Homework 4
Due 5/19/08

This homework calculates the radius of gyration of a ring polymer using some mathematical techniques that are common in theoretical physics. The use of continuous variables simplifies the analysis, and allow one to apply results from the theory of Fourier series. The equipartition theorem from statistical mechanics is also used. This provides a good introduction to many other kinds of problem that use a lot of the same techniques.

1. Consider a polymer chain described by coordinates $\mathbf{r}(s)$, where s is the arclength, and is a real variable with $0 < s < L$. You are used to the coordinates being described as $\mathbf{r}_i$ where i is an integer, but it is easier sometimes to turn the index i into a continuous variable.

We want to calculate the radius of gyration of an ideal *ring* polymer, that is, one with $\mathbf{r}(0) = \mathbf{r}(L)$. We take the Hamiltonian (or energy) at inverse temperature β, and step length l, to be:

$$\beta H = \frac{3}{2l} \int_0^L |\frac{d\mathbf{r}(s)}{ds}|^2 ds$$

Calculate the radius of gyration of this chain as a function of L and l.

Use the following steps.

(a) Write $\mathbf{r}(s)$ in terms of a Fourier series

$$\mathbf{r}(s) = \sum_{k=-\infty}^{\infty} \hat{\mathbf{r}}_k \exp(-2\pi iks/L)$$

and then express H in terms of the new Fourier variables $\hat{\mathbf{r}}_k$. H should decouple when expressed in terms of these new variables.

(b) Write the radius of gyration as

$$R_g^2 = \langle \frac{1}{L} \int_0^L \left| \mathbf{r}(s) - \frac{1}{L} \int_0^L \mathbf{r}(s) ds \right|^2 ds \rangle$$

As in part (a), express this also in terms of the new Fourier variables $\hat{\mathbf{r}}_k$. *Hint: write down the inverse formula for $\hat{\mathbf{r}}_k$ in terms of $\mathbf{r}(s)$. You should notice that the second integral inside of the average for R_g^2 is simply related to one of the $\hat{\mathbf{r}}_k$'s.*

(c) $\hat{\mathbf{r}}_k$ is complex and has a real and imaginary part. Because $r(s)$ is real, use this to relate $\hat{\mathbf{r}}_k$ to $\hat{\mathbf{r}}_{-k}$.

(d) Use the equipartition theorem to calculate $\langle Re(\hat{\mathbf{r}}_k)^2 \rangle$ and $\langle Im(\hat{\mathbf{r}}_k)^2 \rangle$.

(e) Now calculate R_g^2 using the results of parts (b) and (d).