Physics 120/240
Homework 1
Due 4/13/10

This homework has a lot of overlap with introductory statistical mechanics that you've probably already seen, but it may very well bring a new perspective to it.

Problems 1-10:

One important thing to be learned from this is an understanding of the applicability of the "Central Limit Theorem". Where it works and where it doesn't. Another thing is the relationship between what you already know and polymer statistics.

Problem 10 gets you to implement the ideas in these problems numerically.

Problems 11 and 12: *Closely related to 1-10, but with more direct applications to real systems like stretched DNA. 12 requires knowing about simulation techniques so only try this if you're already familiar with such techniques or you're really gung-ho about learning them!*

Problem 13 *is for those more experimentally inclined that want to see how all of this theory is relevant to real systems.*

I encourage you to team up with others for some or all of this homework!

The amount of this homework that you'll want to complete depends on how much of this is already familiar to you. The object is to get you to learn some more physics!

1. Consider N noninteracting Ising spins $\sigma_1, \ldots, \sigma_N$ where each spin is chosen with equal probabilities to have values ± 1. The Hamiltonian (or energy) of this system is

$$E = h \sum_{i=1}^{N} \sigma_i$$

where h is some parameter that can be thought of as a (negative) magnetic field. Using combinatorics (or the binomial distribution), calculate the number states that the system can have at energy E.

2. Define the entropy per spin $s \equiv S_{total}/N$ and the energy per spin as $e \equiv E/N$. Use the simplified Sterling's formula

$$n! \approx n^n e^{-n}$$

to find an expression form $s(e)$ in the limit of large N.

3. The result of the last problem is the entropy in the "microcanonical", or constant energy, ensemble. Let's do the calculation in the "canonical", or constant temperature, ensemble. Consider the same system but now held at constant temperature.

a The partition function Z for this system can be easily calculated. Do this by realizing that the spins are noninteracting so that the system breaks up into N subsystems.

b Now calculate the free energy F.

c By the appropriate differentiation, calculate the energy E.

d Recall that $F = E - TS$. From this and the answer to the last part, calculate S as a function of T (or β). Then find $s(e)$ as before. To do this, you'll have to invert a tanh which can be expressed in terms of a logarithm. Your result should be identical to the one found in the previous problem.

    4.

a Calculate $< E^2 >$. The average is over all possible spin configurations all of which are weighted equally. This can be thought of several different ways. One is an average weighted by the probability distribution in problem 1. This isn't the easiest way to calculate this. Instead write E in terms of the σ_i's which leads to a double sum. Using independence of the spins the cross terms can be eliminated.

b Calculate $< exp(cE) >$ where c is an arbitrary constant. The easiest way to do this is similar to part a; if E is expressed as a sum over spins, this can then be written as a product (similar to the calculation of the partition function). Using independence allows you to decouple all terms.

    5. Find an expression for the probability distribution $P(E)$ near $E = 0$ for large N. Do this by expanding out the logarithms found in problem 2. *Hint: Make sure to go to 2nd order in the expansion of the logs!* Your result should be a Gaussian.

    6. Using the Gaussian approximation of problem 5, recalculate the averages of problem 4. The easiest way to do these is directly, for example

$$< E^2 >= \int_{-\infty}^{\infty} E^2 P(E) dE.$$

Compare your results to the exact ones found in problem 4.

    7. Do a rough sketch of

a the exact $P(E)$ versus E, and also $\ln P(E)$ versus E,

b the Gaussian approximation for both $P(E)$ versus E, and $\ln P(E)$ versus E.

Display the essential features, such as the width of the distribution and how the two cases differ.

    8. Now explain qualitatively from the sketches in the last problem why the approximate results found in problem 6 either work well, or don't.

    9. How do the last eight problems relate to the problem of a random walk? Find a mapping between a random walk and the spin system discussed above. How is the force related to the "spin" β found before?

10. Calculate the probability distribution of a random walk this numerically as follows.

a Write a program that generates a random sequences of -1's and 1's and sums N of them up at a time. You don't have to use the best random number generator in the assignment, for example, you can use the unix "rand" function. Be careful however not to do something like `rand()%2`. That is a big no no. Instead you want something that divides by the right big number to first create a random number that goes between 0 and 1. Use that to decide if the answer should be 1 or -1. This (`ran()` and many useful macros are defined in Josh's `http://physics.ucsc.edu/~josh/120/defs.h`

b Take the resulting sum and assign it to a "bucket" which takes the form of an array. You can allocate all the memory it uses in advance, or do so dynamically using a more general scheme such as Josh's `http://physics.ucsc.edu/~josh/120/hist.c` and `http://physics.ucsc.edu/~josh/120/hist.h`

c After enough averages, you should be able to plot your histogram by writing it to a file and using gnuplot or some other graphing tool.

Alternatively, you can do this in SciPy. Here's a hints file: `http://physics.ucsc.edu/~josh/120.10/home1/binomial_hints.py` The histogram and the random walk generation is done with just a few lines of code. Fill in the lines of code according to the instructions in the file. You should be able to compare your result to the exact result of the binomial distribution, and the Gaussian approximation.

11. *An "ideal" stretched chain.* Consider a chain that doesn't interact with itself, but is connected by rigid links of length a. The links can freely rotate about each other, in the absence of an external force. But now say that the ends of the chain are grabbed by something, and stretched. Experiments like this have been done with "optical tweezers" on biomolecules such as DNA and RNA. The energy of the chain when stretched is $H = \mathbf{f} \cdot \mathbf{R}$. $\mathbf{f}$ is the applied force and $\mathbf{R}$ is the end-to-end distance.

a Write the end to end distance as a sum over vectors describing the separation of adjacent monomers $\mathbf{r}_i$.

b Compare this with the Heisenberg model for non-interacting spins in a field. Figure out the correspondence between the two problems.

c Write down the partition function for an individual "spin", or $\mathbf{r}_i$. Solve the partition function (in three dimensions).

d Relate the average "spin", i.e. $\langle z \rangle$ for a single $\mathbf{r}_i$ to a derivative of the partition function. Then calculate the average end to end distance as a function of the force f. *Hint: How do you relate $\langle z_i \rangle$ to this?*

e Calculate the limiting behavior of your answer for large f and for small f and sketch your results.

f Redo the above for a polymer that lives on a lattice. Each link between adjacent monomers $\mathbf{r}_i/a$ equals $\pm\hat{i}$, $\pm\hat{j}$, or $\pm\hat{k}$. How similar does this model look to the one above?

If you already know how to do Monte Carlo or molecular dynamics simulations

12. Come up with and algorithm, or pseudo-code (or real code if you're psyched enough!) to simulate problem 10, above. You can do this for the continuous case, part (a), or the lattice case part (f). You could try two approaches, Monte-Carlo, or molecular dynamics, the latter being a lot harder for this model with fixed links. It is not clear how to do anything like molecular dynamics for a lattice model, but there have been some attempts to do so.

13. Do a literature search on experimental work showing the stretching of DNA, using for example, optical tweezers. Google Scholar is a good place to start. Good keywords: DNA force optical length. Find a paper that describes how this is done experimentally and briefly summarize it. How do the results compare with theoretical predictions?