Yet another mapping to ASEP — 1D polymer dynamics

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I. INTRODUCTION

Many biological processes can be described by idealized physical models and quantitatively studied through the law of physics and methods of mathematics. A good example is the movement of DNA. Polymer models, constructed by bead and rod or spring, are often utilized to describe DNA[]. In our study of chromosome alignment in meiotic fission yeast, a freely jointed bead rod ring model is adopted[]. Chromosomes during the stage of nuclear oscillation are translated to pinned polymer loop in an external field[]. To further understand the physics of such pinned polymer loop model, here we formulate the problem in 1D, i.e. rods orientate either right or left. Amazingly, we found this simple model can maps to a 1D particle hopping problem, well known as asymmetric simple exclusion process (ASEP)[]. On the other hand, ASEP itself is a well studied paradigmatic model in non-equilibrium statistics with thousands of applications[]. It turns out many real problems can be mapped to ASEP. For instance, ASEP is frequently used to model the traffic transportation[]. Another example is ref. [], MacDonald et al. shown their pioneering work to use ASEP quantitatively modelling kinetic of biopolymerization. Also in ref. [], the reptation movement of polymer in crowded environment is again mapped to ASEP model. In this paper, we will add one more class of problems which can be exactly mapped to ASEP — 1D polymer dynamics. Notice the polymer here is in general polymers in dilute solution rather than the reptating polymer in crowded environment.

In this paper, we will show how to map from a pinned polymer model describing chromosomes to an ASEP particle hopping process. The equivalence between these two models means that methods used to solve one problem can also be mapped to solve the other. As ASEP is a well studied exactly solvable system, we demonstrate that the analytical results can also be translated to the problem of polymer dynamics. In addition, we show that the famous Fermi-Dirac statistics serves as an asymptotic approximation of statistics for rod orientation as well as the density profile of particles. All results shown here are verified by numerical simulations. To further demonstrate the power of this mapping, we study the relaxation of polymer represented by the mapped particle hopping process and compared with the Rouse theory and Brownian Dynamics (BD) simulations. Interestingly, we found the relaxation time of gyration radius varies non-monotonically with the external force, which is consistent with 3D theory and simulations.

The next section we will describe how to build the mapping from polymer and particle and demonstrate how to draw the useful analytical results through the mapping. In section III, the mapping is extended to non-equilibrium aspects to demonstrate its power of prediction. Comparisons of Rouse theory and BD simulations are discussed in detail. Finally, conclusion remarks and outlooks are list in section IV.

II. MAPPING FROM POLYMER TO PARTICLE

In our study of chromosome movements, we use a bead-and-rod model to model the chromosomes. Here, we reformulate the model in 1D instead of 3D. The 1D model is extremely simple but still capture the key properties such as the ability to measure the alignment of beads along the external force field. The exciting thing is we have a peculiar mapping from 1D polymer to particle on lattice sites as shown below.

The chromosome consists of N beads freely jointed by N rods forming a loop; the rod length is chosen to be the Kuhn length a of the chromosome. The position of the ith bead is denote by x_i, and without lost of generality, the spindle pole body which is pinned after transforming to the co-moving frame, is defined to be the 0th bead. An constant external force F is applied on every bead after frame transform with direction defined to be positive along x without loss of generality. The looping topology of the polymer suggests $x_0 = x_N$. We do not consider the volume exclusion in the model of polymer. Define the direction of the ith rod to be $e_i := x_{i+1} - x_i$. In a one-dimensional setting, $x_i = ia$ where $i \in \mathbb{Z}$, and $e_i = \pm a$ for $i = 0, 1, \ldots, N-1$. The internal energy of the polymer reads

$$E = -\sum_{i=1}^{N-1} F x_i = -Fa \sum_{i=1}^{N-1} i$$
$$= -Fa \sum_{i=1}^{N-1} \sum_{j=0}^{i-1} (2Z_j - 1),$$

here $Z_j := (e_j/a + 1)/2$ is a changed variable. By exchanging the order of the double summation and utilizing the looping condition

$$\sum_{j=0}^{N-1} e_j = 0, \tag{1}$$

we arrive at

$$E = E_0 + \Delta E \sum_{j=0}^{N-1} j Z_j \qquad (2)$$

where $E_0 = -N(N-1)\Delta E/2$ and $\Delta E = 2Fa$.

By observing the energy (2), we immediately recognise that the system has a Hamiltonian similar to a system with $N/2$ Fermions in an N equally distributed energy levels $0, \Delta E, \ldots, (N-1)\Delta E$, and Z_j can be interpreted as a binary variable which characterizes whether the energy level j is occupied ($= 1$ if it is occupied, and $= 0$ otherwise). This is actually the inspiration for us to build the mapping from polymer to particles.

A. Brownian bridge

B. Fermi-Dirac statistics of rod orientations

C. Fermion integer number partition theory

D. From rods to a polymer, beauty of Gaussian statistics

III. ASYMMETRIC EXCLUSION PROCESS

Having shown the equilibrium statistics been solved by mapping from polymer to particle, we now come to the discussion about the dynamics. It is intuitively to extend the analogy to nonequilibrium, i.e., the dynamics of pinned polymer corresponds to particle diffusion in a one dimensional lattice. To illustrate the equivalence, we firstly define a typical particle hopping model and build the connection between these two models.

As shown in the section above, we consider a 1D lattice with N lattice sites and exact $N/2$ particles. Only simple exclusive interaction between particle is applied, which means that one lattice site can only occupied by at most one particle and the order of particles is conserved during the particle hopping process. Denote the probability of particle hopping to right and left with p and q respectively, we have the following detailed balance during the hopping

$$p P_n = q P_{n+1} \qquad (3)$$

where P_n is the probability of configuration before particle hopping to the right and P_{n+1} is the probability of configuration after hopping. In addition, the ratio of of probability should be proportional to a Boltzmann factor with the energy difference between these two configurations. Eq 3 can be rewrite as

$$q/p = P_n/P_{n+1} = \exp\left(-\Delta E/k_B T\right) \qquad (4)$$

On the other hand, for a specific particle hopping system, the total hopping rate is determined by the temperature. External force changes nothing but the ratio q/p. Thus we have

$$p + q = cT \qquad (5)$$

where c is a constant. With eq. 5 and eq. 5 we can in principle solve p and q uniquely. The key quantity here is ΔE, which actually connects polymer and particle model. One can learn from the polymer and particle equivalence that one particle hopping the right corresponds to the change of two consecutive rods orientation from right-left to left-right. Thus the energy difference of the two configuration writes

$$\Delta E = 2F\Delta l \qquad (6)$$

where F is the strength of external force and Δl is the rod length. Plug into the above equations one obtain

$$p = \frac{cT \exp\left(-2F\Delta l/k_B T\right)}{1 + \exp\left(-2F\Delta l/k_B T\right)} \qquad (7)$$

$$q = \frac{cT}{1 + \exp\left(-2F\Delta l/k_B T\right)} \qquad (8)$$

Now we have a well defined particle hopping model equivalent to polymer dynamics in the bulk, but the boundary condition is still not specified. It turns out the boundary condition combined with particle number are crucial to determinate the type of corresponding polymer.

IV. TOWARDS UNDERSTANDING DYNAMICS

V. CONCLUSIONS

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