SISSA ISAS

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April 2006 – Entrance Examination: Statistical and Molecular Biophysics - Curriculum in Theory/Computation

Solve one of the following two 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 walker on a one-dimensional lattice with spacing a. At regular time intervals of duration Δt, the walker moves with probability p by one lattice spacing to the right and with probability $q = 1 - p$ by one spacing to the left. The walker is in the origin, $x(0) = 0$ at time $t = 0$.

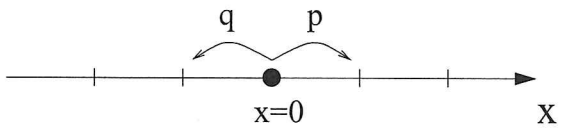


Figure 1: .

Assuming that all steps taken by the walker are uncorrelated:

1. Compute the mean displacement, $\langle x(n) \rangle$ of the walker after n time steps. The mean is intended to be taken over many repetitions of the process.

2. Compute the mean square displacement of the walker, $\langle x(n)^2 \rangle$ after n time steps.

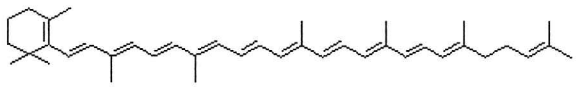
3. For the symmetric case, $p = q = 1/2$, sketch and comment the probability distribution for the position of the walker at sufficiently large times, $Prob[x(n)]$. Can you provide arguments to derive the probability distribution?

4. Repeat calculations [1] and [2] for the case where at each time step the walker moves by **two** lattice spacings to the right with probability $1/3$ and by one lattice spacing to the left with probability $2/3$.

5. Assume now that the steps are slightly correlated, that is the next step has a probability $1/2 + \epsilon$ to be in the same direction of the previous one. Assume ϵ to be a small positive quantity. Repeat calculations [1] and [2] to leading order in ϵ.

2 HOMO-LUMO transition in γ-carotene

γ-Carotene, one of the precursors of vitamin A, is a conjugated system containing 11 double bonds.



The π-electron wavefunctions of this compound may be described within the free electron molecular orbital model (FEMO). Here the inter-electronic repulsions $1/r_{ij}$ are ignored, and the effect of the σ electrons is represented by a (infinite) square-well potential.

1. Calculate the wavelength of light needed to excite the HOMO-LUMO transition of the π electrons for carotene using the simple FEMO. Assume that the effective length of the confinement box is given by

   $$l = (k + 1)a,$$

   where k is the number of carbon atoms in the conjugated π system, and a is about 1.4Å.

   Compare the calculated value with the observed transition at 460 nm.

2. To get a better estimate of the excitation energy one might introduce a perturbing potential of the form

   $$V(x) = A\left(x - \frac{l}{2}\right)^2$$

   that tends to favor the ends of the box. For what value of the constant A the calculated excitation energy is equal to the experimental energy?

Experimental Biophysics curriculum

The candidate has the choice between the following three themes , but should declare up front which one of the three he/she intends to follow.

1) Select a paper from an internationally peer-reviewed scientific journal and describe a proposal for a research program that would lead to the results reported in that paper

2) Select a paper from an internationally peer-reviewed scientific journal and describe a proposal for a research program that would extend to results reported in that paper

3) Write an original research proposal

ATOMIC UNITS AND THEIR SI EQUIVALENTS

Quantity	*Atomic unit*	*SI equivalent*
Mass	$m = 1$ (electron mass)	9.1091×10^{-31} kg
Charge	$\|e\| = 1$ (electron charge)	1.6021×10^{-19} C
Angular momentum	$\hbar = 1$	1.0545×10^{-34} J·s
Permittivity	$\kappa_0 = 4\pi\varepsilon_0 = 1$	1.1126×10^{-10} $C^2 \cdot J^{-1} \cdot m^{-1}$
Length	$\kappa_0\hbar^2/me^2 = a_0 = 1$ (bohr) (Bohr radius)	5.29177×10^{-11} m
Energy	$me^4/\kappa_0^2\hbar^2 = e^2/\kappa_0 a_0 = 1$ (hartree) (twice the ionization energy of atomic hydrogen)	4.35944×10^{-18} J
Time	$\kappa_0^2\hbar^3/me^4 = 1$ (period of an electron in the first Bohr orbit)	2.41889×10^{-17} s
Speed	$e^2/\kappa_0\hbar = 1$ (speed of an electron in the first Bohr orbit)	2.18764×10^{6} $m \cdot s^{-1}$
Electric potential	$me^3/\kappa_0^2\hbar^2 = e/\kappa_0 a_0 = 1$ (potential energy of an electron in the first Bohr orbit)	27.211 V
Magnetic dipole moment	$e\hbar/m = 1$ (twice a Bohr magneton)	1.85464×10^{-23} $J \cdot T^{-1}$