SISSA ISAS

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

Statistical and Molecular Biophysics PhD Program

Entrance Exam 2006 - October Session

Address Problem 1 if you intend to follow the Experimental Curriculum of the PhD Program.

Solve one of problems 2-4 (no extra credit is given to solve more than one problem) if you intend to follow the theoretical curriculum of the PhD program. Write solutions clearly and concisely. State each approximation used. Diagrams welcome.

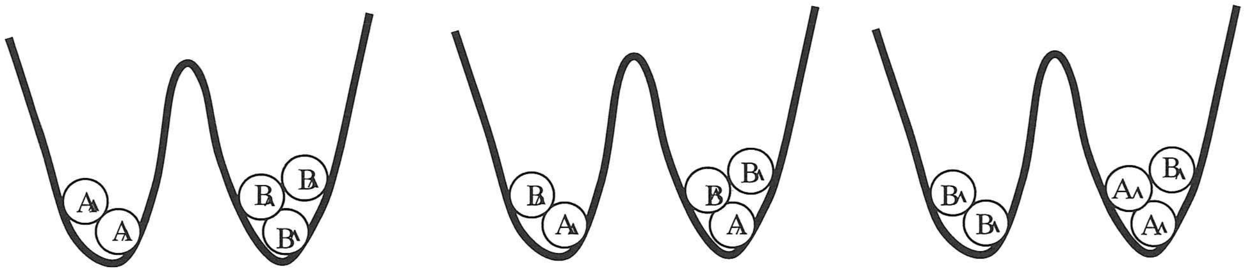
Number page, problem and question clearly. Do not write your name in the problem sheet but use envelope.

Problem 1.

The candidate will describe an experimental technique of her/his choice in Biophysics, Biophysical Chemistry, Biotechnology or Nanotechnology (in this latter case the Biocomponent may be missing) clearly but briefly (approximately in the number of words contained in three typewritten pages), explaining the following three aspects: (one page each) 1) What the technique is all about 2) why the technique is of general interest and what problems it solves and 3) Why the candidate finds the technique particularly interesting or intriguing (i.e. how the technique relates to the culture of the candidate). Finally the candidate will summarize the whole in a half page of writing. A paper that will contain also numbers with units (for instance about sensitivity levels and noise sources) will be rated higher than a paper that contains only vague statements. If the candidate culture does not allow for too specific writing please pay attention to the paper's organization and logic that will need to be present especially in absence of numbers.

Problem 2.

Consider a system made of 5 particles that live on a one dimensional free energy profile. The profile has two wells that accommodate respectively 2 and 3 particles. The 5 particles are of two different types, A and B, and there are 2 particles of type A and 3 of type B. Hence, the system can exist in one of the three configurations depicted below:



State 1 **State 2** **State 3**

Transitions between these three configurations are obtained exchanging at random two particles, one in the first well and the other in the second.

1.Assuming that: (i) the free energy of the three configurations is the same; (ii) all the transitions require the crossing of a free energy barrier of identical height and (iii) the probability not to perform any exchange transition in a unit of time τ is equal to 1/2, compute the transition matrix for the system.

2.What is the stationary probability distribution of the system?

3.Assuming the system is prepared at time zero in the state 1, compute the probability that the system at time $t=i\ \tau$ (after i units of time) is observed in the state 1,2 and 3.

4.We now consider an observable defined as the number of particles of type A in the first well (we denote this number by n). Compute the average value $<n>$ and, for the same initial condition of point 3, the autocorrelation function $<n(0)n(t)>$

5. If the unit of time τ introduced in point 1 is equal to one ns, what is the order of magnitude of the barrier (in units of k_BT) that the system has to cross in order to perform an exchange transition? (Hint: the attempt frequency in most microscopic systems is of the order of 10^{-13} seconds)

Problem 3.

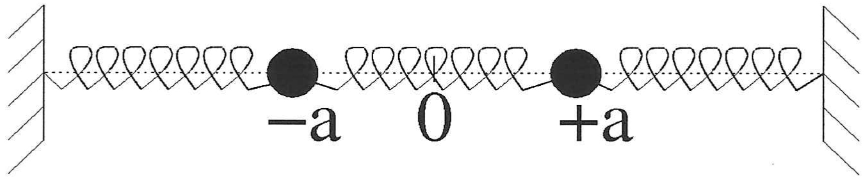
Calculate the Hückel π-electron energy and the energy levels of at least three neutral unsaturated molecules containing four carbon atoms.

Compare the π-electron energies of the three systems with that of two ethylene molecules. Determine which molecule has the largest delocalization energy according to Hückel theory.

For at least one of them determine the coefficients of the molecular π-orbitals and draw a simple sketch of them.

Problem 4.

Consider two particles of mass m_1 and m_2 constrained to move on a line. As shown in the figure, three springs of equal strength connect the particles with themselves and with a nearby wall and act so to penalize deviations of the particles from their rest positions at x_1=-a and x_2=+a.



The potential energy for the system is therefore

$$U(x_1, x_2) = \frac{k}{2}(x_1 + a)^2 + \frac{k}{2}(x_2 - a)^2 + \frac{k}{2}(x_2 - x_1 - 2a)^2$$

1. Characterize the normal modes of the system. In particular discuss the case where the masses m_1 and m_2 are equal.

2. Assume that the system fluctuates in thermal equilibrium at temperature t. The springs can be considered sufficiently strong that the particles never collide against the nearby wall. Provide an expression for the probability distribution of the positions, $P(x_1, x_2)$.

3. Calculate the mean square value of the mid point of the particles, $\left\langle \left(\frac{x_1 + x_2}{2} \right)^2 \right\rangle$ and of the relative displacement of the particles $\langle (x_1 - x_2)^2 \rangle$.

4. How does the mass of the particles affect the results of the previous question?

5. Calculate the mean square displacement of the first particle, $\langle (x_1 - a)^2 \rangle$.