Queen Mary
University of London

BSc/MSci EXAMINATION

PHY-319 Quantum Mechanics A

Time Allowed: 2 hours 15 minutes

Date: Wednesday 23rd May 2007

Time: 10:00

Answer ALL questions in section A. Answer ONLY TWO questions from section B. Section A carries 40 marks, each question in section B carries 30 marks. An indicative marking-scheme is shown in square brackets [ ] after each part of a question.

COMPLETE ALL ROUGH WORKINGS IN THE ANSWER BOOK AND CROSS THROUGH ANY WORK WHICH IS NOT TO BE ASSESSED.

NUMERIC CALCULATORS ARE PERMITTED IN THIS EXAMINATION.

YOU MAY RETAIN THE EXAMINATION PAPER AT THE END OF THE EXAMINATION.

Useful information:

$m_e = 9.11\text{x}10^{-31}\text{kg} = 0.511\text{MeV/c}^2$ $\qquad u = 1.66\text{x}10^{-27}\text{kg}$

$\hbar = 1.05\text{x}10^{-34}\text{Js} = 6.58\text{x}10^{-16}\text{eVs}$ $\qquad c = 3\text{x}10^8\text{ms}^{-1}$

$h = 6.63\ \text{x}10^{-34}\text{Js} = 4.13\text{x}10^{-15}\text{eVs}$

DO NOT TURN TO THE FIRST PAGE OF THE QUESTION PAPER UNTIL INSTRUCTED TO DO SO BY THE INVIGILATOR

Section A, Questions A1 to A3 – This section to be answered by all candidates

A1) a) Write down the 1D Time Dependent Schrödinger Equation. [2]

i) What condition allows us to derive the Time Independent Schrödinger Equation? [1]

ii) Write down the 1D Time Independent Schrödinger Equation and the resulting form of the wavefunction $\Psi(x,t)$ [2]

b) A particle exists in an eigenstate $\Psi(x,t)$.

i) What is the Born interpretation of $\Psi(x,t)$? [4]

ii) For an observable, q, represented by an operator $\hat{Q}$, write an expression for the expectation value of q, namely $\langle q \rangle$. [2]

iii) Write down an expression for the uncertainty in q, namely, Δq. [2]

iv) Write down the Heisenberg uncertainty principle in mathematical form. [1]

A2) Sketch the ground state and first excited state wavefunctions, and their probability densities, for the following systems:

a) A particle in a finite square well. [2]

b) A quantum mechanical simple harmonic oscillator. [2]

c) A particle bound by a forbidden region and a linearly varying potential (the "quantum bouncer"). [2]

(Include as much additional information in your sketches as you can)

d) Dr K. states: "All of these systems display a feature which is classically not expected." Explain this statement. [2]

A3) At $t = 0$ a wave packet moving in one dimension is prepared in a state corresponding to the wave function shown in fig.1.

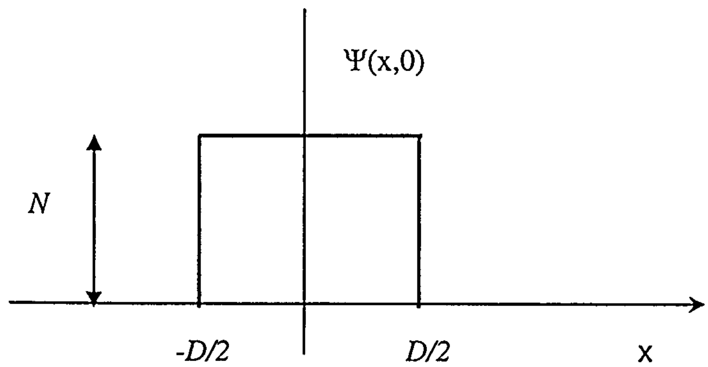

Fig.1: A wave packet at t = 0

a) By normalising the wave function, $\Psi(x,0)$, prove that $N = \frac{1}{\sqrt{D}}$ [4]

b) Evaluate $\langle x \rangle$ and $\langle x^2 \rangle$, and hence prove that the uncertainty in position, Δx, is $\frac{D}{2\sqrt{3}}$. [10]

c) What is the probability of finding the particle in the range $-\Delta x \le x \le +\Delta x$? [4]

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Section B, Questions B1 to B4 – Answer two questions only from this section.

B1) This question concerns two quantum mechanical dynamical systems: The Simple Harmonic Oscillator (SHO) and the "Quantum bouncer".

a) Consider a SHO of mass m, energy E and angular frequency ω_0.

i) Write an expression for the potential $V(x)$ and sketch it. [3]

ii) Obtain an expression for the classical turning point, x_0. [1]

iii) Prove that the solutions, ψ_0 and ψ_1, given below, satisfy the Time-Independent Schrödinger Equation for a SHO, obtaining E_0 and E_1.

$\psi_0 = N_0 e^{-\frac{ax^2}{2}}$ $\qquad \psi_1 = N_1 x e^{-\frac{ax^2}{2}}$ given that $a = \frac{m\omega_0}{\hbar}$ [7]

iv) Write a general expression for the allowed energy eigenvalues, E_n, of the SHO. [1]

The molecular vibrational energy spectra of diatomic molecules can be described using the harmonic approximation.

v) Hydrogen Fluoride (HF) is composed of one Hydrogen atom ($m_H = 1u$) and one Fluorine atom ($m_F = 19u$). Given that is has a broad absorption peak at 3.44μm, calculate the effective spring constant (in Nm^{-1}) of the H-F bond. [3]

b) Now consider a neutron of mass m and energy E, bouncing vertically, under gravity ($\beta = mg$), off a horizontal mirror (a Quantum bouncer).

i) Write an expression for the potential $V(x)$ and sketch it. [3]

ii) Obtain an expression for the classical turning point, x_0. [1]

By writing the Time Independent Schrödinger Equation for the quantum bouncer, and by using the substitution: $x = ay + b$

iii) Eliminate the x-independent terms in the Schrödinger Equation, proving that $b = x_0$ [5]

iv) Obtain Airy's equation, showing that $a = \sqrt[3]{\frac{\hbar^2}{2m\beta}}$ where $\beta = mg$ [6]

NOTE: if $x = ay + b$, then $\frac{d^2\psi(x)}{dx^2} = \frac{1}{a^2}\frac{d^2\psi(y)}{dy^2}$

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B2) Consider a particle confined to a one dimensional finite square well (see fig.2)

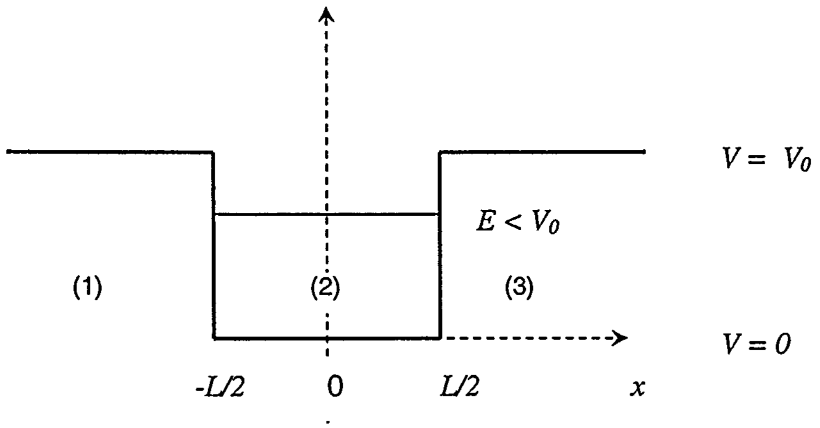

Fig.2: A particle inside a finite square well, width L and depth V_0.

a) Explain why we expect definite parity solutions for such a potential. [3]
b) By writing the Schrödinger equation in the three regions and applying appropriate boundary conditions:

i) Obtain both the positive and negative parity solutions in the three regions.[9]
ii) Obtain the consistency conditions for the bound states, namely:

$$\frac{\kappa}{k} = \tan\left(\frac{kL}{2}\right) \text{ for positive parity and } \frac{\kappa}{k} = -\cot\left(\frac{kL}{2}\right) \text{ for negative parity}$$

where $\kappa = \sqrt{\frac{2m}{\hbar^2}(V_0 - E)}$ and $k = \sqrt{\frac{2m}{\hbar^2}E}$ [8]

c) Using the dimensionless parameters $\eta = \frac{L}{2}\sqrt{\frac{2m}{\hbar^2}E}$ and $\zeta_0 = \frac{L}{2}\sqrt{\frac{2m}{\hbar^2}V_0}$.

i) The consistency conditions in part **b)ii)** can be rewritten as:

$$\tan(\eta) = \sqrt{\left(\frac{\zeta_0}{\eta}\right)^2 - 1} \text{ for even parity and } -\cot(\eta) = \sqrt{\left(\frac{\zeta_0}{\eta}\right)^2 - 1} \text{ for odd parity}$$

Depict these graphically, explaining how you calculate the number of bound states in part **c)ii)** as well as how the values given in part **c)iii)** could be obtained. [4]
ii) Calculate the number of electron bound states for a 1nm wide, 30eV deep well. [3]
ii) If the consistency conditions are solved graphically, yielding $\eta_1 = 1.465$, $\eta_2 = 2.93$ and $\eta_3 = 4.715$, calculate the energy separation, in eV, between the $n = 2$ and $n = 3$ states. [3]

Questions continue overpage

B3) This question concerns the two experimental demonstrations which were carried out during the course.

a) Linear conjugated molecules can be modelled as 1D infinite potential wells.

i) Modelling these systems as a 1-dimensional escape-proof boxes of width $L = Na$, containing N electrons obtain the *theoretical prediction* for the energy gap:

$$\Delta E = \frac{\hbar^2 \pi^2}{2ma^2} \frac{(N+1)}{N^2}$$

where m = mass of the electron and typically, for conjugated molecules, a = 0.12nm. **[6]**

ii) Give a brief account of an experiment demonstrated during the course where this simple model was compared to results obtained from actual conjugated molecules. Include descriptions of the experimental method, the data analysis and the results obtained, as well as any discrepancies between theory and experiment. **[9]**

b) In a scanning tunnelling microscope (STM) the electrons can be assumed to tunnel through a barrier of approximately constant height given by the work function, φ, and width the tip-substrate distance, L. In this situation, the tunnelling current can be approximated by:

$$I = I_0 e^{-2\kappa L} \text{ where } \kappa = \sqrt{\frac{2m\varphi}{\hbar^2}}$$

i) Draw three energy-position diagrams for the tunnelling between the tip and the substrate in an actual STM: one under no bias, one with the platinum tip (φ_{Pt} = 6.3 eV) positively biased with respect to the substrate and one with the gold substrate (φ_{Au} = 5.1 eV) positively biased with respect to the tip. If we wish to measure the work function of the tip, which of these applies? **[6]**

ii) Give a brief account of the experiment demonstrated during the course, where the tip of the STM is oscillated about its average position with amplitude ΔL, giving rise to an oscillation in the tunnelling current, amplitude ΔI. In particular, explain how the tip work function, φ, is obtained from the data. **[9]**

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B4) A stream of particles with energy $E > V_0$ is incident from the left on the downward step potential shown in figure 4.

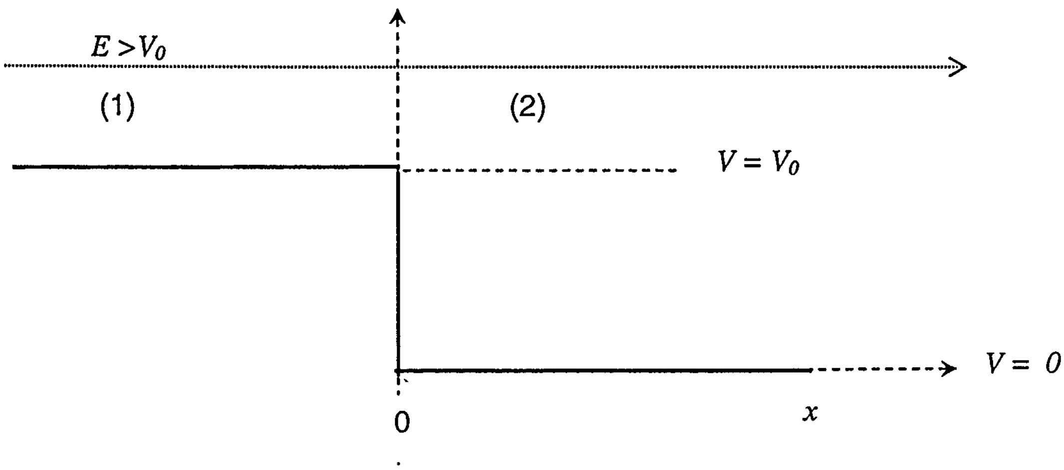

Fig.4: A stream of particles incident on a downwards step potential.

a) Write down the Schrödinger equation in regions 1 and 2 and obtain the solutions for both regions. **[10]**

b) By applying appropriate boundary conditions obtain the transmission and reflection coefficients, namely:

$$T = \frac{4kq}{(k+q)^2} \quad \text{and} \quad R = \left(\frac{k-q}{k+q}\right)^2$$

where $$k = \sqrt{\frac{2m}{\hbar^2}(E - V_0)} \quad \text{and} \quad q = \sqrt{\frac{2m}{\hbar^2}E}$$ **[12]**

c)

i) Verify that the above transmission and reflection coefficients satisfy conservation of particles. [3]

ii) Given that the particles are 128eV electrons and that the potential step is 32eV deep, calculate the transmission and reflection coefficients. [5]

End of Examination Paper **Dr T.Kreouzis**