**Homework 5**

Optional

# Statistical Mechanics of Linear Systems & Quadratic Path Integrals

1. Examine a general linear system, say an arbitrary network of springs under the influence of constant forces. You can write the Hamiltonian for this as

$$H = \frac{1}{2}\sum_{i,j=1}^{n} x_i M_{i,j} x_j + \sum_{i=1}^{n} N_i x_i$$

where $\mathbf{M}$ is a real symmetric matrix and $\mathbf{N}$ is a real vector. Two degrees of freedom, say $x_0$ and $x_1$ are *held fixed*. Besides these two constraints, the system is free to fluctuate at temperature $T$. So you can define the partition function with $x_1$ and $x_2$ held fixed by

$$Z(x_1, x_2) = \int e^{-H/T} dx_2 dx_3 \dots dx_n$$

Calculate $Z(x_1, x_2)/Z(0, 0)$ as follows

   (a) Minimize $H$ keeping $x_1$ and $x_2$ fixed to obtain a formal expression for $x$'s at the minimum. Your result should involve the inverse of a matrix.

   (b) Taylor expand H around this minimum to *all orders*. This is not as hard as it might sound.

   (c) Rewrite $Z(x_1, x_2)$ in terms of integrals over the difference between the $x_i$'s and $x_{min,i}$.

   (d) Calculate $Z(x_1, x_2)/Z(0, 0)$ by noticing a large cancellation of integrals. You should then have a formal answer involving matrices and their inverses. The important thing to note is the dependence on temperature and $x_1$ and $x_2$.

   (e) For an arbitrary $x_m$, how does $\langle x_m \rangle$ depend on temperature? How is it related to the zero temperature result?

2. The results of the last problem can be thought of in terms of path integrals which involve an infinite number of variables indexed by $s$. Instead of integration being over $d\mathbf{r}_3 d\mathbf{r}_4 \dots d\mathbf{r}_m$, it is often written $\delta\mathbf{r}(s)$ In analogy to the previous problem, consider a partition function

$$Z(r_0, r_L) = \int e^{-\frac{3}{2l}\int_0^L |\frac{dr}{ds}|^2 ds - \int_0^L v(r(s)) ds} \delta\mathbf{r}(s)$$

This represents a polymer chain in an external potential $v(\mathbf{r})$. It is often called the Greens function for the polymer. Here the ends are fixed at $r(0) = r_0$ and $r(L) = r_L$. Consider the case of a one dimensional quadratic potential $v(\mathbf{r}) = \frac{k}{2}x^2$. It also represents the imaginary time path integral of an electron in a quadratic potential.

Calculate $Z(r_0, r_L)/Z(0,0)$ in analogy to the last problem as follows.

(a) Make the analogy to classical mechanics with $s \to t$. $L \to T$, $3/l \to m$. Then miminimizing the exponent of above, is like minimizing an action $\int Ldt$ with Lagrangian $L = T - V$. Find $T$ and $V$, and with this interpretation, write down Newton's second law for this system.

(b) Solve Newton's equations with the appropriate boundary conditions. This represents the "classical path" for the system.

(c) Using the result of the last problem, calculate $Z(r_0, r_L)/Z(0,0)$. The calculation should only involve the above classical path. The result is a little complicated, but should be no more than a few lines long. This is a much easier approach than more standard methods for calculating Greens functions.

3. Consider the Hamiltonian of the first problem. We can add an external force to it at one point say the $m$th degree of freedom.

$$H \to H + f_m x_m$$

(a) Write down a formal expression for the partition function in this case, and also $\langle x_j \rangle$ where $j$ is also arbitrary.

(b) Relate

$$\frac{\partial \langle x_j \rangle}{\partial f_m}$$

to the two point correlation function $\langle x_m x_j \rangle$. *Hint: try differentiating.*

(c) Consider a polymer chain with the ends both fixed at zero. Apply a force $f$ to the middle of the chain at arclength $L/2$. Calculate $\langle \mathbf{r}(L/2) \rangle$. *Hint: use the result for average values found in the first problem.*

(d) Using this calculate the scaling of $\langle |\mathbf{r}(s) - \mathbf{r}(0)|^2 \rangle$ as a function of $s$.