SISSA ISAS
SCUOLA INTERNAZIONALE SUPERIORE DI STUDI AVANZATI - INTERNATIONAL SCHOOL FOR ADVANCED STUDIES
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April 2011 – Entrance Examination: Physics and Chemistry of Biological Systems

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 – Equilibrium and stationary flux

Consider a system that can exist in three states, A, B and C. The probability at time t to observe the system in A, B or C is denoted as $p_A(t)$, $p_B(t)$ and $p_C(t)$respectively. The time evolution of these probabilities is described by the rate equations:

$$\begin{aligned}
\frac{dp_A}{dt} &= -k_{AB}p_A + k_{BA}p_B \\
\frac{dp_B}{dt} &= -\left(k_{BA} + k_{BC}\right)p_B + k_{AB}p_A + k_{CB}p_C \\
\frac{dp_C}{dt} &= -k_{CB}p_C + k_{BC}p_B
\end{aligned}$$

- What is the equilibrium probability to observe the system in B? (hint: use the normalization condition $p_A + p_B + p_C = 1$)
- What is the net probability flux between A and B in equilibrium conditions?
- How many time constants role the relaxation of the system towards equilibrium? Express these time constants as a function of the rates k.

Assume now that a source is placed in A and a sink in C, in such a way that $p_C(t) = 0$ and $p_A(t) = p_S$.

- Write an equation describing the time evolution of $p_B(t)$. Solve this equation with an initial condition $p_B(0) = 0$.
- What is the stationary probability to observe the system in B?
- What is the net probability flux between A and B in stationary conditions?

Problem n. 2 – Ideal Gas

Consider a macroscopic vessel (for example a cylindrical vessel closed by a piston of neglegible mass and that can slide without friction) containing an ideal gas in normal conditions (P=1 atmosphere $\sim 10^5$ Pascal, temperature T=300K). The molecular weight of the gas is 40 g/mol and the gas particles have diameter $d = 0.4$nm.

1. Estimate the the typical velocity of a gas particle, $\bar{v}$ and estimate the typical distance, λ, between nearby gas particles.
2. The gas particles experience fequent collisions with each other inside the vessel. Provide an estimate of the rate at which a given gas particle experiences these collisions. For simplicity you can assume that all collisions are "head-on" (i.e. particles meet coming from opposite directions) and that all particles have velocity $\bar{v}$.
3. Estimate the mean free path, l, that is the mean distance that a gas particle covers between two consecutive collisions with the other gas particles.
4. Compare λ and l and discuss their dependence on the temperature T, pressure P.

Useful data: $K_B = 1.38\,10^{-23} J/K$, $N_{Avogadro} = 6.02\,10^{23}$

Problem n. 3 – Force-stretch repsonse of an elastic elastomer

This problem is motivated by the study of the elastic repsonse of polymers (elastomers). Consider a strip of elastomer, of undeformed size $L_x \times L_y \times L_z$, tested in uniaxial extension. This means that the faces parallel to the z-axis are force-free, while the z-component of the displacement $\mathbf{u}$ are prescribed on the two faces perpendicular to z. We take $u_z = 0$ on the face $z = 0$ and $u_z = L_z + \lambda L_z$ on the face $z = L_z$, so that $\lambda \geq 1$ is the imposed stretch. Assuming that the elastomer is incompressible and governed by the Neo-Hookean elastic energy density

$$W(\mathbf{F}) = \frac{\mu}{2}|\mathbf{F}|^2 \tag{1}$$

where $\mu > 0$ is a material parameter and the matrix $\mathbf{F} = \nabla \mathbf{y}$ is the gradient of the map $\mathbf{y}$ describing the deformation of the strip, find:

1. the equilibrium force-stretch response (i.e., find the z-component of the force required to stretch the strip by λ, and plot it as a function of λ);
2. the initial Young modulus of the elastomer (i.e., the slope of the force-stretch curve at $\lambda = 1$);
3. the physical meaning of the material parameter μ.

Problem n. 4 Bioinformatics: sequence alignment

1. discuss the impact that sequence alignment of proteins and nucleic acids has had for the understanding and characterization of the salient properties of these biomolecules.
2. discuss the key concepts at the basis of such methods. Elaborate on the use of scoring matrices and gap penalties and explain how they are calculated.
3. Outline in detail one of the algorithms that are used for pairwise sequence alignment (e.g. dynamic programming, ...) and discuss how the statistical relevance of an alignments is estimated.
4. Ouline a possible strategy to carry out multiple sequence alignment.