Problem Set # 3

Problem 1: An early Wormlike Chain model, from Marko-Siggia (1995) for force vs. extension is given below.

$$F_{WLC} := \frac{k_b \cdot T}{L_p} \cdot \left[\frac{1}{4 \cdot \left(1 - \frac{x}{L_c}\right)^2} - \frac{1}{4} + \frac{x}{L_c} \right]$$

On the Stellar web-site we've loaded a real DNA stretching curve obtained with an optical trap. Fit this data trace to this model and extract a contour length, L_c and persistence length L_p for this data curve. Plot your fit with the data (force vs. extension) and list your results for these two parameters. What region of the curve fits well? Where does the model have trouble? A good way to determine where a fit deviates from the data is to create a "residual trace" where you subtract the data from the fit. If the residuals are near zero, your fit is good. Make a residual trace and multiply by a factor that amplifies this trace relative to your curves (such as a factor of 5). Plot this along with your data and fit curve.

Problem 2: In translational diffusion three directions are included to generate a diffusion constant x= sqrt($6D_\theta$ t). For rotational diffusion, we only need to specify two angles in order to make a vector. Use this information to write down a relation for angular diffusion. Given that the rotational drag for a sphere is $\gamma_\theta = 8\pi\eta a^3$ where "a" is the radius, write an expression for D_θ in rad^2/s. How long will it take a 10μm diameter cell to rotate and randomize its orientation through $\theta = \pi/2$ degrees?

Problem 3: Draw the configurations for a 5 beaded polymer chain on a 2D lattice where chains are 5nm long and angles between chains are 90 degrees or straight. How many total microstates are there? If we group microstates by energy levels determined by the number of bead contacts which stabilize the molecule, see below for a bead contact in the ground state, how many energy levels are there and how many microstates are in each energy level? Write out a partition function, Q, for this system. If the energy of one bead contact group is $\varepsilon = 0$, and no bead contact $\varepsilon = 500$kcal/mole, compute the average end to end distance at room temperature. What is the average end to end distance at 400 degrees kelvin, what is it at very high temperatures?
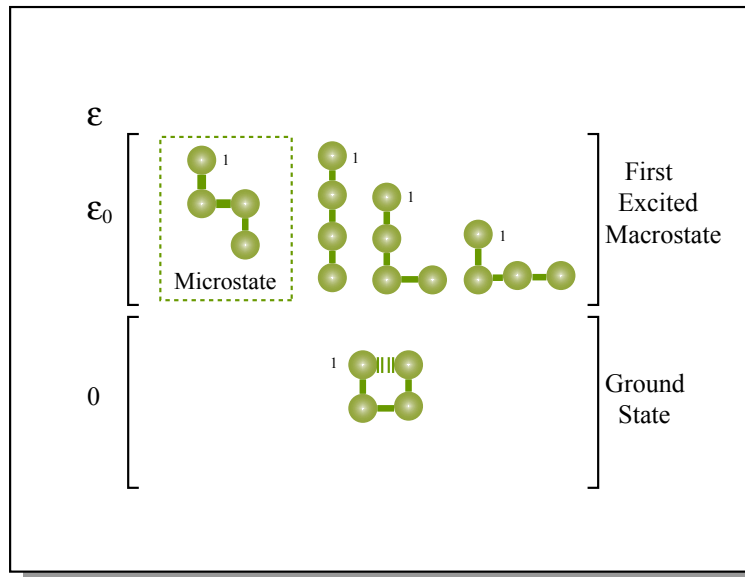
Figure by MIT OCW.

Problem 4: Consider a Gaussian model for a freely jointed chain in 3D, with N links of length b. The probability that the end of the chain is at location [x,y,z] when the beginning of the chain is at [0,0,0] can be obtained as:

$$P(x, y, z) = \left(\frac{3}{2\pi \, Nb^2} \right)^{\frac{3}{2}} e^{-\frac{3(x^2+y^2+z^2)}{2Nb^2}}$$

We see that the most probable location for the end of the chain is still at the origin. Now lets ask what is the most probably end to end distance, r_o, of the Gaussian chain? Is it zero?

Think through this problem by making an analogy to shooting arrows at a round target:
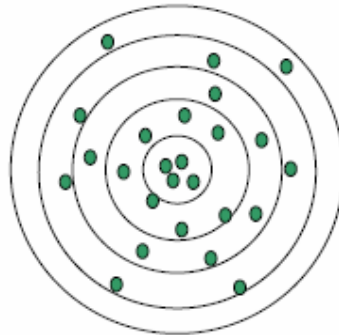
Now if you have great aim, the probability is maximum at the center of the target. But if you ask which ring has the most arrows, it may not be the center of the target. Why?

Use these lines of thought to find a value for r_o which maximizes the entropy, i.e., the probability of configurations where the end of the chain is located at a distance r_o from the origin.