SISSA ISAS

SCUOLA INTERNAZIONALE SUPERIORE DI STUDI AVANZATI - INTERNATIONAL SCHOOL FOR ADVANCED STUDIES

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Solve **one** of the following problems (no extra credit is given for attempts to solve more than one problem). Write out solutions clearly and concisely. State each approximation used. Diagrams welcome. Number page, problem, and question clearly. Do not write your name on the problem sheet, but use extra envelope.

Problem 1

Consider a gas of independent particles. Each particle can be in a state $k = 0, 1, 2, \ldots$. In a time interval dt, for each particle one of the following processes may occur:

- with probability ηdt the state *spontaneously* increases by one: $k \to k+1$

- with probability $k dt$ the state *spontaneously* decreases by one: $k \to k-1$

• Write the master equation for this process and find the stationary state distribution $P_0(k)$ of k. (*Hint:* use the generating function $P(z) = \sum_{k=0}^{\infty} P(k)\, z^k$.) Now consider a case where we switch on the interaction between particles by introducing the following additional process:

- in a time interval dt with probability ξdt particle i collides with a particle j chosen at random, and if $k_j > 1$ then $k_i \to k_i + 1$, otherwise k_i is unchanged. The interaction leaves k_j unchanged.

Consider the mean field approximation where the probability $P_\xi(k,t)$ has the same functional form of $P_0(k)$ but the average $\langle k \rangle = c(t)$ depends on time.

• Discuss qualitatively the behavior of the system, within this approximation, as a function of the interaction parameter ξ for $\eta \ll 1$.

• Will the gas always reach the same stationary state independently of the initial condition?

Problem 2

Consider a system with two energy levels, $E_A = 0$, $E_B = \epsilon > 0$ occupied by N particelle that are in thermal equilibrium at a temperature $T = 1/\beta$ ($K_B = 1$).

1. Calculate the probability, P_n to find n particles in the ground state (state A). Assume that the particles are classical (i.e. subject to Boltzmann statistics). Then calculate the average energy for the system , $\langle E \rangle$, specific heat and average number of particles in the ground state $\langle n \rangle$ as a function of β. Summarise your results in a qualitative sketch for the behaviour of the calculated quantities.

2. Repeat the above calculation for particles obeying Bose statistics. Compare the behaviour of the calculated quantities for $T \to 0$ and $T \to \infty$ for the two cases of Boltzmann and Bose statistics.

3. Assume that detailed balance is satisfied, and that $W(n \to n')$ indicates the rate of transition from n to n' particles in the ground state. Calculate

$$\frac{W(n \to n-1)}{W(n-1 \to n)} \tag{1}$$

   in the classical and quantum (Bose) case and discuss the differences.

4. Assume that

$$W(n \to n-1) = \frac{1}{W(n-1 \to n)} \,. \tag{2}$$

   and that all transition rates $W(n \to n')$ are zero if $|n - n'| > 1$. At time $t = 0$ the system is prepared with all particles in the excited state (state B). Calculate how P_n increases at early times ($t \approx 0$) in the classical and quantum case.

Problem 3

Please provide a concise and reasoned answer (about 200 words) to at least three of the following questions.

1. Describe the structural properties of a α helix.
2. Outline the principles of a method for electronic structure calculations.
3. What are the main experimental tools for the determination of the 3D structure of proteins?
4. What are the main differences between RNA and DNA?
5. What is the physical basis for the catalytic power of enzymes?
6. Describe briefly the nature of hydrogen bond interactions.
7. What are the basic ingredients of an alignment between the sequences of two proteins?
8. How can one built a 3D structural model of a protein based on another protein whose structure is known and whose primary sequence is very similar?
9. Describe briefly the nature of hydrophobic interactions.
10. Outline the principles of molecular dynamics simulations.