Ex5440: One dimensional XY model

Submitted by: Yuval Friedman

The problem:

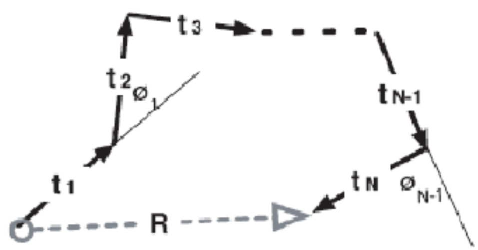
Polymer in two dimensions: Configurations of a polymer are described by a set of vectors $\mathbf{t}_i$ of length a in two dimensions (for i = 1,...,N), or alternatively by the angles ϕ_i between successive vectors, as indicated in the figure below. The energy of a configuration $\{\phi_i\}$ is

$$\mathcal{H} = -\kappa \sum_{i=1}^{N-1} \mathbf{t}_i \cdot \mathbf{t_{i+1}} = -\kappa a^2 \sum_{i=1}^{N-1} \cos\phi_i$$

(a) Show that the correlations $\langle \mathbf{t}_n \cdot \mathbf{t}_m \rangle$ decay exponentially with distance and obtain an expression for the "persistence length" ξ; you can leave the answer in terms of simple integrals.

Hint: Show $\mathbf{t}_n \cdot \mathbf{t}_m = a^2 \mathrm{Re}\{\mathrm{e}^{i\sum_{j=n}^{m-1}\phi_j}\}$.

(b) The end-to-end distance $\mathbf{R}$ is defined as illustrated in the figure. Calculate $\langle R^2 \rangle$ in the limit $N \gg 1$.



The solution:

(a) We begin by evaluating $\langle \cos\phi_i \rangle$ using the partitition function:

$$\mathbf{Z} = \int_{-\pi}^{\pi} \mathrm{e}^{\beta\kappa \mathbf{a^2} \sum_{\mathbf{i=1}}^{\mathbf{N-1}} \cos\phi_\mathbf{i}} \mathrm{d}\phi_\mathbf{1} \cdots \phi_\mathbf{N-1} = \left(\int_{-\pi}^{\pi} \mathrm{e}^{\beta\kappa \mathbf{a^2} \cos\phi} \mathrm{d}\phi \right)^{\mathbf{N-1}} \tag{1}$$

$$\langle \cos\phi_i \rangle = \frac{1}{\mathbf{Z}} \int_{-\pi}^{\pi} \mathrm{e}^{\beta\kappa a^2 \sum_{j=1}^{N-1} \cos\phi_j} \cos\phi_i \mathrm{d}\phi_1 \cdots \phi_{N-1} = \frac{\int_{-\pi}^{\pi} \mathrm{e}^{\beta\kappa a^2 \cos\phi} \cos\phi \mathrm{d}\phi}{\int_{-\pi}^{\pi} \mathrm{e}^{\beta\kappa a^2 \cos\phi} \mathrm{d}\phi} \tag{2}$$

We continue by caculating the angle between the vectors: $\mathbf{t}_n$ and $\mathbf{t}_m$. To do so, we should use the fact that we are given only the angles between two succesive vectors, so the angle ϕ_{nm} between vectors $\mathbf{t}_n$ and $\mathbf{t}_m$ will be a sum of all angles between those indexes:

$$\phi_{nm} = \phi_n + \phi_{n+1} + ... + \phi_{m-1} = \sum_{i=n}^{m-1} \phi_i \tag{3}$$

So the correlation between those vectors will be:

$$\langle \mathbf{t}_n \cdot \mathbf{t}_m \rangle = a^2 \langle \cos\phi_{nm} \rangle = a^2 \langle \cos(\sum_{i=n}^{m-1} \phi_i) \rangle = a^2 \mathrm{Re}\{\langle \mathrm{e}^{i\sum_{i=n}^{m-1}\phi_i} \rangle\} \tag{4}$$

Knowing that different $\cos\phi_i$ have the same distribution function gives:

$$\langle \mathrm{e}^{i\sum_{i=n}^{m-1}\phi_i}\rangle = \langle \mathrm{e}^{i\phi_n}\rangle \cdot \langle \mathrm{e}^{i\phi_{n+1}}\rangle \cdot ...\langle \mathrm{e}^{i\phi_{m-1}}\rangle = \prod_{i=n}^{m-1}\langle \mathrm{e}^{i\phi_i}\rangle = \langle \mathrm{e}^{i\phi_i}\rangle^{|m-n|} \tag{5}$$

Because $\langle \sin\phi_i\rangle = 0$, $\langle \mathrm{e}^{i\phi_i}\rangle$ becomes $\langle \cos\phi_i\rangle$, so:

$$\langle \mathbf{t}_n \cdot \mathbf{t}_m\rangle = a^2 \mathrm{Re}\{\langle e^{i\phi_i}\rangle^{|m-n|}\} = a^2\langle \cos\phi_i\rangle^{|n-m|} = a^2 e^{-|n-m||ln\langle\cos\phi_i\rangle|} = a^2 e^{-|n-m|a/\xi} \tag{6}$$

Where the persistence length is:

$$\xi = \frac{a}{|\ln\langle\cos\phi_i\rangle|} \tag{7}$$

Persistance length is a parameter quantifying the stiffness of the polymer: the polymer is less flexible when the persistance length grows.

Substituting (2) into (7) we get:

$$\xi = a\Big|\ln\Big(\int_{-\pi}^{\pi}\mathrm{e}^{\beta\kappa a^2\cos\phi}\cos\phi\mathrm{d}\phi\Big) - \ln\Big(\int_{-\pi}^{\pi}\mathrm{e}^{\beta\kappa a^2\cos\phi}\mathrm{d}\phi\Big)\Big|^{-1} \tag{8}$$

(b) Substituting $r = n - m$ and taking the sum to infinity for $N \gg 1$ we get:

$$\langle R^2\rangle = \sum_{n=1}^{N}\sum_{m=1}^{N}\langle \mathbf{t}_n\cdot\mathbf{t}_m\rangle = a^2\sum_{n=1}^{N}\sum_{m=1}^{N}\langle\cos\phi_i\rangle^{|n-m|} = Na^2\sum_{r=-\infty}^{\infty}\langle\cos\phi_i\rangle^{|r|} =$$
$$Na^2(1+2\sum_{r=1}^{r=\infty}\langle\cos\phi_i\rangle^r) = Na^2(1+\frac{2}{1-\langle\cos\phi_i\rangle}) = Na^2\frac{1+\langle\cos\phi_i\rangle}{1-\langle\cos\phi_i\rangle} \tag{9}$$

And in terms of the persistence length:

$$\xi = \frac{a}{|\ln\langle\cos\phi_i\rangle|} \implies \langle\cos\phi_i\rangle = \mathrm{e}^{-\frac{a}{\xi}} \tag{10}$$

So:

$$\langle R^2\rangle = Na^2\frac{1+\mathrm{e}^{-\frac{a}{\xi}}}{1-\mathrm{e}^{-\frac{a}{\xi}}} = Na^2\frac{\mathrm{e}^{\frac{a}{2\xi}}+\mathrm{e}^{-\frac{a}{2\xi}}}{\mathrm{e}^{\frac{a}{2\xi}}-\mathrm{e}^{-\frac{a}{2\xi}}} = Na^2\coth(\frac{a}{2\xi}) \tag{11}$$