Science I (Quiz 1) **[22 marks]**

(1) Define the Hamiltonian of an interacting N-particle system. [1]

(2) What are Hamilton's equations of motion? Why do we need them? [2]

(3) Show that for an isolated system, the Hamiltonian is a constant of motion. [2]

(4) Compare the phase space trajectories of an isolated and a closed one-dimensional harmonic oscillators. [3]

(5) What is Boltzmann's entropy formula? What is its significance? [1]

(6) How do you define the entropy of a closed system? Calculate the entropy of an ideal gas when it is (a) isolated and (b) closed. Compare these entropies. [1+3+3+1]

(7) What is the physical significance of energy fluctuations in a closed system? [5]

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Science I (Quiz 2) [21 marks]

(1) Define action. What is the principle of least action? Why do we need it? [2]

(2) Write the Lagrangian for a system of N ideal gas atoms confined in a cubic box of volume V and kept at a temperature T. Determine the Lagrange's equation of motion for the i^{th} atom in this system. [2]

(3) Using the Lagrangian function, discuss the law of conservation of angular momentum. [4]

(4) State at least four properties of a wave function. [2]

(5) Starting from the one-dimensional random walk model, derive the diffusion equation. [3]

(6) The solution P(x,t) of the one-dimensional diffusion equation was discussed in the class. Using the normalized P(x,t), calculate the following averages: $\langle x \rangle$ and $\langle x^2 \rangle$ [4]

(7) Draw the ground state and first excited state wave functions and probability densities of a quantum particle confined in a one-dimensional? [3]

(8) Write the time-independent Schrodinger equation for a one-dimensional quantum system. [1]

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Mid Semester Exam (Monsoon 2019)

Science I

Time: 90 min **Total: 25 marks**

(1) 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). [5]

(2) What are Hamilton's equations of motion? Why do we need them? [1]

(3) Compare the phase space trajectories of an isolated and a closed one-dimensional harmonic oscillators. [2]

(4) What is Boltzmann's entropy formula? What is its significance? [1]

(5) 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. [6]

(6) What are thermodynamic potentials? Under what conditions spontaneous processes minimize these potentails? [3]

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(7) Using the second law of thermodynamics, show that the process of flow of heat from a colder object to a hotter object is not spontaneous. You may assume that these two objects are in contact and they are isolated from the surroundings. [2]

(8) How is chemical potential related to the Gibbs free energy of system? [1]

(9) Discuss the following: (a) phase stability (b) phase diagram (c) phase boundary (d) phase transition (e) triple point. [4]

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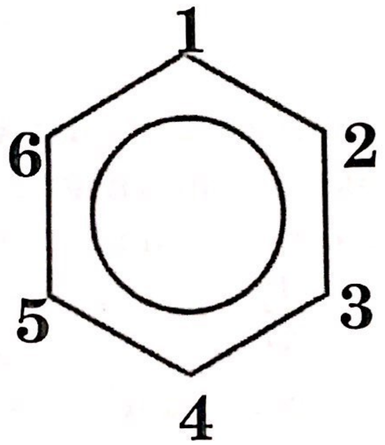
End Semester Exam (Monsoon 2019)

Science I

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

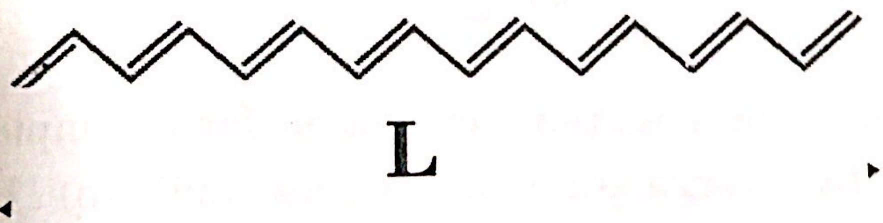
(1) The following figure shows the structure of a benzene molecule, whose carbon atoms are numbered from 1 to 6. Using the paricle on a ring model, calculate the probability of finding a pi-electron between carbons 1 and 4 of the benzene molecule (you can assume that these pi-electrons are free particles on the ring). 1/2 [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). 0

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



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(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]

$$\psi(x) = A e^{-\frac{m\omega x^2}{2\hbar}}$$

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). $A = \frac{1}{\sqrt{2\pi}}$ $\Delta x \cdot \Delta p$ $\langle x \rangle \cdot \langle p \rangle$

(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?

(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]

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(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]**

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