1 Supplement Materials

1.1 Monte Carlo Simulation

The 1D simulation is performed using Monte Carlo algorithm under the particle scenario. The analogy of 1D polymer loop to the Fermions particle system is shown in Figure. 1.

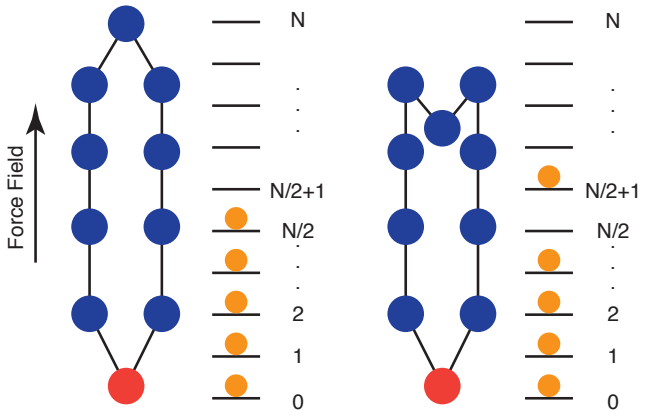

Figure 1: Sketch for analogy of 1D polymer loop to Fermions system. Ground state and its corresponding on the left and the first excitation state on the right.

$N/2$ Fermions are filled in N energy levels. One occupying state of Fermion system can exactly map to one polymer conformation. Standard Metropolis scheme[1] was exploited to do the sampling. More specifically, the simulation contains the following steps:

Step 1: initializing the system with the ground state, i.e. all Fermions sit on the lower half N energy level.

Step 2: randomly select a particle and perform a jumping trial to the empty slot with the probability $p = min\{1, exp\{-(U_{new} - U_{old})/k_B\tilde{T}\}\}$. Here $\tilde{T}$ is the dimensionless temperature defined in the main text. k_B is Boltzmann constant. U_{new}, U_{old} is the energy potential of new and old occupying state which can be calculated

$$U = -2\gamma a v_0 \sum_{i=1}^{N} j n_j \tag{1}$$

where $n_j = 1$ if the jth energy level is occupied and $n_j = 0$ if not.

Step 3: repeat step 2 for enough steps to thermalize the system until it is equilibrated.

Step 4: sampling the system and transfer it to the polymer configuration scheme to do the statistical analysis for the average and variance of bead position.

Basically, 10^4 independent samples after enough thermalization steps are utilized to collect the statistical results.

1.2 Brownian Dynamics Simulation

To control the number of free parameters, we choose the ideal bead-rod polymer model to describe the dynamics of chromosomes in nucleus, without considering the exclusive volume effect. As we will see later that the system can be reduced to a one free parameter model, i.e. $\tilde{T}$.

The simulation of model bead connected with rigid rod utilize the technique of Brownian Dynamics[2]. The dynamical equation of beads representing chromosome segments is

$$\dot{\mathbf{r}_i} = \frac{1}{\xi}(\mathbf{F}_i^b + \mathbf{F}_i^c + \mathbf{F}_i^e + \mathbf{F}_i^{pseudo}) \tag{2}$$

where $\mathbf{r}_i$ is the position vector of the i^{th} bead, ξ is friction coefficient, $\mathbf{F}_i^b$ is random force, $\mathbf{F}_i^c$ is constraint force caused by rigid rod constraints and $\mathbf{F}_i^e$ is external force. $\mathbf{F}_i^{pseudo}$ is pseudo force added to ensure the right statistics [3, 2].

The random force, which characterizes the fluctuation origin of beads dynamics, is a standard Brownian force which satisfies the following conditions

$$\left\langle \mathbf{F}_i^b \right\rangle = \mathbf{0}, \tag{3a}$$

$$\left\langle \mathbf{F}_i^b(t)\mathbf{F}_j^b(t') \right\rangle = 2k_B T_c \xi \delta_{ij} \delta(t - t') \tag{3b}$$

k_B is Boltzmann constant and T_c is the *characterizing temperature* which characterize the level of randomness arise from the thermal motion of solvent molecules and other interactions between the chromosome and proteins in the nucleus.

The constraint force for a specific bead in a bead-rod ring is

$$\mathbf{F}_i^c = \lambda_i \mathbf{u}_i - \lambda_{i-1}\mathbf{u}_{i-1} \tag{4}$$

where λ_i is strength of tension on the rod between i^{th} and $(i+1)^{\text{th}}$ bead, $\mathbf{u}_i$ is the unit vector along this rod and $\mathbf{u}_N$ connects N^{th} bead and the 1^{th} bead.

In case of constant force field, the external force is constant $\mathbf{F}_i^e = -\xi\mathbf{v}$ acting on every bead except for the pinned one representing the SPB.

The pseudo force is calculated using

$$\mathbf{F}_i^{pseudo} = -\frac{\partial U_{met}}{\partial \mathbf{r}_i}; U_{met} = \frac{1}{2}k_B T_c \ln(\det \mathbf{G}) \tag{5}$$

where $\mathbf{G}$ is the metric matrix of the bead-rod system[5].

Since the rods present in our model are rigid rods, additional constrained equations are needed to keep the rod length unchangeable

$$(\mathbf{r}_{i+1} - \mathbf{r}_i)^2 - a^2 = 0 \tag{6}$$

where a is rod length.

Dimensionless variables can be obtained by rescaling the parameters $\mathbf{r}' \to \mathbf{r}/a$, $t' \to t/(\xi a^2/k_B T_c)$, and $\mathbf{F}' \to \mathbf{F}/(k_B T_c/a)$. The only free parameter left in the model is the dimensionless temperature $\tilde{T}$, prescribed by

$$\tilde{T} = \frac{k_B T_c}{Fa} = \frac{k_B T_c}{\xi v a} \tag{7}$$

Numerical scheme employed to solved the set of constrained differential equations (2) and (6) is the predictor-corrector algorithm, which is used widely in bead-rod simulations[2, 6, 4]. Basic steps include calculating a prediction of $\mathbf{r}_i(t + \delta t)$ without considering the constraint force followed by a correction step, i.e. solving the algebra constraint equations to get constraint forces and re-plugin to the original equations for the corrected $\mathbf{r}_i(t + \delta t)$. The differential equations are solved using Euler iterative method with a time step $\delta t = 10^{-4}$. Statistical results are all obtained based on the ensemble of no less than 10^9 steps after equilibrium.

References

[1] Kurt Binder and Dieter Heermann. *Monte Carlo simulation in statistical physics: an introduction*. Springer Science & Business Media, 2010.

[2] C. Cruz, F. Chinesta, and G. Régnier. Review on the Brownian Dynamics Simulation of Bead-Rod-Spring Models Encountered in Computational Rheology. *Archives of Computational Methods in Engineering*, 19(2):227–259, May 2012.

[3] EJ Hinch. Brownian motion with stiff bonds and rigid constraints. *Journal of Fluid Mechanics*, pages 219–234, 1994.

[4] Tony W. Liu. Flexible polymer chain dynamics and rheological properties in steady flows. *The Journal of Chemical Physics*, 90(10):5826, 1989.

[5] Matteo Pasquali, David C Morse, and Brownian Dynamics. An efficient algorithm for metric correction forces in simulations of linear polymers with constrained bond lengths. 116(5), 2002.

[6] Madan Somasi, Bamin Khomami, Nathanael J. Woo, Joe S. Hur, and Eric S.G. Shaqfeh. Brownian dynamics simulations of bead-rod and bead-spring chains: numerical algorithms and coarse-graining issues. *Journal of Non-Newtonian Fluid Mechanics*, 108(1-3):227–255, December 2002.