Yet another problem maps to ASEP — 1D polymer dynamics

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abstract text

I. INTRODUCTION

Many biological processes can be characterized 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 transformed 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 coincide 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. BUILD THE MAPPING

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.

A. Mapping from polymer to particle

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 lost of generality. The looping topology of the polymer suggests $x_0 = x_N$. Define the orientation of the ith rod to be $e_j := (x_{j+1} - x_j)/a$. In a one-dimensional setting, $x_i = a \sum_{j=0}^{i} e_j$ where $e_j = \pm 1$ and $i, j \in \{0, 1, \ldots, N-1\}$. We do not consider the volume exclusion effect and bending energy in the model of polymer. The internal energy of the polymer reads

$$E = -\sum_{i=0}^{N-1} F x_i = -Fa \sum_{i=0}^{N-1} \sum_{j=0}^{N-1} e_j, \tag{1}$$

In addition, the looping condition gives

$$\sum_{j=0}^{N-1} e_j = 0. \tag{2}$$

We now build the mapping from polymer to particle. Notice that the state rod orientation is binary, i.e. $e_j \in$

$\{-1, +1\}$. We map it to the state of a lattice site which is also binary, i.e. either occupied by particle ($Z_j = 1$) or empty ($Z_j = 0$). The relation of Z_j and e_j is defined by a simple variable transformation $Z_j := (e_j + 1)/2$. The position of polymer beads is obtained by the back transformation

$$x_i = a \sum_{j=0}^{j=i} e_j = a \left(2 \sum_{j=0}^{j=i} Z_j - i \right) \qquad (3)$$

Several examples of polymer configurations maps to particles on lattice sites are given in Fig. 1. It is not difficult to see the boundary condition of lattice for the particle hopping model is reflecting boundaries. We will discuss more about this in section III A.

B. Fermi-Dirac statistics of rod orientations

By exchanging the order of the double summation in eq. (1) and utilizing the looping condition we arrive at

$$E = E_0 + \Delta E \sum_{j=0}^{N-1} j Z_j, \qquad (4)$$

where $E_0 = -N(N-1)\Delta E/2$ and $\Delta E = 2Fa$. The looping condition (2) implies a hard constraint of the total number of the Fermions $\sum_{j=0}^{n-1} Z_j = N/2$.

By observing the energy (4), we immediately recognise that the system has a Hamiltonian similar to a system with $N/2$ Fermions in an N equally distributed energy levels $0, \Delta E, \dots, (N-1)\Delta E$, 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). Clearly when the lowest energy corresponds to $Z_j = 1 \ \forall j < N/2$ and $Z_j = 0$ otherwise. When the system is in contact with an external thermal bath with temperature T, it is possible to be in any configuration. The equilibrium Gibbs measure indicates that the probability of the system in a configuration $\{Z_j\}_{j=0}^{N-1}$ is

$$\mathbb{P}\left\{ \{Z_j\}_{j=0}^{N-1} \right\} \propto \exp \left[-\frac{E_0 + \Delta E \sum_{j=0}^{N-1} j Z_j}{k_B T} \right] \qquad (5)$$

where k_B is the Boltzmann factor.

The fixed total number or particle to $N/2$ corresponds to a picture of *canonical ensemble* []: the system does not exchange particles with its environment. While formally the equilibrium distribution is solved by (5). But here the difficulty of obtaining the analytic solution due to the degeneracy of the system, i.e., some (total) energy levels contain multiple microscopic states.

An alternative approach is to first release the fixed-number constraint, and use the *grand canonical ensemble* which allows exchange of particles with external reservoir [], derive the probability distribution of the microscopic

states to construct an random walk model, and then finally use the to re-enforce the fixed-number constraint []. Below we outline the analysis and the results of this approach. In this one-dimensional case, after releasing the fixed-number constraint, the probability distribution of Z_j can be derived [] to be a Fermi–Dirac distribution

$$\mathbb{P}\{Z_j = 1\} = \left\{ 1 + \exp \left[\frac{\Delta E (j - \mu)}{k_B T} \right] \right\}^{-1}, \qquad (6a)$$

$$\mathbb{P}\{Z_j = 0\} = 1 - \mathbb{P}\{Z_j = 1\}, \qquad (6b)$$

with a chemical potential $\mu = (N-1)/2$ obtained from a symmetry argument. Noting the relation of Z_j and the configuration of the orientation of jth rod $e_j = (2Z_j - 1)$, the probabilities (6a) are used to compute the distribution of e_j. In this context, the famous Pauli exclusion principle—Z_j can be either 0 or 1—corresponds to an almost trivial statement of each rod: either it points to the right ($Z_j = 1$) or to the left ($Z_j = 0$). We emphasize that only in the picture of grand canonical ensemble, the probability distribution of each rod are mutually independent; with a hard constraint of the particle number, Z_j's are not independently distributed. In fact, the independence is the key for an analytic solutions of the equilibrium properties, such as (5), are possible.

Knowing the probability distribution of the orientation of each rod, a random walk is then built, satisfying the first and the second moments of the individual rods. Specifically, we construct a Gaussian random walk, which satisfies the conditional probability

$$\rho(x_{i+1}|x_i) = \exp \left\{ -\frac{[x_{i+1} - x_i - a\mathbb{E}[Z_j]]^2}{4\text{var}[Z_j]\, a^2} \right\}, \qquad (7)$$

on a continuum domain $x \in \mathbb{R}$. Finally, the "bridge" condition in section [XXX] is imposed to re-enforce the fixed-number condition (2).

C. Number partition theory

Although the approach detailed in the above section accurately estimates the mean and variance of equilibrium position of jth bead, it is an approximated theory. The random walk is continuous in space and the positions of the beads resides on an lattice. In addition, the distribution of the position of any bead in the random-walk picture is always a Gaussian [], but in the discrete lattice model it is not: for example, in low temperature, the polymer would be mostly staying in its fully stretched configuration (see Fig. 1) and the distribution of the positions of the beads are always bounded by the natural length of the rods.

Analytic solutions are possible in this particular model. We outline the key ideas in the followings, and leave the more detailed and technical analysis in a separate article [XXX].
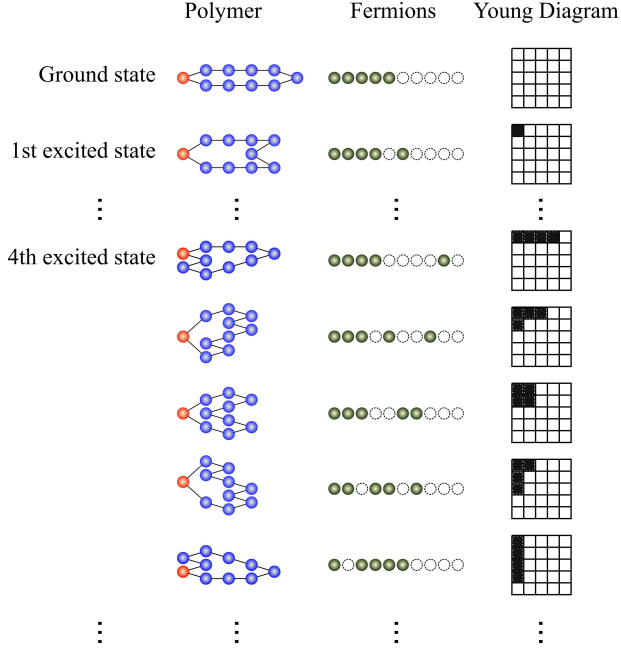
FIG. 1. Schematic diagram. (a) Polymer blahblihblah (b) Fermion blahblihblah (c) Young diagram didadi...

Our idea is to change the basis of the Fermionic system from its microscopic configurations $\{Z_0, Z_1, \ldots, Z_{N-1}\}$ to the energy of the system. Clearly, the energy can only take values $E_0, E_0 + \Delta E, \ldots, E_0 + N^2 \Delta E/4$; in this picture, the probability space is a one-dimensional lattice with finite support. Without lost of generality, we let the constant energy $E_0 = 0$ and $\Delta E = 1$ by choosing a proper unit. The difficulty of this basis is to determine the degeneracy of the microscopic states which have the same energy $E \in \{0, 1, \ldots N^2/4\}$, sometimes referred to as the "density of the state" in statistical mechanics [] and condensed matter physics []. We let the number of microscopic states with energy E to be $g(E)$; once $g(E)$ is known, the partition function of the system can be formally derived in the canonical ensemble picture

$$\mathcal{Z}(T) = \sum_{E=0}^{N^2/4} g(E) \exp\left(-\frac{E}{k_B T}\right), \qquad (8)$$

and the equilibrium property of the system can be derived from $\mathcal{Z}$.

With a little surprise, we discovered that $g(E)$ in this problem is closely related to the problem of integer partition in number theory []. The connection can be made by formulating the problem in the following way. We consider to label the micro-state of the system by how many energy unit a Fermion is excited from its ground state. Mathematically, we denote E_i to be the excited energy of the particle with i^{th} highest energy. The total energy

of the system is

$$E = \sum_{i=1}^{N} E_i, \qquad (9a)$$

and construction we have a constraint

$$N/2 \geq E_1 \geq E_2 \geq \ldots \geq E_{N/2} \geq 0. \qquad (9b)$$

Equations (9) constitutes a restricted partition of the integer E: $g(E)$ is the possible ways to partition an integer E into $N/2$ non-increasing parts [].

A very neat way to label the microscopic configuration is to use the Young diagram [], showing in the right panel of Fig. 1. The black box in row i denotes the excited energy E_i. With the constraint (9b), each row can have at most $N/2$ black boxes, and the number of black boxes in $(i+1)^{\text{th}}$ row cannot exceed the that in i^{th} row. Then, $g(E)$ is the number of possibility of arrangement of E black boxes onto the $N/2 \times N/2$ "checkerboard".

Once the this relation is identified, fruitful results from the number theory [] can be used to solve our problem. For example, denote the ways to put E black boxes onto an $K \times L$ checkerboard with non-increasing number of black boxes per row by $\pi(K, L, E)$. A recursive relation exists []

$$\pi(K, L, E) = \pi(K, L-1, E) + \pi(K-1, L, E-L), \qquad (10)$$

which allows very efficient computations of the $g(E) = \pi(N/2, N/2, E)$. In addition, the generating function

$$\Phi(q) := \sum_{E=0}^{N^2/2} g(E) q^E \qquad (11)$$

is identified to be the Gaussian binomial coefficient

$$\Phi(q) \equiv \binom{N}{N/2}_q := \frac{\prod_{j=1}^{N}(1-q^j)}{\left[\prod_{j=1}^{N/2}(1-q^j)\right]^2}, \qquad (12)$$

which allows us to formulate the partition function of the original polymer problem (**??**).

We finally remark that along this line of analysis, the probability distribution analogous to (6a) can also be formulated. Not surprisingly, for a finite (and small N), the exact results are different from (6a). Several other physical quantities at equilibrium can be efficiently computed without resorting to Monte Carlo simulation. We will present a more detailed analysis separately [XXX].

III. EXTEND THE MAPPING TO NON-EQUILIBRIUM

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 on a one dimensional lattice. To illustrate the equivalence, we firstly define a typical particle hopping model and build the connection between these two models.

A. Asymmetric Exclusion Process

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 r and l respectively, we have the following detailed balance during the hopping

$$rP_n = lP_{n+1} \qquad (13)$$

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 (13) can be rewrite as

$$l/r = P_n/P_{n+1} = \exp\left(-\Delta E/k_B T\right) \qquad (14)$$

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 l/r. Thus we have

$$l + r = cT \qquad (15)$$

where c is a constant. With eq. (15) and eq. (14) we can in principle solve l and r 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

$$\Delta E = 2Fa \qquad (16)$$

Plug into the above equations one obtain

$$l = \frac{cT \exp\left(-2Fa/k_B T\right)}{1 + \exp\left(-2Fa/k_B T\right)} \qquad (17a)$$

$$r = \frac{cT}{1 + \exp\left(-2Fa/k_B T\right)} \qquad (17b)$$

One has to careful to notice that the process of a group of particles hoping to right is not correspond to the stretching process of the polymer. It is actually correspond to a spatial motif of polymer configuration moving along the polymer. 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 together with particle number are crucial to determinate the type of corresponding polymer.

It is not difficult to find that the pinned polymer loop corresponds to exactly $N/2$ particles hopping on N lattice sites with reflecting boundaries, as discussed in detail for modeling chromosome in this paper. The mapping can be generalized to other cases, e.g. un-pinned polymer loop corresponds to $N/2$ particles on N lattice sites with periodic boundaries, free polymer chain corresponds to an open lattice filled by arbitrary number of particles. We start and focus on the case of pinned polymer loop in this paper because of its direct biological relevance. Other cases will be discussed in our future work.

B. Relaxation Time

With the ASEP analogy of polymer dynamics, we are ready to go deeper to analyze the non-equilibrium properties of the polymer system. One of the typical quantities people interested about dynamics is relaxation time, denote by τ here. The protocol here is as following, firstly the trajectories of particle on ASEP is recorded and then transformed to bead position of polymer by eq. (3), finally relaxation time is fitted from auto-correlation function (ACF) of interested observables such as gyration radius R_g.

To get trajectories of hopping particle, we employ the Kinetic Monte Carlo simulation[], which is very fast and efficient compare to Molecular Dynamics simulation of polymer. By transform to the picture of polymer, we obtain the dynamical behavior illustrate in Fig. **??**.

ACF of gyration radius is calculated based on the information of beads position. It is not surprising that the $ACF(Rg)$ decays exponentially with time lag. However, we also observe a effect of multiple relaxation modes which is predicted in Rouse model, especially in the case of strong external force. Practically, relaxation time is fitted in the decaying regime where the slope is most flat, which corresponds to the longest relaxation mode.

We interested in how the relaxation time varies with the external force field. So we fixed the temperature T and total hopping rate cT in our model and simulate the relaxation behavior for different external force. One would intuitively expect a monotonic decreasing as F grows. Surprisingly, we found a non-monotonic behavior contrast to the expectation, i.e. there is peak which marks a slowest relaxation time in a weak external force regime. See in Fig. **??**. To verify the non-monotonic behavior is not artificially introduced by the reduction of the model, we perform a 3D Brownian dynamics simulation of pinned bead-rod loop with the same settings. We successfully reproduced the same behavior of relax-

ation time varies with external force — non-monotonic, as illustrate in Fig. **??**

The non-monotonic behavior can be better understood in the corresponding particle hopping picture. In the strong force case, all particles sit on the left half of the lattice sites. Only the right-most particle is free to hop right. In fact, because of the strong hopping bias to the left, even this particle is not easy to move. Thus a faster relaxation behavior is observed caused by the strong constraint. On the other hand, when there is totally no external force applied on the polymer beads, which means there is no bias for the particle hopping. In this case, the particle will finally evenly distributed on the lattices sites. The freedom of particle to move is confined by its neighbors, which is only 2 lattice sites in average. Since the total hopping rate is fixed, the relaxation time is proportional to the accessible distance. In comparison, in the moderate force regime, particle distributed denser on the left part of lattice and sparser on the right part. The freedom for those particles on the right side to move is larger than the case of no external force, and the constraint is not so strong that these particles can still easily move around. These conditions lead to a longer relaxation time than the case with no force.

IV.   CONCLUSIONS

In conclusion, we demonstrate that 1D polymer can be exactly mapped to a particle hopping on lattice sites, i.e. ASEP. We discussed the case of pinned polymer loop in detail, shown the analytical equilibrium statistics drawing from the mapping. Furthermore, the dynamics of polymer is also illustrated in the mapped particle hopping picture. Interestingly, we found the relaxation time varies with external force non-monotonically. An quantitative explanation is given by picture of particles hopping on the lattices sites.

The mapping from polymer to particle is not restricted in the case of pinned polymer loop. Other generalizations can be investigated with the same mapping, which leads to ASEP model with different boundaries and particle numbers. We emphasize the generality of this mapping which can be applied to a huge class of polymer problems. Moreover, the polymer dynamics beyond 1D is also possible to model by multi-species ASEP model. There are still a lot of fascinating open questions to discover in the future.