_0\vec{n} = a_0(n_x, n_y)$, where a_0 is the lattice constant and $n_{x,y}$ are integers.

Disregard the spin quantum number and write down the second-quantised Hamiltonian for this problem in terms of the creation and annihilation operators $\hat{a}^\dagger_{\vec{n}}$, $\hat{a}_{\vec{n}}$ for an electron on the site $\vec{n} = (n_x, n_y)$.

Work out the Brillouin zone, diagonalise the Hamiltonian and obtain the one-electron energy spectrum $\epsilon(\vec{k})$ as function of the quasi-momentum $\vec{k} = (k_x, k_y)$.

At half-filling, when the Fermi level is at the middle of the band, i.e. $E_F = 0$, determine the shape of the Fermi surface. Does the Fermi surface pass through the corner point $\vec{k}_0 = (\pi/a_0, 0)$? By expanding $\epsilon(\vec{k})$ around $\vec{k}_0$ (let $\vec{k} = \vec{k}_0 + \vec{p}$, $\vec{p}$–small) determine what kind of a stationary point it is. Identify the remaining stationary points of the same nature.