SISSA ISAS

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

I-34014 Trieste ITALY - Via Beirut 4 - Tel. [+]39-40-37871 - Telex:460269 SISSA I - Fax: [+]39-40-3787528

Entrance Examination Physics and Chemistry of Biological Systems October 2011

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. All essays/solutions should be written in English. Do not write your name on the problem sheet, but use extra envelope.

Problem n. 1 – Interacting molecules on a lattice

One molecule of type A and N_B molecules of type B are free to move on a lattice of N equivalent sites. Molecules of different types feel an on-site attractive interaction energy ϵ (i.e. the energy of two molecules of different types on the same site is $-\epsilon$). Molecules of the same type feel no mutual interaction, and each site of the lattice can contain an arbitrary number of molecules. The system is at equilibrium at temperature T.

1. For $N_B = 1$ and $\epsilon = 0$ (i.e. non-interacting molecules) compute the probability to find the molecule of type A and the molecules of type B on the same site.

2. For $N_B = 1$ and $\epsilon \neq 0$ compute the probability to find the molecule of type A and the molecule of type B on the same site as a function of the interaction energy ϵ and of the system temperature T.

3. For $N_B > 1$ and $\epsilon \neq 0$ compute the probability to find at least one molecule of type B on the same site as the molecule of type A. *Hint: the probability distribution of each of the B molecules is independent from the other B molecules.*

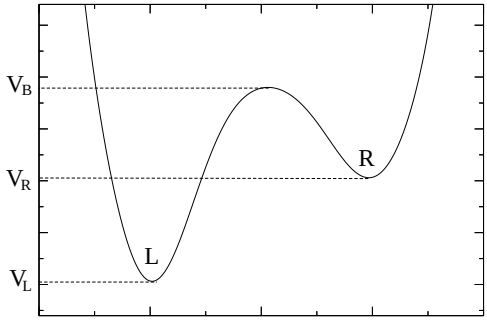
4. In the limit of large number of lattice sites and at fixed concentration c of molecules of type B (i.e. $N \to \infty$ and $N_B = cN$) compute the concentration c_{50} for which the probability of finding at least one molecule of type B on the same site as the molecule of type A is equal to 50%.

5. Now assume that each site cannot contain more than one molecule of type B (i.e. there is an infinitely strong repulsion among B molecules). Is the c_{50} increased or decreased?

6. Calculate an explicit expression for the c_{50} in the last point.

Problem n. 2 – Two interacting particles on a one-dimesional potential

Consider a single particle moving on the one-dimensional potential depicted in figure, at a temperature $T = 1$.



Denote by $p_L(t)$ (resp. $p_R(t)$) the probability of observing the particle in the minimum labelled by L (resp. R). If $V_B - V_L \gg 1$ and $V_B - V_R \gg 1$, $p_L$and p_R satisfy the rate equation

$$\begin{aligned} \frac{dP_L}{dt} &= -k_{LR}P_L + k_{RL}P_R \\ \frac{dP_R}{dt} &= k_{LR}P_L - k_{RL}P_R \end{aligned}$$

where k_{LR} (resp. k_{RL}) is the rate for a transition between L and R (resp., between R and L)

- Compute the equilibrium probability to observe the particle in L.
- Assume now that $k_{LR} = 130$ s^{-1} and $k_{RL} = 100$ μs^{-1}. Provide an approximate estimate of $V_R - V_L$.
- Consider now N identicle non-interacting particles moving on the same potential. Compute the equilibrium probability to observe *at least one* particle in L.

Take now $N = 2$ and assume that the two particles interact with a constant energy E_{int} when they are both in L or when they are both in R, while they don't interact when they are one in L and the other in R.

- Compute the equilibrium probability to observe the two particles in L.
- Write a rate equation in the probability of observing the system in the three relevant states. Provide an approximate expression of the rates as a function of k_{LR}, k_{RL} and E_{int} (assume $V_B - V_L - E_{int} \gg 1$ and $V_B - V_R - E_{int} \gg 1$).

Problem n. 3 – Logistic Equation and Allee effect

The following nonlinear ordinary differential equation is often used to describe continuous-time growth rates of a population x

$$\frac{dx}{dt} = rx(1-x), \qquad x \geqslant 0, \tag{1}$$

where $r > 0$ is a parameter.

- Study the solution, that is, verify whether it is consistent with "being a population", compute the steady states, and analyze their stability character (e.g. through a linearization of the ODE or through qualitative arguments). Analyze the asymptotic behavior, drawing a qualitative plot of the solution in a (t, x) plane.
- What happens for $r < 0$?
- Can you solve Eq. (1) explicitely?

A generalization of Eq. (1) is given by the following equation

$$\frac{dx}{dt} = rx\left(1-(x-\alpha)^2\right), \qquad x \geqslant 0, \qquad 0 < \alpha < 1, \quad r > 0 \tag{2}$$

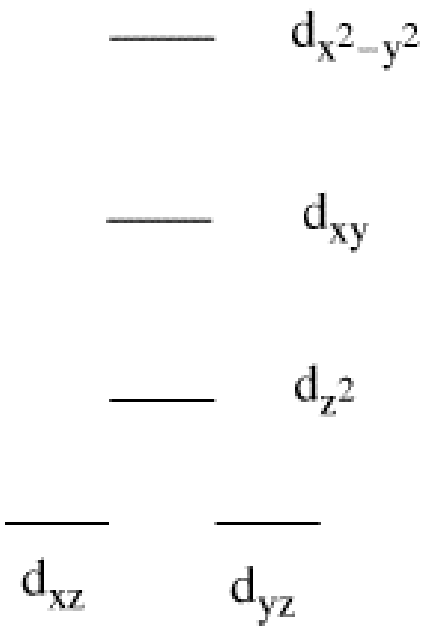
Explain why this equation is more suitable than (1) to represent an effective growth rate $\frac{\dot{x}}{x}$ which is maximal at intermediate concentrations of x (so-called Allee effect).

Problem n. 4 – Alkene coordination to transition metals

The Zeise's salt is a compound of formula $K[PtCl_3(C_2H_4)] \cdot H_2O$. The anion of this salt exhibits a square planar geometry and contains a η^2-ethylene ligand.

Using the Hueckel approximation write the energy and the coefficients of the π-molecular orbitals of ethylene.

Considering that the splitting of the d orbital in a square planar field



draw the geometry of the platinum complex and its coordination ligands. Which is the difference in the geometry of ethylene when it is isolated or coordinated to the platinum ion? Considering that Pt is d^{10}, which is the spin state of the coordination compounds?

How would you expect the geometry of the $[PtC_3H_5Cl_2]^-$ on the basis of the shape and the coefficients of the molecular π-orbitals of the allyl radical as obtained from the Hueckel approximation?

Problem n. 5 – Bioinformatics: sequence-structure relationships in proteins

Protein relatedness can be assessed at the sequence and structural level. Discuss the principles and algorithmic strategies of bioinformatics approaches that are available to:

1. detect evolutionary relationships in proteins based on similarity of their primary sequence and
2. to cluster them them in structural classes.
3. Finally, discuss the sequence-structure relationship in proteins.