Quantum Mechanics A PHY-319 Problems 2

Issue: Tuesday 17th January 2012 **Hand-in:** 16:00 Thursday 26th January 2012
Hand-In questions **1** and **2**.

Please post your solutions in the box outside the 1st floor departmental offices

QUESTION 1.

For an infinite square well potential ($V = 0$ in the range $-\frac{L}{2} \leq x \leq \frac{L}{2}$) the normalised even parity energy eigenstates are:

$$\Psi_n(x,t) = \sqrt{\frac{2}{L}} \cos\left(\frac{n\pi}{L} x\right) e^{\frac{-iE_n t}{\hbar}} \text{ for } -\frac{L}{2} \leq x \leq \frac{L}{2} \text{ with } n = 1,3,5\ldots$$
$$= 0 \quad \text{elsewhere}$$

a) By substituting into the Time-Dependent Schrödinger Equation (TDSE) inside the well, obtain the energy eigenvalue, E_n, for which $\Psi_n(x,t)$ is a solution.

b) The particle in the well is in eigenstate $\Psi_n(x,t)$. Obtain the probability of finding it in the range $0 \leq x \leq \frac{L}{4}$. What does the probability of finding it in this range tend to for large n?

e) Sketch the probability density $|\Psi_1(x,t)|^2$ for the states n = 1, 3 and 5. Also in your sketch, indicate what the probability density would look like for large n.

f) Calculate the momentum uncertainty, Δp, given that $\hat{P} = -i\hbar \frac{\partial}{\partial x}$.

Some useful maths: $\cos^2\theta = \frac{1}{2}(1 + \cos 2\theta)$ and $\sin\left(\frac{n\pi}{2}\right) = (-1)^{\frac{(n-1)}{2}}$ for n odd

QUESTION 2.

The organic molecule hexatriene has the form shown in figure 1 (below).
Six of the electrons (the π electrons) are shared between the 6 carbon atoms: they are "delocalised", i.e. free to move along the backbone of the molecule. Model the potential that confines them to the molecule as a 1-dimensional square well of width L = 0.72nm

a) Find the values of the first 4 energy levels in eV.

b) Assuming each level can accommodate 2 electrons, (due to the Pauli exclusion principle) in the ground state of the molecule the lowest three levels are filled but the rest are empty.

Suppose the molecule is exposed to electromagnetic radiation of just the right wavelength to excite an electron from the n = 3 to the n = 4 level. What is this wavelength (in nm)? Compare your result with the experimentally measured value λ = 258nm.

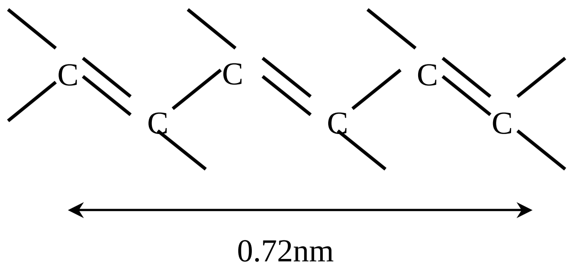

Fig.1: Hexatriene

Exercise Class Questions.

1) Further revision exercises in the use of complex numbers:

a) prove that for A, B complex, $AB^* + BA^* = 2\,\mathrm{Re}\,A^*B = 2\,\mathrm{Re}\,B^*A$

b)Write down the complex conjugate, Ψ^*, and the mod-squared, $|\Psi|^2$, of the following wave functions (all symbols except i are real unless otherwise stated):

i) $\psi(x) = A\psi_1(x) + B\psi_2(x)$, with A, B complex and $\psi_n(x)$ real.

ii) $\Psi(x,t) = \psi_1(x)e^{-\frac{iE_1t}{\hbar}} + \psi_2(x)e^{-\frac{iE_2t}{\hbar}}$, with $\psi_n(x)$ real.

2) Given that:

$$\Psi_n(x,t) = N\sin\left(\frac{n\pi}{L}x\right)e^{\frac{-iE_nt}{\hbar}} \quad \text{for } 0 \le x \le L \quad \text{with } n = 1,2,3...$$
$$= 0 \qquad \text{elsewhere}$$

Calculate the probability density of the state function:

$$\Psi(x,t) = \frac{1}{\sqrt{2}}\{\Psi_1(x,t) + \Psi_2(x,t)\}$$

Is this a stationary state?

3) The normalised ground state wavefunction for the simple harmonic oscillator can be written as:

$$\Psi(x,t) = \psi(x)e^{\frac{-iE_0t}{\hbar}} \text{ with } \psi(x) \text{ given by } \psi(x) = \left(\frac{a}{\pi}\right)^{\frac{1}{4}} e^{-\frac{ax^2}{2}}$$

a) Calculate the positional uncertainty Δx .

b) Given that: $\hat{P} = -i\hbar\frac{\partial}{\partial x}$, calculate the momentum uncertainty Δp .

c) What is the uncertainty product $\Delta p \Delta x$?

Some more useful maths:

$$\int_{-\infty}^{\infty} e^{-Cx^2}dx = \sqrt{\frac{\pi}{C}} \qquad \int_{0}^{\infty} xe^{-Cx^2}dx = \frac{C}{2} \qquad \int_{-\infty}^{\infty} x^2e^{-Cx^2}dx = \frac{1}{2}\sqrt{\frac{\pi}{C^3}}$$