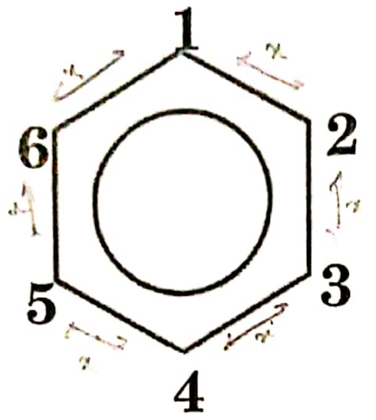
End Semester Exam (Monsoon 2019)

Science I

Time: 3 hours **Total: 40 marks**

(1) The following figure shows the structure of a benzene molecule, whose carbon atoms are numbered from 1 to 6. Using the paricle on a ring model, calculate the probability of finding a pi-electron between carbons 1 and 4 of the benzene molecule (you can assume that these pi-electrons are free particles on the ring) . [3]



(2) The following figure shows a conjugated polyene (a molecule with alternating single and double carbon-carbon bonds) of length L. Assume that you can model a pi-electron of this molecule as a free particle in a box bounded by infinite potentials.

(a) Calculate the probability that an electron in the state with n=1 will be found between x=0.25L and x=0.75L (with x=0 at the left-end of the molecule).

(b) Calculate the energy gap between the ground state and the first excited state of a pi-electron. [4]

L

$\int_{0.25}^{0.75} \frac{\psi^*(x)\hat{A}\psi(x)}{\psi(x)\psi^*(x)}$

$P(x) = \frac{4\pi r^2|\psi(x)|dV}{}$

$\frac{4r^2}{r^3}$

(3) A quantum particle of mass m is confined in an infinite one-dimensional square well potential with walls at $x = -L/2$ and $x = L/2$, where L is the length of the box. Write the wave functions for the ground state (n = 1), first excited state (n = 2) and the second excited state (n = 3). **[4]**

(4) The ground state wavefunction of a one-dimensional quantum harmonic oscillator is given by **[6]**

$$\psi(x) = A\, e^{-\frac{m\omega x^2}{2\hbar}} \qquad \int \psi^*(x)\psi(x) = 1$$

where A is the normalization constant. (a) By normalizing this wavefunction, determine A. (b) calculate the product of the uncertainty in x (denoted by Δx) and uncertainty in momentum (denoted by Δp). $(\Delta x)(\Delta p) = \frac{\hbar}{2\pi}$

(5) (a) Write the Schrodinger equation for a hydrogen atom. **[4]**

(b) Discuss the three quantum numbers involved in the hydrogen atom model. How would you understand different atomic orbitals using these quantum numbers? n, l, m

(6) The equation of state of a van der Waals gas is given by

$$(P + a\frac{n^2}{V^2})(\frac{V}{n} - b) = RT$$

where P is the pressure, V is the volume, T is the temperature, R is the gas constant, n is the number of moles of the gas, a and b are positive constants. Determine the second and third virial coefficients of this gas (Note: The equation of state of an ideal gas is $PV = nRT$ and you may need to use molar density in the virial expansion). **[3]**

(7) Determine the equations of motion for a simple pendulum using the (a) Lagrangian mechanics and (b) Hamiltonian mechanics. **[4]**

(8) Determine the Lagrangian for a coplanar double pendulum (recall the assignment problem). [3]

(9) For a closed system at a constant temperature T, derive the relationships between the partition function and (a) internal energy (b) heat capacity (c) entropy and (d) Helmholtz free energy. [4]

(10) What are thermodynamic potentials? Why do we need them? [1]

(11) Discuss the following: (a) phase stability (b) phase diagram (c) phase boundary (d) phase transition (e) triple point. [2]

(12) Derive the one-dimensional diffusion equation using the one-dimensional random walk model. [2]