UNIVERSITY OF LONDON

IMPERIAL COLLEGE OF SCIENCE, TECHNOLOGY AND MEDICINE

BSc/MSci EXAMINATION (MATHEMATICS) MAY – JUNE (2004)
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This paper is also taken for the relevant examination for the Associateship

M4A8 Quantum Mechanics II

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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.

 M4A8: 6 Pages

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

$$\hat{H} = -\frac{\hbar^2}{2m}\left[\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}\right] + U(\vec{r}, t) \ ,$$

with $\vec{r} = (x, y, z)$. The potential is abruptly changed at time $t = 0$, so that

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

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

The particle in a harmonic potential, $U_i(\vec{r}) = \frac{1}{2}m\omega^2|\vec{r}|^2$, is suddenly subjected to an additional force F in the z–direction $U_f(\vec{r}) = U_i(\vec{r}) + Fz$. Determine the probability $w(F)$, as a function of the force F, that the particle remains in the ground state. Sketch $w(F)$.

[You may use the result that the normalised ground–state wave–function for a one–dimensional harmonic oscillator is

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

without proof.]

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 $(n = 0, 1, 2...)$.

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

$$U(x) = Kx^4 \ ,$$

where K is a constant. [Express the result in terms of the constant

$$I_0 = \int_0^1 du\sqrt{1-u^4}$$

but do not calculate this integral.]

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

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

(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. Two spin–1/2 electrons interact via the exchange interaction J and are sujected to the time–dependent magnetic field $H(t)$

$$\hat{H} = J\hat{\vec{s}}_1 \cdot \hat{\vec{s}}_2 - \mu H(t) S^z,$$

where S^z is the z–component of the total spin operator $\hat{\vec{S}} = \hat{\vec{s}}_1 + \hat{\vec{s}}_2$.

In terms of the wave-functions $\{|\uparrow\uparrow\rangle, |\uparrow\downarrow\rangle, |\downarrow\uparrow\rangle, |\downarrow\downarrow\rangle\}$, construct the basis of the singlet and triplet states diagonalising $\hat{\vec{S}}^2$ and S^z. In this basis solve the time–dependent Schroedinger equation (set $\hbar = 1$ in this question):

$$i\frac{\partial}{\partial t}\psi(t) = \hat{H}(t)\psi(t) \ .$$

Next assume that the system was initially (at $t = -\infty$) polarised along the x–axis, so that $S^x\psi_+ = \psi_+$. Also assume that the integral

$$\int_{-\infty}^{\infty} dt \ H(t) \equiv H_0$$

converges.

Then calculate the probability w_+ that the system will remain in the same state at $t = +\infty$. Calculate the probabilities w_- and w_0 that, at $t = +\infty$, the system is in the state ψ_- such that $S^x\psi_- = -\psi_-$ or in the state ψ_0 such that $S^x\psi_0 = 0$, respectively.

Show that the sum of the three probabilities is equal to 1 and explain why. Does any of the probabilities depend on the strength J of the exchange interaction?

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

$$\hat{H}_0 = \sum_{\alpha=1}^{2} \left[\frac{\hat{p}_\alpha^2}{2m} + \frac{1}{2} m\omega^2 \hat{x}_\alpha^2 \right] ,$$

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

The annihilation and creation operators are defined by:

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

Show that the creation and annihilation operators satisfy the commutation relations

$$[\hat{a}_\alpha, \hat{a}_\beta^\dagger] = \delta_{\alpha\beta}$$

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

An external non-linear perturbation

$$\hat{V} = \alpha\hat{x}_1\hat{x}_2 + \beta\hat{x}_1^2\hat{x}_2{}^2$$

is now applied to the oscillator.

Express $\hat{V}$ 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 $\hat{V}$.

5. Electrons hop between neighbouring sites of a one–dimensional lattice (chain). The hopping integrals alternate along the chain being t_1 on even links and t_2 on odd links.

Sketch the lattice and indicate the hopping processes on the sketch. Suitably numbering the sites and chosing the unit cell, write down the second–quantised Hamiltonian of the problem.

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.

If there is one (spin–1/2) electron per site, is the system an insulator or a conductor? Will your conclusion change if $t_1 = t_2$?

