Statistical Physics II
Problem Set 4

Due: Tuesday, May 6, **before** the lecture

5. **Gaussian Chain** **(8 points)**

The *Gaussian chain* is a standard model for the large-scale behavior of polymers. It consists of N monomers, located at the (in general time dependent) positions $\mathbf{R}_1, \dots, \mathbf{R}_N$ and connected via harmonic springs. In thermal equilibrium, the statistical distribution of bond vectors $\mathbf{b}_n = \mathbf{R}_{n+1} - \mathbf{R}_n$ reads

$$\psi(\{\mathbf{b}_i\}) = \prod_{i=1}^{N-1} \left(\frac{3}{2\pi b^2}\right)^{3/2} \exp\left(-\frac{3}{2b^2}\mathbf{b}_i^2\right).$$

a) Compute the distribution of monomer-monomer distances,

$$\Phi(\mathbf{R}_n - \mathbf{R}_m) = \int \delta\left(\sum_{l=m+1}^{n} \mathbf{b}_l - (\mathbf{R}_n - \mathbf{R}_m)\right)\psi(\{\mathbf{b}_i\})\mathrm{d}\{\mathbf{b}_i\},$$

as well as the mean square distance $\langle(\mathbf{R}_n - \mathbf{R}_m)^2\rangle$.
Hint: The end result of the former is

$$\Phi(\mathbf{R}_n - \mathbf{R}_m) = \left(\frac{3}{2\pi b^2|n-m|}\right)^{3/2} \exp\left(-\frac{3}{2b^2}\frac{(\mathrm{R}_n - \mathrm{R}_m)^2}{|n-m|}\right).$$

b) The *radius of gyration* measures the overall size of the polymer coil and is defined as follows,

$$R_\mathrm{g}^2 = \frac{1}{N}\sum_{n=1}^{N}\langle(\mathbf{R}_n - \mathbf{R}_\mathrm{cm})^2\rangle,$$

where $\mathbf{R}_{\mathrm{cm}} = \sum_n \mathbf{R}_n/N$ denotes the center of mass. Show that $R_{\mathrm{g}}^2 = \sum_{n,m=1}^{N}\langle(\mathbf{R}_n - \mathbf{R}_m)^2\rangle/2N^2$ and use this relation to calculate R_{g}^2.

Hint: All sums can be evaluated explicitly, but may be approximated by integrals. Estimate the order of the approximation error.

c) Calculate the structure factor

$$S_{\mathbf{q}} = \frac{1}{N}\sum_{n,m=1}^{N}\left\langle \mathrm{e}^{i\mathbf{q}(\mathbf{R}_n-\mathbf{R}_m)}\right\rangle$$

for the Gaussian chain and rewrite it in the scaling form $S_{\mathbf{q}} = Nf(\mathbf{q}^2R_{\mathrm{g}}^2)$. Analyze its asymptotic behavior in the limits $\mathbf{q}^2R_{\mathrm{g}}^2 \ll 1$ and $\mathbf{q}^2R_{\mathrm{g}}^2 \gg 1$. Sketch $S_{\mathbf{q}}$ qualitatively and give reasons why $S_{\mathbf{q}} \approx N/(1+\mathbf{q}^2R_{\mathrm{g}}^2/2)$ provides an acceptable approximation.