

Report: Rouse theory of pinned polymer loop

Wenwen Huang

May 10, 2016

1 Model

Consider a pinned polymer loop modeled by bead-spring, the dynamical equation for a single bead is

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

where ξ is the friction coefficient of bead in solution, \mathbf{r}_j is the bead position of the j th 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

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

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

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

In addition to the dynamical equation, the boundary condition for a pinned polymer loop writes

$$\mathbf{r}_0 = \mathbf{r}_N = 0 \quad (4)$$

2 Normal Coordinate

Eq. (1) can be rewrite in the term of vector contains all beads

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

where $\mathbf{R} = [\mathbf{r}_1, \mathbf{r}_2, \dots, \mathbf{r}_N]^T$, and similar for $\mathbf{F}^e, \mathbf{F}^b$.

Notice that the connecting matrix \mathbf{A} is real and symmetric, consider a similarity transfer

$$[\Omega^{-1}A\Omega]_{jk} = \lambda_k \delta_{jk} \quad (6)$$

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

3 Constant Force Field

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

References