Rouse theory of pinned polymer loop

Wenwen Huang

September 11, 2016

Consider a pinned polymer loop modeled by beads and connecting springs, the dynamical equation for a single bead is

$$\xi \frac{d\mathbf{r}_j}{dt} = -k_H \sum_k A_{jk}\mathbf{r}_k + \mathbf{f}_j^e + \mathbf{f}_j^b \tag{1}$$

where ξ is the friction coefficient of bead in solution, $\mathbf{r}_j$ is the bead position of the jth bead, k_H is the spring constant with a linear Hookean spring assumed. $\mathbf{f}_j^e$ is the external force exerted on beads, $\mathbf{f}_j^b$ is typical brownian force satisfying

$$\left\langle \mathbf{f}_j^b \right\rangle = \mathbf{0}; \left\langle f_{i\alpha}^b(t) f_{j\beta}^b(t') \right\rangle = 2\xi k_B T \delta_{ij}\delta_{\alpha\beta}\delta(t-t') \tag{2}$$

$\mathbf{A}$ is the connecting matrix, in case of pinned polymer loop, it has the form of following

$$\mathbf{A} = \begin{bmatrix} 2 & -1 & 0 & \cdots \\ -1 & 2 & -1 & \cdots \\ \vdots & \ddots & \ddots & \vdots \\ \cdots & -1 & 2 & -1 \\ \cdots & 0 & -1 & 2 \end{bmatrix} \tag{3}$$

Since the polymer is a loop and pinned, so we write down the additional constraints besides the dynamical equation. Without loss of generality, the pinned point is set at the origin.

$$\mathbf{r}_0 = \mathbf{r}_N = 0 \tag{4}$$

The dynamical equation of all beads can be written in the vector term of Eq. (1)

$$\xi \frac{d}{dt}\mathbf{R} = -k_H \mathbf{A}\mathbf{R} + \mathbf{F}^e + \mathbf{F}^b \tag{5}$$

where $\mathbf{R} = [\mathbf{r}_1, \mathbf{r}_2, \cdots, \mathbf{r}_N]^T$, and similar vector notation are also applied for $\mathbf{F}^e$, $\mathbf{F}^b$. Notice that the connecting matrix $\mathbf{A}$ is real and symmetric, consider a similarity transfer

$$\left[\Omega^{-1} A \Omega\right]_{jk} = \lambda_k \delta_{jk} \tag{6}$$

here Ω is a unitary matrix, thus λ_k is the eigenvalue of matrix $\mathbf{A}$.

We now consider the pinned polymer loop in a constant force field, i.e. $\mathbf{f}_j^e = f^e \mathbf{e}_z$.

References