Imperial College London

UNIVERSITY OF LONDON

BSc and MSci EXAMINATIONS (MATHEMATICS)

May-June 2006

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

M4A8

Quantum Mechanics II

Date: Monday, 22nd May 2006 Time: 2 pm – 4 pm

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

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

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

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

For $t < 0$ the particle is in the eigen-state $\psi_n^{(i)}(x)$ of the initial Hamiltonian. Write down an expression for the probability that the particle is in the eigen-state $\psi_m^{(f)}(x)$ of the final Hamiltonian for $t > 0$. In particular, obtain the probability w that the particle remains in the ground state.

Calculate the probability that the particle remains in the ground state for the case when the initial and final potentials are given by

$$U_i(x) = \frac{1}{2}m\omega_1^2 x^2 \quad \text{and} \quad U_f(x) = \frac{1}{2}m\omega_2^2 (x - x_0)^2 \ ,$$

respectively.

[You may use without proof the result that the normalised ground-state wave-function for a harmonic oscillator is

$$\psi_0(x) = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} e^{-m\omega x^2/2\hbar} \ . \ ]$$

2. For a quantum particle of mass m in a one–dimensional potential well, the WKB quantisation rule is

$$2\int_{a_1}^{a_2} p(x)dx = 2\pi\hbar(n+1/2),$$

where $p(x)$ is the classical momentum and a_1 and a_2 are the classical turning points $(n = 0, 1, 2, \ldots)$.

(i) Within this framework, determine the WKB energy levels, E_n, for a particle in the potential of the form

$$U(x) = F|x| \ ,$$

where F is a constant.

(ii) For large $n \gg 1$, the energy difference, $\Delta E_n = E_{n+1} - E_n$, between neighbouring level scales has $\Delta E_n \sim n^\beta$. Determine β. Show how the same result can be obtained by using the classical frequency $\omega = 2\pi/T$, where the classical period is given by

$$T = 2m\int_{a_1}^{a_2} \frac{dx}{p(x)} \ .$$

Is the resulting β positive or negative? Explain why.

(iii) Next, assume that there are N non-interacting electrons (i.e. spin-$1/2$ particles obeying the Pauli principle) placed into the above potential well. For $N \gg 1$, estimate the Fermi energy and the total ground–state energy of the system.

3. (i) Two spin-1/2's interact via a fully anisotropic exchange interaction:

$$\widehat{H} = J^x\,\widehat{s}_1^x\,\widehat{s}_2^x + J^y\,\widehat{s}_1^y\,\widehat{s}_2^y + J^z\,\widehat{s}_1^z\,\widehat{s}_2^z \ ,$$

where $\widehat{s}_i^\alpha$'s $(i = 1, 2,\ \alpha = x, y, x)$ are the spin-$1/2$ operators and J^α's are the exchange constants.

Use the basis $\{\,|\uparrow\uparrow\rangle\ ,\ |\uparrow\downarrow\rangle\ ,\ |\downarrow\uparrow\rangle\ ,\ |\downarrow\downarrow\rangle\}$ to obtain all the eigenstates and the eigenvalues of the Hamiltonian $\widehat{H}$.

(ii) Four identical Bose particles occupy two different quantum states $\psi_i(\xi)$, $i = 1, 2$. The wave-functions $\psi_i(\xi)$ are normalised and mutually orthogonal. Determine the normalised four-particle wave-function $\Psi(\xi_1, \xi_2, \xi_3, \xi_4)$ such that three of the four particles are in the same quantum state and the fourth particle is in a different quantum state.

4. The Hamiltonian of a two–dimensional harmonic oscillator of mass m and frequency ω is given by:

$$\widehat{H}_0 = \sum_{i=1}^{2} \left[\frac{\widehat{p}_i^2}{2m} + \frac{1}{2} m\omega^2 \, \widehat{x}_i^2 \right] \, ,$$

where $\widehat{x}_i$ and $\widehat{p}_i$ are canonical coordinate and momentum operators with the commutation relation $[\widehat{x}_i, \widehat{p}_j] = i\delta_{ij}$ (in units such that $\hbar = 1$).

The annihilation and creation operators are defined by:

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

Show that the creation and annihilation operators satisfy the commutation relations

$$[\widehat{a}_i, \widehat{a}_j^\dagger] = \delta_{ij}$$

and derive the second-quantised Hamiltonian for the two-dimensional harmonic oscillator.

An external non-linear perturbation

$$\widehat{V} = \alpha \, \widehat{x}_1^2 \, \widehat{x}_2^2 + \beta(\widehat{x}_1\widehat{x}_2^3 + \widehat{x}_1^3\widehat{x}_2) + \gamma(\widehat{x}_1^4 + \widehat{x}_2^4)$$

is now applied to the oscillator.

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

Using the commutation relations (or otherwise), find the first-order correction to the ground-state energy due to the perturbation $\widehat{V}$.

5. Electrons hop between neighbouring sites of a one-dimensional lattice (chain). The hopping integral is equal to t for all links. The single-electron energies alternate along the chain and are equal to ϵ_1 on the even sites and ϵ_2 on the odd sites.

(i) Sketch the lattice and indicate the hopping processes on the sketch. By suitably numbering the sites and choosing the unit cell, write down the second–quantised Hamiltonian of the problem.

(ii) Diagonalise the Hamiltonian in momentum space. Hence derive the expressions for the energy bands. How many energy bands are there? Sketch the energy bands and determine the magnitude of the energy gap at the Brillouin zone boundary.

(iii) If there is one (spin-$1/2$) electron per site, is the system an insulator or a conductor? Will your conclusion change if $\epsilon_1 = \epsilon_2$?