Swaraj

Mid Semester Examination I – Monsoon 2018
IIIT-Hyderabad

Subject: Science I

Full Marks: 40 Time: 90 min

Use of non-programmable scientific calculator is allowed

1) (a) Derive the one-dimensional diffusion equation starting from the one-dimensional random walk model. [2]

(b) Solve the one-dimensional diffusion equation using the Fourier transformation method. Plot (in a single plot) the solutions of the diffusion equation at time $t = 0$, $t \to \infty$, and $t = t_1$, and $t = t_2$ such that $\infty > t_2 > t_1 > 0$. [5+2]

2) Calculate the mean displacement and the mean square displacement of
   a) a random walker in one-dimension after N steps starting from the origin.
   b) a solute, which is restricted to move in one dimension, surrounded by solvent molecules whose diffusion is described by the one-dimensional diffusion equation (after N steps starting from the origin).
   c) a one-dimensional solute in a solvent whose dynamics is described by the Langevin's equation. [6+6+5]

3) (a) Define the Hamiltonian function for an isolated classical system consisting of N interacting particles. (b) What is phase space? (c) How do you describe the microscopic dynamics of this system using the Hamiltonian function? [1+1+2]

4) Consider the random walk problem in one dimension, the probability of a displacement between s and $s+ds$ being

$$w(s)ds = (2\pi\sigma^2)^{\frac{-1}{2}} e^{-(s-l)^2/2\sigma^2} ds$$

After N steps,

(a) What is the mean displacement $\langle x \rangle$ from the origin?

(b) What is the dispersion of $\langle (x - \langle x \rangle)^2 \rangle$?

(Here, l and σ are constants.)

[10]

$p^2 (p+q)^N$ $\frac{K\sqrt{Dt}}{1} + \frac{ix}{2\sqrt{Dt}}$

$p^2 (N)(p+q)^{N-1}$ $\left(\frac{2KDt + ix}{2\sqrt{Dt}}\right)^2$

$Np^2 + p^2(N^2 - N)$

$Np^2 + p^2N^2 - pN$

$N(p^2 - p)$.

Mid Semester Examination-II Monsoon 2018
IIIT-Hyderabad
Subject: Science I

Total: 45 marks **Time: 1.5 hrs**

1) When a particle with spin 1/2 is placed in a magnetic field H, its energy level is split into $-\mu H$ and $+\mu H$ and it has a magnetic moment μ or $-\mu$ along the direction of the magnetic field, respectively. Suppose a closed system consisting of N such particles is in a magnetic field H and is kept at a constant temperature T. Find the internal energy, the entropy, the specific heat capacity and the total magnetic moment M of this system. (7)

2) N monomeric units are arranged along a straight line to form a chain molecule. Each monomeric unit is assumed to be capable of being either in an α state or in a β state. In the former state, the length is a and the energy is E_α. The corresponding values in the latter state are b and E_β. Derive the relation between the length L of the chain molecule and the tension X applied between the both ends of the molecule. (Hint: assume that it is a closed system at constant tension). (10)

3) Calculate the number of accessible microstates and the entropy of an isolated system of N ideal gas atoms confined in a cubic box of volume V. (4)

4) A cylinder of radius R and length b rotates about its axis with a constant angular velocity ω. Evaluate the density distributions of an ideal gas enclosed in the cylinder. Ignore the effect of gravitation. Carry out classical calculations assuming that thermal equilibrium is established at T. (Hint: The Hamiltonian that describes the motion in a rotating coordinate system is $H^* = H - \omega L$, where H is the Hamiltonian in the coordinate system at rest and L denotes the angular momentum). (10)

5) Derive the equation of state for a) an ideal gas and b) a dilute real gas consisting of N identical particles in a cubic box of volume V maintained at temperature T. (4 + 6)

6) Derive the relationship between the energy fluctuation and heat capacity of a closed system. (4)

End Semester Examination (Monsoon 2018)
IIIT-Hyderabad
Subject: Science I

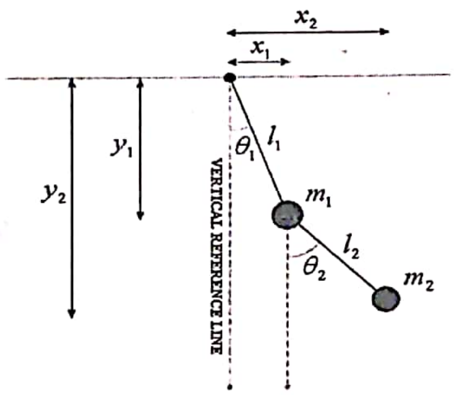
Total: 60 marks **Time: 3 hrs**

1) Consider a classical system of N noninteracting identical homonuclear diatomic molecules enclosed in a box of volume V at temperature T. The Hamiltonian for a single molecule is taken to be

$$H(p_1, p_2, r_1, r_2) = \frac{1}{2m}(p_1^2 + p_2^2) + \frac{1}{2}K|r_1 - r_2|^2$$

where $\mathbf{p_1}$, $\mathbf{p_2}$, $\mathbf{r_1}$, $\mathbf{r_2}$ are the momenta and coordinates of the two atoms in a molecule, m is the mass of each atom, and K is a positive constant. Find
(a) the Helmholtz free energy of the system;
(b) the heat capacity at constant volume;
(c) the mean square molecule diameter $\langle|\mathbf{r_1}-\mathbf{r_2}|^2\rangle$. [10]

2) Determine the equation of motion of a coplanar double pendulum (shown below) using the (a) Lagrangian mechanics and (b) Hamiltonian mechanics. [12]



3) a) An electron is moving freely inside a one-dimensional infinite potential box with walls at $x = 0$ and $x = L$. The width of the box is 2×10^{-10} m. If the wave function of the first excited state is $\psi(x) = \sqrt{\frac{2}{L}}\sin\left(\frac{2\pi x}{L}\right)$, what is the probability of finding the electron between $x = 0$ and $x = 10^{-10}$ m in that state.

b) Calculate the expectation values of position $\langle x\rangle$ and of the momentum $\langle p_x\rangle$ of a particle in the one-dimensional box when it is in the n^{th} state. [3 + 3]

4) Calculate the entropy of an isolated one-dimensional classical harmonic oscillator of energy E. [4]

5) (a) What are Euler angles? Why do we need them? You need to write the final rotation matrix in terms of Euler angles.

(b) Using space-fixed and rotated frames of reference, determine the rotation matrix for a rotation about an arbitrary axis by an arbitrary angle. [5+3]

6) Calculate the mean square displacement of a solute in a solvent using (a) the random walk model (b) the diffusing equation and (c) the Langevin dynamics. You may assume that the system is one dimensional. [4+4+4]

7) (a) Using a phase diagram, discuss (a) phase boundaries (b) phase transitions (c) phase stability (d) triple point.
(b) How do you determine the equation of a phase boundary? You may consider any phase boundary of your choice. [4+4]

$\langle \Delta m \rangle = n_1 - n_2 = 2n_1 - N$

$\langle (\Delta m)^2 \rangle =$ $P(x,t)$

$$\frac{dP}{dT} = \frac{S_\beta - S_\alpha}{V_\beta - V_\alpha} = \frac{\Delta S_{tran}}{\Delta V_{trans.}}$$