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ONE-DIMENSIONAL CHAIN WITH HERNIAS

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Abstract. The density-matrix renormalization-group method has been applied to the modified $d = 1$ Rubinstein-Duke model for polymer dynamics, where hernias are considered. This simple model demonstrates the crossover from reptation to Rouse dynamics.

Introduction

In the past decade the motion of long linear polymers has been successfully treated by stochastic lattice models of hopping reptons. In a gel or in a polymer melt, the motion of a polymer is largely confined to reptation in a tube, which restricts sideways motion. In a dilute solution in a fluid, the polymer has however a much larger degree of freedom. So one distinguishes in polymer dynamics between reptation, which is the motion in a fixed confining tube and Rouse dynamics, which applies to polymers in a fluid [1]. Both forms of motion have distinct characteristics, if only one form of motion is present. Rouse dynamics leads to a diffusion coefficient decaying as N^{-1} for long chains, where N is the number of moving units (the reptons) of the chain. Reptation on the other hand is much slower and the diffusion coefficient decays as N^{-2} . Similar behavior is observed for the renewal time which increases as N^2 for Rouse dynamics and as N^3 for reptation. There has been a dispute on the precise values of the exponents, since there seemed to be a discrepancy between the theoretical exponents given here and the experimentally observed values. This issue has been clarified recently by means of a careful finite-size scaling analysis. A less studied question is the crossover from Rouse dynamics to reptation.

Therefore it is interesting to study the asymptotic behavior of the diffusion coefficient and the renewal time when both mechanisms are present. This note addresses the crossover problem, albeit in a simplified setting. Apart from Rouse dynamics and reptation there is a form of motion which holds the middle between the two. It is the formation and annihilation of hernias. A hernia is a sideways motion of a repton, which does not modify the confining tube. In dimensions $d = 2$ and higher, hernias are believed to have only a marginal influence on the diffusion coefficient and renewal time, by and large because the hernias grow and shrink not affecting the backbone of the tube. Only hernias close to the end of the chain can change the tube substantially.

However in dimension $d = 1$, the situation is different. Sideways motion is not possible of course, but a one-dimensional chain is full of hernias, since the chain can only progress back and forth and every step in the forward direction, followed by a step backward is a hernia. Considering the chain as a random walker, one finds that the number of hernias is of the same order as the number of links between the reptons. Now, if the hernias are fixed and if they can only disappear or be created by the retraction and extension of the ends of the chain, the basic motion is that of reptation. In this note a one-dimensional model is studied which includes reptation and hernia annihilation and creation. It shows crossover from the reptation exponents to the Rouse exponents as a function of the creation/annihilation rate of the hernias. The crossover regime is described by a crossover function, which we determine for the model.

1. The model

The model is a one-dimensional chain of $N+1$ reptons, connected by N links, y_1, \dots, y_N . The links are either in the forward direction, $y_i = 1$, or in the backward direction $y_i = -1$, or have the value $y_i = 0$. The cases $y_i = \pm 1$ are considered as taut links, while $y_i = 0$ is a slack link or an element of stored length. The basic motion rule is the hopping of this stored length unit along the chain, by interchanging with slack links. If it moves in the forward direction, its transition rate is biased by a factor $B > 1$, while the hopping rate in the backward direction is decreased by the factor $B^{-1} < 1$. The biases represent an external field driving the reptons of the chain. At the end of the chain the links may change from slack to taut and vice versa, thereby adding or subtracting an element of stored length, again with a bias depending on the direction of the transport of length. These motion rules form the much studied Rubinstein-Duke (RD) model [2]. Our new element is that we allow a neighboring pair of opposite taut links to change into a pair of slack links and vice versa. We describe this as the annihilation viz. creation of a hernia. The transition rate for hernia creation/annihilation is h , multiplied with a bias based on the sign of motion of the middle repton of the hernia.

Without hernia motion the RD model is a typical case of reptation. The tube, which is here the sequence of taut links, can only be changed from the ends. This is a slow process, since a taut link at distance l from the end can only disappear from the tube by at least l^2 elementary steps. So the inner taut links survive at least N^2 repton moves, if the change could renew itself in a systematic way. The change of configuration is however a diffusive process in configuration space and therefore the average renewal time is N^4 measured in single repton moves, or N^3 in chain updates. So the reptation renewal time $\tau \sim N^3$. Obviously hernia creation and annihilation speed up the renewal of the chain and the point of this note is to see how they can overtake the reptation mechanism.

Our model is, as all the hopping models, governed by the Master Equation for the probability distribution $P(Y)$ where Y stands for the complete configuration y_1, \dots, y_N . It has the form

$$\frac{\partial P(Y, t)}{\partial t} = \sum_{Y'} [W(Y | Y')P(Y', t) - W(Y' | Y)P(Y, t)] \equiv \sum_{Y'} M(Y, Y')P(Y', t) \quad (1)$$

The W 's are the transitions rates and the matrix M contains the gain terms (in the off-diagonal elements) and the loss terms (on the diagonal). Conservation of probability implies that the sum over the columns of the matrix vanishes. So the matrix has a zero eigenvalue and the eigenfunction corresponding to this eigenvalue is the stationary state of the system, to which every other initial state ultimately decays. The matrix is non-symmetric, due to the bias, which gives different rates to a process and its inverse. So one has to distinguish between left and right eigenfunctions. The left eigenfunction belonging to the zero eigenvalue is trivial (all components equal); the problem is to find the right eigenfunction as the stationary state probability distribution.

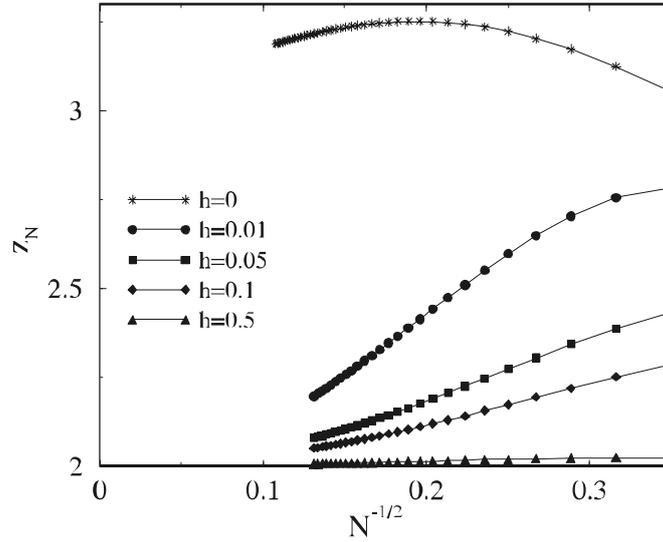


Fig. 1. Plot of z_N as function of $N^{-1/2}$ for several values of the transition rate h for hernia creation/annihilation

The renewal time is given by the slowest decaying eigenstate. Thus the gap in the spectrum near 0 is the inverse renewal time. All eigenvalues must of have of course a negative real part, otherwise probability would grow unlimited. The form (1) stresses the similarity to quantum mechanical problems. Indeed the linear structure of the polymer chain makes it a one-dimensional quantum problem, however, with a non-hermitian hamiltonian. Our approach to the solution exploits this ana-

logy by applying the so-called DMRG method [3] for quantum problems to find the properties of the transition matrix M . In previous publications this method has been described in detail [4]. Here we present only the results.

2. Scaling exponents

One of the advantages of the DMRG method is that it calculates the properties, e.g. the gap, for a growing length N of the chain. The drawback is that the calculations are lengthy and the values of larger N come in slowly. But the procedure is stable and can run for months without interference. This make the results very well suited for a finite size analysis. We convert the gap as function of N to a renewal time $\tau(N)$. In Figure 1 we present the local exponent z_N , defined as

$$z_N = \frac{\ln[\tau(N+2)] - \ln[\tau(N)]}{\ln(N+2) - \ln(N)} \quad (2)$$

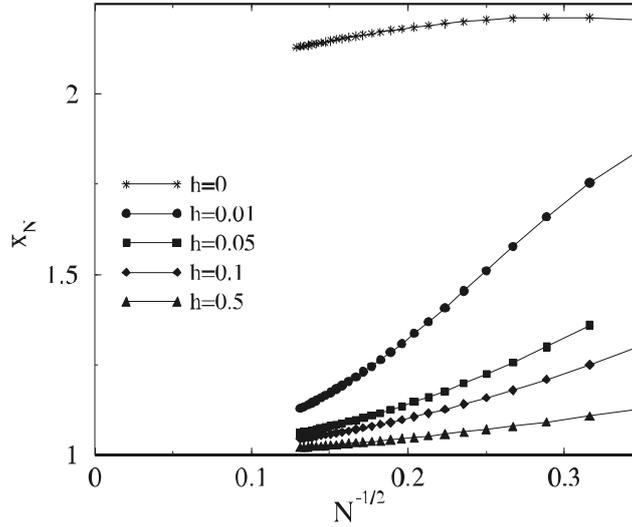


Fig. 2. Plot of x_N as function of $N^{-1/2}$ for several values of the transition rate h for hernia creation/annihilation

The DMRG method gives very accurate values such that the small differences in (2) do not spoil the accuracy. Conventionally the renewal time refers to the unbiased (or undriven) system. The various curves correspond to different values of h . We have found earlier [4] that the proper way to plot it as function of N , is to use $N^{-1/2}$ on the horizontal axis. Some features are noteworthy:

- It takes very large values N to reach the asymptotic regime. This is the origin of the earlier mentioned controversy between theory and experiment. In particular

the plateau in the $h = 0$ curve (the pure reptation case) may easily lead to the conclusion that the exponent has settled on the (too large) value.

- The influence of the parameter h is quite strong for long chains in particular for small values of h . We come back on this point when we discuss the crossover behavior.
- The asymptotic behavior of the exponent (for $N \rightarrow \infty$) differs for $h = 0$ from all the other curves. While the theoretical value $z_\infty = 3$ for reptation, is compatible with the data, it is definitely excluded for the curves $h \neq 0$. They rather point to the common value $z_\infty = 2$.

In Figure 2 we plot in the same way the local exponent x_N for the diffusion coefficient. The diffusion coefficient is obtained by the Einstein relation from the drift velocity in the limit of small driving fields [4]. The drift velocity is easily found from the probability distribution of the stationary state. The picture has the same message as the previous one. It is clear that, without hernia motion ($h = 0$), the exponent evolves towards the value 3, while for any non-zero value of h , it rather aims at a value 2. Again one has large corrections to scaling which make it difficult to conclude the exponent e.g. from log-log plots.

3. Crossover scaling

The point of crossover scaling is to represent the data for various values of h in one single curve. Anticipating the asymptotic values of the two regimes: $h \rightarrow 0$ and a fixed $h \neq 0$, the following representation is adequate for the renewal time

$$\tau(N, h) = N^3 g(h^\alpha N) \quad (3)$$

The crossover scaling function $g(x)$ should have a finite value $g(0)$ and behave for large argument as $g(x \rightarrow \infty) \sim 1/x$, in order that the expected asymptotic behavior results for the two regimes: reptation dominated and hernia dominated. In Figure 3 we have plotted the same curves as in Figure 1 but against the combination $h^{1/2} N$. The observed data collapse is the proof for crossover scaling.

In Figure 4 we do the same for the diffusion coefficient in the form

$$D(N, h) = N^{-2} f(h^\alpha N) \quad (4)$$

Now the crossover scaling function f approaches again a finite value at $x = 0$ and for large arguments, it should behave as $f(x \rightarrow \infty) \sim x$. The data collapse for the choice $\alpha = 1/2$, but not as nice as for the renewal time. So further finite-size corrections are visible.

The exponent $\alpha = 1/2$ is the best exponent for data collapse, but its precise value cannot be deduced from the data. Our preference for $\alpha = 1/2$ is based on the simple estimate of the times to remove a hernia for the two mechanisms. As we

mentioned, pure reptation requires N^2 single repton moves to remove a hernia. For the competing process of annihilating a hernia, it takes $1/h$ repton steps. The fastest process dominates and the crossover scaling function should be a function of the ratio $h N^2$.

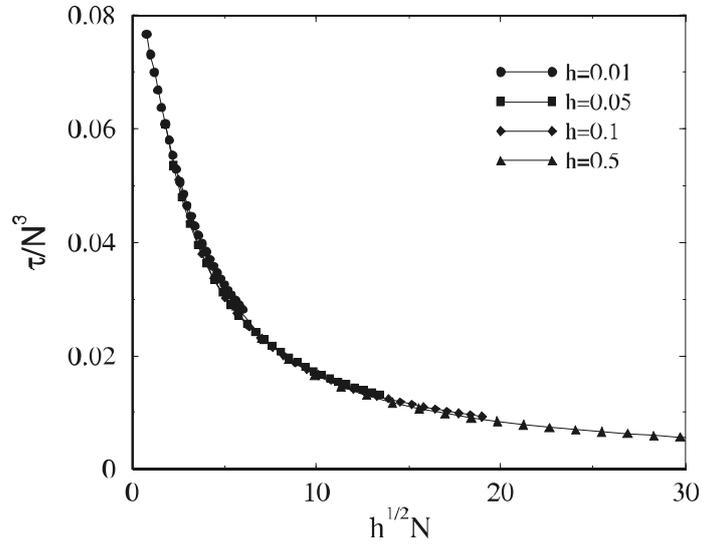


Fig. 3. The scaling form for the renewal time for various values of h

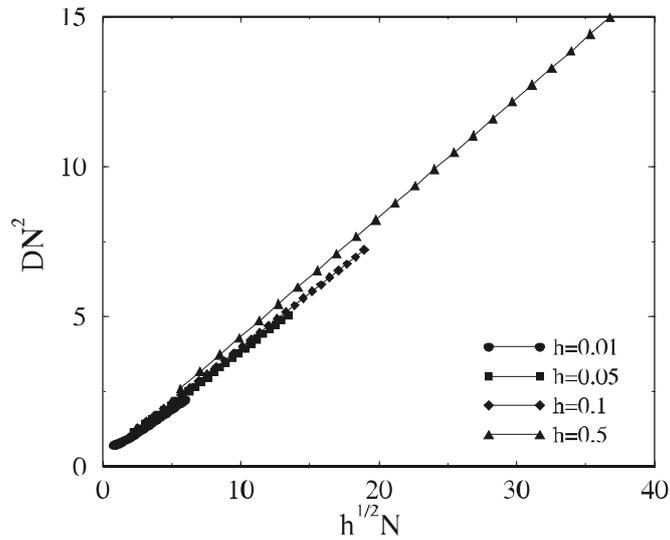


Fig. 4. The scaling form for the diffusion coefficient for various values of h

Conclusions

We have presented a simple model which demonstrates the crossover from reptation to Rouse dynamics. In our one-dimensional model hernia annihilation and creation play the same role as the tube changes which are allowed in Rouse dynamics. Longer calculations, which will sharpen up the results and the conclusions, are in progress.

In a paper by Sartoni and van Leeuwen [5], the one-dimensional reptation with hernia creation and annihilation was connected with a simpler model of two types of particles which move independent of each other along the chain. They also conclude that the diffusion coefficient decays as N^{-1} , but they have to stick to a hernia creation and annihilation rate equal to the hopping rate of the reptons. Here we could vary this rate at will and therefore study the crossover behavior.

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