Rouse theory of pinned polymer loop

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1 Model

Consider a pinned polymer loop modeled by beads and connecting springs, see in the sketch Fig. 1. Without loss of generality, the bead labeled by 0 is

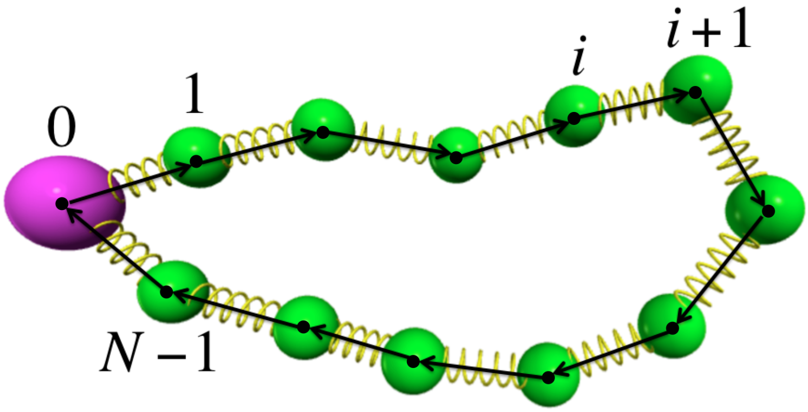

Figure 1: Sketch of pinned bead spring model, magenta bead represent the pinned SPB, green beads represent chromosome segments.

assumed be pinned at the origin and there are N beads in total in the loop. We can write the pinned condition as

$$\mathbf{r}_0 = \mathbf{0} \tag{1}$$

So the dynamical equation for a single bead except the pinned one in the loop can be written as

$$\xi \frac{d\mathbf{r}_i}{dt} = -k_H \sum_k A_{ik} \mathbf{r}_k + \mathbf{f}_i^e + \mathbf{f}_i^b \tag{2}$$

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

$$\left\langle \mathbf{f}_i^b \right\rangle = \mathbf{0}; \left\langle f_{i\alpha}^b(t) f_{j\beta}^b(t') \right\rangle = 2\xi k_B T \delta_{ij} \delta_{\alpha\beta} \delta(t - t') \tag{3}$$

$\mathbf{A}$ is the connecting matrix. It is not difficult to find that in the case of the setting above, i.e. pinned loop, $\mathbf{A}$ is a $(N-1) \times (N-1)$ matrix and has the following form

$$\mathbf{A} = \begin{bmatrix} 2 & -1 & 0 & \cdots \\ -1 & 2 & -1 & \cdots \\ \vdots & \ddots & \ddots & \vdots \\ \cdots & -1 & 2 & -1 \\ \cdots & 0 & -1 & 2 \end{bmatrix} \tag{4}$$

Notice that we do not take into account any complex terms of interaction such as bending stiffness and exclusive effect in this simple model. This is because analytical results are tractable in such a simple setting. The impact of these complex interaction terms will be studied numerically by Brownian Dynamics Simulation.

2 Solution

For convenience, we use the vector notation and rewrite Eq. (2) as

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

where $\mathbf{R} = [\mathbf{r}_1, \mathbf{r}_2, \cdots, \mathbf{r}_{N-1}]^T$, and similar vector notation is also applied for $\mathbf{F}^e$, $\mathbf{F}^b$. In order to solve this set of dynamical equations, we first notice that the connecting matrix $\mathbf{A}$ is a very special type of matrix called tridiagonal Toeplitz matrix[]. Luckily, it is always exactly diagonalizable. To do this, let us introduce a similarity transfer that

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

here $\mathbf{\Omega}$ is normalized to be a unitary matrix, and λ_k is the eigenvalue of matrix $\mathbf{A}$. We skip the calculation details here and just give out the results as following

$$\lambda_k = 4 \sin^2 \left(\frac{k\pi}{2N} \right), k = 1, 2, \cdots, N-1 \tag{7}$$

$$\Omega_{jk} = \Omega_{kj} = [\Omega^{-1}]_{jk} = [\Omega^{-1}]_{kj} = \sqrt{\frac{2}{N}} \sin \left(\frac{jk\pi}{N} \right) \tag{8}$$

With this we can multiply both sides of Eq. (5) by $\boldsymbol{\Omega}^{-1}$ arrive at

$$\xi\frac{d(\boldsymbol{\Omega}^{-1}\mathbf{R})}{dt} = -k_H\boldsymbol{\Omega}^{-1}\mathbf{A}\boldsymbol{\Omega}\boldsymbol{\Omega}^{-1}\mathbf{R} + \boldsymbol{\Omega}^{-1}\mathbf{F}^e + \boldsymbol{\Omega}^{-1}\mathbf{F}^b \tag{9}$$

Notice that $\boldsymbol{\Omega}^{-1}\mathbf{A}\boldsymbol{\Omega} = \mathbf{D}$ and use the notation such that $\tilde{\mathbf{R}} = \boldsymbol{\Omega}^{-1}\mathbf{R}$, we get the set of decoupled equations

$$\xi\frac{d\tilde{\mathbf{r}}_j}{dt} = -k_H\lambda_j\tilde{\mathbf{r}}_j + \tilde{\mathbf{f}}_j^e + \tilde{\mathbf{f}}_j^b \tag{10}$$

Eq. (10) can be solved easily by standard methods. The general solution can be written as following

$$\tilde{\mathbf{r}}_j(t) = \tilde{\mathbf{r}}_j(0)e^{-\frac{k_H\lambda_j}{\xi}t} + \frac{1}{\xi}\left(\int_0^t \tilde{\mathbf{f}}_j^e e^{-\frac{k_H\lambda_j}{\xi}(t-t')}dt' + \int_0^t \tilde{\mathbf{f}}_j^b e^{-\frac{k_H\lambda_j}{\xi}(t-t')}dt'\right) \tag{11}$$

Here the transformed brownian force also fulfills

$$\left\langle \tilde{\mathbf{f}}_j^b \right\rangle = \mathbf{0}; \left\langle \tilde{f}_{i\alpha}^b(t)\tilde{f}_{j\beta}^b(t') \right\rangle = 2\xi k_B T\delta_{ij}\delta_{\alpha\beta}\delta(t-t') \tag{12}$$

Given the solution of Eq. (11), the position of each bead can be obtain by the inverse transformation $\mathbf{R} = \boldsymbol{\Omega}\tilde{\mathbf{R}}$. Next section, we will discuss the solution for two different cases of external force separately, i.e. constant external force and periodic external force.

2.1 Constant Force Field

We now consider the pinned polymer loop in a constant force field, i.e. $\mathbf{f}_j^e = f^e\mathbf{e}_z$. Plug in to the Eq. (11), obtain

$$\tilde{\mathbf{r}}_j(t) = \tilde{\mathbf{r}}_j(0)e^{-\frac{k_H\lambda_j}{\xi}t} + \frac{\tilde{f}^e\mathbf{e}_z}{k_H\lambda_j}\left(1 - e^{-\frac{k_H\lambda_j}{\xi}t}\right) + \frac{1}{\xi}\int_0^t \tilde{\mathbf{f}}_j^b e^{-\frac{k_H\lambda_j}{\xi}(t-t')}dt' \tag{13}$$

Do the inverse transfer we obtain the position of every bead

$$\mathbf{r}_i(t) = \sum_j \Omega_{ij}\tilde{\mathbf{r}}_j(t) \tag{14}$$

We are interested in the equilibrium statistics of the polymer, such as the mean and variance of the each bead position. The mean position of each bead can be obtained easily by combining Eq. (13) and Eq. (14) and let $t \to \infty$, we get

$$\langle \mathbf{r}_i^\infty \rangle = \sum_j \Omega_{ij}\frac{\tilde{f}^e\mathbf{e}_z}{k_H\lambda_j} = \frac{\tilde{f}^e\mathbf{e}_z}{2Nk_H}\sum_{k,j}\frac{\sin\left(\frac{ik\pi}{N}\right)\sin\left(\frac{ik\pi}{N}\right)}{\sin^2\left(\frac{k\pi}{2N}\right)} \tag{15}$$

If $N \gg 1$, the summation of j can be approximated by the integral so we get

$$\langle \mathbf{r}_i^{\infty} \rangle = \frac{\tilde{f}^e \mathbf{e}_z}{k_H} \sum_{l=1}^{\frac{N+1}{2}} \frac{\sin\left(\frac{i(2l-1)\pi}{N}\right)}{(2l-1)\pi \sin^2\left(\frac{(2l-1)\pi}{2N}\right)} \tag{16}$$

One can clearly see from Eq. (16) that $\langle \mathbf{r}_i \rangle = \langle \mathbf{r}_{N-i} \rangle$ as we expected. And the components of mean position perpendicular to the force field direction are vanished. In order to calculate the variance of bead position, it is nontrivial to firstly calculate the two time correlation of normal coordinate position, as following

$$\begin{aligned} \langle \tilde{\mathbf{r}}_m(t) \tilde{\mathbf{r}}_n(t') \rangle = & \langle \tilde{\mathbf{r}}_m(0) \tilde{\mathbf{r}}_n(0) \rangle \, e^{-\frac{k_h \lambda_m}{\xi} t - \frac{k_h \lambda_m}{\xi} t'} \\ & + \frac{(\tilde{f}^e)^2}{k_H^2 \lambda_m \lambda_n} \left(1 - e^{-\frac{k_H \lambda_m}{\xi} t}\right) \left(1 - e^{-\frac{k_H \lambda_n}{\xi} t'}\right) \\ & + \frac{3 k_B T}{k_H \lambda_m} e^{-\frac{k_H \lambda_m}{\xi} t} \delta_{mn} \end{aligned} \tag{17}$$

Utilize Eq. (17) we get the second moment of bead position

$$\left\langle \mathbf{r}_i^2(t) \right\rangle = \sum_{m,n} \Omega_{im} \Omega_{in} \langle \tilde{\mathbf{r}}_m(t) \tilde{\mathbf{r}}_n(t) \rangle \tag{18}$$

Finally, let $t \to \infty$, we get the equilibrium variance of bead position

$$\mathrm{var}\left[\mathbf{r}_i^{\infty}\right] = \left\langle (\mathbf{r}_i^{\infty})^2 \right\rangle - \langle (\mathbf{r}_i^{\infty}) \rangle^2 = \frac{3 k_B T}{2 N k_H} \sum_k \left[\frac{\sin\left(\frac{ik\pi}{N}\right)}{\sin\left(\frac{k\pi}{2N}\right)} \right]^2 \tag{19}$$

Notice that we also have the symmetry that $\mathrm{var}\left[\mathbf{r}_i^{\infty}\right] = \mathrm{var}\left[\mathbf{r}_{N-i}^{\infty}\right]$. Moreover, it is important to point out the variance does not depend on the external force. So the statistical distance between two beads will not change no matter the external force filed is strong or weak. This is essentially because infinite extensible Hookean springs are employed in this simple model.

Besides the equilibrium statistics, dynamical properties are also tractable. Our my interested quantity is the relaxation time of the pinned polymer. In order to do that, let us calculate the autocorrelation function of diameter vector, defined as $\mathbf{r}_d = \mathbf{r}_{\frac{N}{2}} - \mathbf{r}_0 = \mathbf{r}_{\frac{N}{2}}$. Utilize Eq. (17) we get

$$\langle \mathbf{r}_d(t) \mathbf{r}_d(0) \rangle = \sum_{m,n} \Omega_{\frac{N}{2}m} \Omega_{\frac{N}{2}} \langle \tilde{\mathbf{r}}_m(t) \tilde{\mathbf{r}}_n(0) \rangle \tag{20}$$

From Eq. (17) we can readily get the relaxation time

$$\tau = \frac{\xi}{k_H \lambda_1} = \frac{\xi}{4k_H \sin(\pi/2N)} \tag{21}$$

when N is large we can expand the sin term arriving at $\tau = \frac{\xi N^2}{k_H \pi^2}$, which coincides as the unpinned polymer chain. Like the variance of bead position, the relaxation time does not depend on the external force too.

2.2 Periodic Force Field

We now consider the pinned polymer loop in a constant force field, i.e. $\mathbf{f}_j^e = f \sin(\omega t)\mathbf{e}_z$. Plug in to the Eq. (11), obtain

$$\begin{aligned}\tilde{\mathbf{r}}_j(t) =& \tilde{\mathbf{r}}_j(0) e^{-\frac{k_H\lambda_j}{\xi}t} + \frac{\tilde{f}\xi\mathbf{e}_z}{\omega^2\xi^2 + k_H^2\lambda_j^2}\left(\frac{k_H\lambda_j}{\xi}\sin(\omega t) - \omega\cos(\omega t) - \omega e^{-\frac{k_H\lambda_j}{\xi}t}\right) \\ &+ \frac{1}{\xi}\int_0^t \tilde{\mathbf{f}}_j^b e^{-\frac{k_H\lambda_j}{\xi}(t-t')}dt'\end{aligned} \tag{22}$$

In the case of periodic force field, each bead is constantly moving according to the driven force, so there is no equilibrium position for the bead position.

3 Simulation

There are three pairs of chromosomes in Fission Yeast. The Kuhn length of chromomsomes is estimated to be 200 nm. And the compaction ratio is 100 bp/nm. For the genome of size 12.6 Mbp, we have ≈ 1260 monomers for the polymer model.

Experimentally, moving speed of the bead is observed 2.5μm/min. So the force extert on the bead can be estimated by the Stoke's law $f = 6\pi\mu R v$, where μ is the viscosity of the solution and R is the radius of bead. $R =$ 50nm is used in our estimation. The viscosity of the solution is estimated as about 1000 times of μ_{water}. So we get the strength of force field is about $f^e = 3.5 \times 10^{-14}$N.

In the Brownian Dynamics Simulation, the varables are rescaled to dimensionless by $\mathbf{r}' = \mathbf{r}/a$, $t' = t/(\gamma a^2/k_B T)$, and $\mathbf{F}' = \mathbf{F}/(k_B T/a)$. By insert the estimation of parameters above, we obtain $\mathbf{r}' = \mathbf{r}/(200\text{nm})$, $t' = t/(8.15\text{s})$, $\mathbf{F}' = \mathbf{F}/(2.06 \times 10^{-14}\text{N})$.

The osillation period measured in the experiment is ≈ 10 min. Accordingly, we can obtain the external force field used in the simulation. For constant force $f^e = 1.7$, for periodic force $f^e = 2.67 \sin(8.53 \times 10^{-2} t)$.

References