Queen Mary University of London

B.Sc./M.Sci Examination

XXXX Xth May 2011   XX:XX

PHY319   Quantum Mechanics A   *Duration 2 hours 30 minutes*

YOU ARE NOT PERMITTED TO START READING THIS QUESTION PAPER UNTIL INSTRUCTED TO DO SO BY AN INVIGILATOR.

Answer ALL questions in section A. Answer ONLY TWO questions from section B. Section A carries 50 marks, each question in section B carries 25 marks. An indicative marking-scheme is shown in square brackets [ ] after each part of a question

CALCULATORS ARE PERMITTED IN THIS EXAMINATION. PLEASE STATE ON YOUR ANSWER BOOK THE NAME AND TYPE OF MACHINE USED.

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

CANDIDATES SHOULD NOTE THAT THE EXAMINATION AND ASSESSMENT REGULATIONS STATE THAT POSSESSION OF UNAUTHORISED MATERIALS AT ANY TIME WHEN A CANDIDATE IS UNDER EXAMINATION CONDITIONS IS AN ASSESSMENT OFFENCE. PLEASE CHECK YOUR POCKETS NOW FOR ANY NOTES THAT YOU MAY HAVE FORGOTTEN THAT ARE IN YOUR POSSESSION. IF YOU HAVE ANY THEN PLEASE RAISE YOUR HAND AND GIVE THEM TO AN INVIGILATOR NOW.

EXAM PAPERS CANNOT BE REMOVED FROM THE EXAM ROOM

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Useful information:

$$AB^* + BA^* = 2\,\mathrm{Re}\,A^*B = 2\,\mathrm{Re}\,B^*A$$

$$\int_{-\infty}^{\infty} x^2 e^{-Cx^2}\,dx = \frac{1}{2}\sqrt{\frac{\pi}{C^3}}$$

$$\sinh\theta = \frac{e^{\theta} - e^{-\theta}}{2}$$

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SECTION A: answer <u>all</u> questions

A1) **a)** Write down the one-dimensional, time-dependent Schrödinger equation for a particle in a potential $V(x,t)$.
b) What condition allows us to derive the time-independent Schrödinger equation?
c) Write down the one-dimensional, time-independent Schrödinger equation. **[5]**

A2) **a)** Write down an expression for the probability of detecting a particle in state $\Psi(x,t)$, at time t, in the interval $a \le x \le b$.
b) Hence write down the normalisation condition for $\Psi(x,t)$. **[5]**

A3) An observable, q, is represented by an operator, $\hat{Q}$.
a) Write an expression for the expectation value of the observable, $\langle q \rangle$, in a state $\Psi(x,t)$.
b) Write an expression for the uncertainty in the observable, Δq.
c) Write expressions for the operators relating to position and momentum ($\hat{X}$ and $\hat{P}$) and for the squares of the operators.
d) If $\Psi(x,t)$ is an eigenstate, write an equation relating it to the observable and its operator. **[10]**

A4) **a)** If a potential is symmetric i.e. it obeys $V(-x) = V(x)$, what are the consequences on the parity of the allowed eigenstates?
b) Sketch the ground and first excited state wavefunctions and probability densities of the infinite square well to illustrate your answer in part (a). **[5]**

A5) A system has angular momentum $l = 2$, write down the corresponding values of m_l which are allowed. **[5]**

Questions A6 to A9 refer to particle prepared at $t = 0$ in the state $\Psi(x,0)$ shown in figure 1.

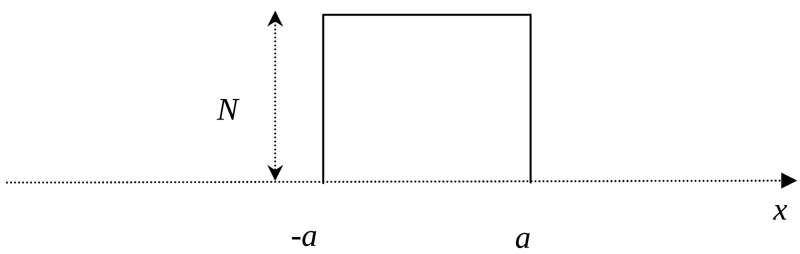

Figure 1: A particle prepared in a state $\Psi(x,0)$.

This can be written as: $\Psi(x,0) = N$ for $-a \le x \le a$ and $\Psi(x,0) = 0$ elsewhere

A6) By normalising the wave function, $\Psi(x,0)$, show that: $N = \dfrac{1}{\sqrt{2a}}$ **[5]**

A7) Prove that the position uncertainty, Δx, is given by: $\Delta x = \dfrac{a}{\sqrt{3}}$ **[5]**

A8) Show that the probability of detecting the particle in the interval $-\Delta x \le x \le \Delta x$ is $\dfrac{1}{\sqrt{3}}$ **[5]**

A9) Discuss whether the wavefunction shown in figure 1 contains any features generally deemed incompatible with a wavefunction. What consequences would such features have? **[5]**

Section B: answer two questions only, each question carries 25 marks.

Question B1

The harmonic approximation is used to describe certain features of the molecular energy spectrum of diatomic molecules.

a) Draw an energy-internuclear separation diagram, corresponding to the ground and first excited electronic states, for a diatomic molecule. Include any additional energy levels present (vibrational, rotational), and label any transitions with the part of the electromagnetic spectrum they correspond to. Use your diagram to explain what is meant by harmonic approximation. **[10]**

b) The normalised ground state, $\Psi_0(x,t)$, and first excited state, $\Psi_1(x,t)$, wavefunctions of the harmonic oscillator can be written as:

$$\Psi_0(x,t) = \left(\frac{a}{\pi}\right)^{\frac{1}{4}} e^{-\frac{ax^2}{2}} e^{-\frac{iE_0 t}{\hbar}} \quad \text{and} \quad \Psi_1(x,t) = \sqrt{2}\left(\frac{a^3}{\pi}\right)^{\frac{1}{4}} x e^{-\frac{ax^2}{2}} e^{-\frac{iE_1 t}{\hbar}} \quad \text{where } a = \frac{m\omega_0}{\hbar}$$

i) What are the values of E_0 and E_1 in terms of ω_0? **[2]**

Suppose an oscillator is prepared in a state $\Psi(x,t)$ given by a linear combination of the ground state and first excited state wavefunctions, namely:

$$\Psi(x,t) = \frac{1}{\sqrt{2}}\{\Psi_0(x,t) - \Psi_1(x,t)\}$$

ii) Show that $|\Psi(x,t)|^2 = \sqrt{\frac{a}{\pi}} e^{-ax^2}\left\{\frac{1}{2} + ax^2 - \sqrt{2}\sqrt{a}\,x\cos\omega_0 t\right\}$

[7]

iii) Prove that the expectation value of position, $\langle x \rangle$, oscillates with frequency ω_0 and amplitude $\frac{1}{\sqrt{2}\sqrt{a}}$. **[6]**

N.B. You may wish to refer to the useful information at the front of the examination paper

Question B2

In a scanning tunneling microscope (STM) the electrons can be assumed to tunnel through an approximately rectangular tunnelling barrier, whose height is given by the tip work function, φ, and whose width is the tip-substrate distance, L.

a) Draw the following energy-position diagrams for tunnelling between the tip (φ_{Pt} ~ 6 eV) and the substrate (φ_{Au} ~ 5.5 eV) in an STM:
i) Under no external bias (open circuit case).
ii) With the tip and substrate connected with a conductor (short-circuit case).
iii) With the tip at a small (~100 meV) positive bias compared to the short circuit case.
iv) With the substrate at a small (~100 meV) positive bias compared to the short circuit case.
[8]

During the course we studied quantum mechanical tunnelling by considering a beam of particles of energy E incident on a rectangular potential barrier of height V_0 and width L as shown in figure 2.

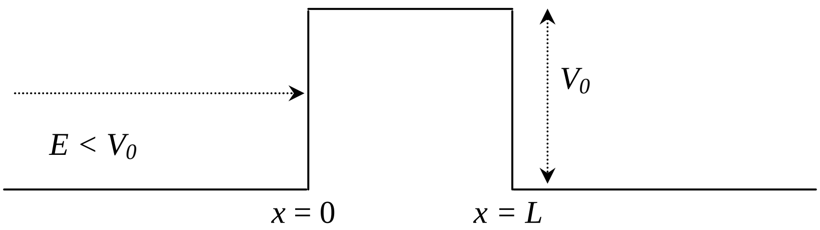

Figure 2: A rectangular potential barrier.

The tunneling transmission coefficient, T, for such a barrier when $E < V_0$ is given by:

$$T = \frac{4\kappa^2 k^2}{\left(\kappa^2 + k^2\right)^2 \sinh^2(\kappa L) + 4\kappa^2 k^2} \quad \text{where } \kappa = \sqrt{\frac{2m}{\hbar^2}\left(V_0 - E\right)} \qquad \text{and } k = \sqrt{\frac{2m}{\hbar^2}E}$$

b) Show that in the classically strongly forbidden case (a tall, thick barrier) the transmission coefficient reduces to: $T \approx \dfrac{16E\left(V_0 - E\right)e^{-2\kappa L}}{V_0^2}$ **[8]**

c) Solve the Schrödinger equation in the region $0 \le x \le L$ for both $E < V_0$ and $E > V_0$. Hence show how the expression relating to the tunneling transmission coefficient for $E < V_0$ can be modified to give the transmission coefficient for $E > V_0$. **[9]**

N.B. You may wish to refer to the useful information at the front of the examination paper

Question B3

a) Electronic states in the Hydrogen atom are described by four quantum numbers, namely n, l, m_l and m_s.

i) Explain the meaning of the four quantum numbers and how their values are constrained (either on their own, or by one another).

ii) Write expressions for $\left|\vec{L}\right|^2$ and L_z using the relevant quantum numbers and other quantities.

[10]

The technique of separation of variables is used repeatedly in quantum mechanics. It is based on writing a function of several variables as the product of two or more functions, for example:

$$\psi(r,\theta,\varphi) = R(r)Y(\theta,\varphi)$$

During the course we used this to write the Hydrogen wavefunction as the product of a radial wavefunction and a spherical harmonic. An example of a normalised spherical harmonic is given by:

$$Y_l^{m_l} = -\frac{1}{2}\sqrt{\frac{3}{2\pi}}\sin\theta\, e^{i\varphi}$$

b) Explain how you would obtain the values of l and m_l for this spherical harmonic simply by inspection. **[3]**

c) Using the expressions for the angular momentum operators $\hat{L}^2$ and $\hat{L}_z$ given below, obtain the actual values of l and m_l for the spherical harmonic considered in part (b). **[12]**

$$\hat{L}_z = -i\hbar\frac{\partial}{\partial\varphi} \quad \text{and} \quad \hat{L}^2 = -\frac{\hbar^2}{\sin\theta}\frac{\partial\left(\sin\theta\frac{\partial}{\partial\theta}\right)}{\partial\theta} - \frac{\hbar^2}{\sin^2\theta}\frac{\partial^2}{\partial\varphi^2}$$

Question B4

A stream of particles of mass m and energy $E > 0$ is incident from the left on the downward step potential shown in figure 3.

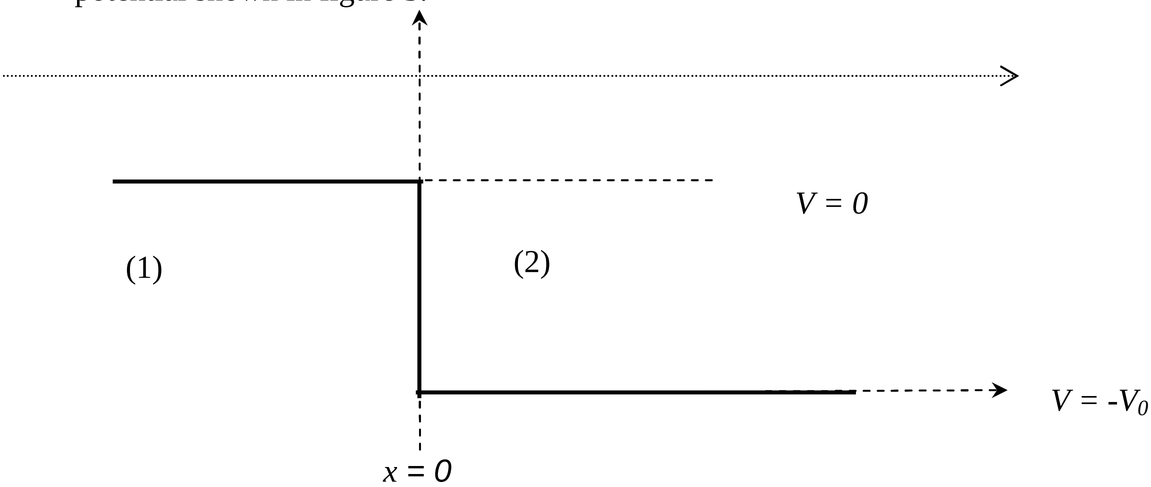

Figure 3: A stream of particles incident on a downwards step potential (split into two regions).

a) Write down the Schrödinger equation in regions 1 and 2 and obtain solutions, $\Psi(x,t)$, for both regions. **[5]**

b) Given that the particle flux can be expressed as $j(x,t) = \frac{1}{m}\mathrm{Re}\left[\Psi^* \hat{P}\Psi\right]$, where $\hat{P}$ is the momentum operator, obtain the incident, reflected and transmitted flux using the solutions obtained in part (a). **[5]**

c) Prove that the reflection coefficient, R, can be written as: $R = \left(\frac{k-q}{k+q}\right)^2$

where $k = \sqrt{\frac{2m}{\hbar^2}E}$ and $q = \sqrt{\frac{2m}{\hbar^2}(E + V_0)}$ **[7]**

d) i) Figure 3 is an example of an idealised, piece-wise continuous potential. Sketch a more realistic potential depicting this situation. By considering your sketch, explain how we obtain *realistic* solutions for such an *idealised* potential. **[4]**

ii) Discuss any consequences for the reflection coefficient if the particles were incident from the right to the left in figure 3. **[4]**

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