Quantum Mechanics I

Physical Chemistry Tutorials

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Question 1

A particle of mass m is constrained to move in a one-dimensional potential well with $V(x)=0$ for $0 \le x \le L$ and $V(x)=\infty$ elsewhere.

a) Show that the function

$$\psi(x) = a\cos(n\pi x/L) + b\sin(n\pi x/L)$$

Where a and b are constants and n is a number is a solution of the Schrödinger equation for the system.

b) Using the boundary conditions at x=0 and L, show that a=0 and find the allowed values of n and the corresponding energies.

c) Evaluate the constant b that ensures correct normalization of the wavefunction $\psi(x)$.

d) Sketch $\psi(x)$ and $\psi(x)^2$ for the lowest three values of n. Comment of the physical significance of these two functions.

e) An electron is confined to a one-dimensional box of length 15 nm. How many energy levels lie between 3.5 and 8.0 $kJmol^{-1}$? (m_e=9.110E-31 kg)

Question 2

The Schrödinger equation for a one-dimensional harmonic oscillator may be written

$$-\frac{\hbar^2}{2\mu}\frac{d^2\psi}{dx^2} + \frac{1}{2}kx^2\psi = E\psi$$

where μ is the effective mass of the oscillator and x is the displacement from equilibrium.

a) Show that the wavefunction $\psi = Ae^{-\alpha x^2}$, where A is a constant and $\alpha = \frac{\sqrt{k\mu}}{2\hbar}$ satisfies the Schrödinger equation.

b) Find the energy associated with the wavefunction given in a) and comment on the result obtained.

c) Make a sketch showing the variation of the potential energy with x. On your diagram, show the energies and wavefunctions associated with the four lowest states of the harmonic oscillator. In what ways does the behaviour of the quantum harmonic oscillator differ from that expected from classical mechanics?

Question 3

The Hamiltonian for a particle of mass m, confined to a ring of radius r can be written

$$H = -\frac{\hbar^2}{2mr^2}\frac{d^2}{d\phi^2}$$

where ϕ is the angle in the plane of the ring and the potential is a constant, taken as zero.

a) Show that the wavefunction $\psi(\phi) = Ne^{in\phi}$ satisfies the Schrödinger equation, and normalise the wavefunctions.

b) The appropriate boundary conditions for motion on a ring can be written $\psi(\phi) = \psi(\phi + 2\pi)$. Show that imposition of this boundary condition to the wavefunctions given in a) leads to quantised energy levels and derive an expression for the energy levels.

c) What is the Born interpretation of the wavefunction? What conclusions can be draw by adopting the Born interpretation of the wavefunction given in a)?

Question 4

a) What is meant by wave-particle duality? State de Broglie's relation between wavelength and momentum and explain qualitatively the connection between de Broglie's relation and the Heisenberg Uncertainty Principle.

b) Calculate the momentum of a photon of yellow light from a sodium lamp (wavelength 589 nm).

c) In low-energy electron diffraction, a beam of electrons is accelerated through a potential of 100 V before striking a sample. Show that the momentum, p, of the electron is given by $p = \sqrt{2m_e eV}$, where V is the accelerating potential, m_e is the mass of the electron, and e the electronic charge. Hence calculate the wavelength o of the electrons at the sample. Compare this value with the typical spacing between atoms in a metal.

d) Using the equipartition principle, write down an expression for the average kinetic energy of a helium atom Hence estimate a typical wavelength for a helium atom at 298K.