Drift velocity for a chain of beads in one dimension

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The one-dimensional motion of a chain of *N* beads is studied to determine its drift velocity when an external field is applied. The dependences of the drift velocity with the chain length and field strength are addressed. Two cases are considered, chains with all their beads charged and chains having an end bead charged. In the last case, an analytical expression for the drift velocity is proposed for all *N*. Results are tested with the help of Monte Carlo simulations.

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I. INTRODUCTION

A chain in one dimension can move by contracting and stretching in a wormlike fashion. This mechanism, named reptation in polymer physics, plays a key role in the dynamics of entangled polymer melts and in many chemical, biological, and industrial processes. In the dynamics of entangled polymers, neighboring chains constrain a given chain to diffuse only along a confining tube and then the chain executes a one-dimensional random walk [1,2]. Thus, a chain can progress by leaving part of the initial tube and creating a new part as it reptates.

The idea of reptation was originally introduced by de Gennes [3]. Later, Rubinstein presented a unidimensional model (the repton model) to analyze the chain dynamics under reptation [4]. This model was adapted by Duke to study electrophoresis of DNA chains in a gel [5] and then the consequences of applying an external field was addressed for a variety of cases [6–12]. Electrophoresis is a very important tool in molecular biology that is regularly used for separating long chain macromolecules according to their size.

Recently, Guidoni *et al.* introduced a slightly modified repton model with hardcore reptons in one dimension [13,14]. The dynamics diffusion of both repton models are identical. However, the hardcore reptons model is more flexible regarding the jump probabilities of particles at the ends of chains relative to those for the central ones allowing the study of cases that cannot be addressed with the original repton model [4]. In this work we focus on the drift velocity as a function of the chain length for the hardcore reptons model. We deduced exact analytical expressions for some cases of interest using an approach that simplifies the calculations respect to the standard methods used in the literature [15]. We also verified the Einstein relation comparing the present results with the chain diffusivity as a function of the chain length recently derived [16,17].

II. MODEL

Let us consider a chain in a one-dimensional lattice consisting of *N* particles that can hop to the nearest site only if this site is empty. There can be only one particle per lattice site. Particles can hop to the right or left but no more than one site can be empty between two of them [13,14]. When external force are not applied, the jumping rules of the model are as follows:

(i) If the particle is located at the end of the chain and its nearest site is occupied by another particle, the end particle jumps with a probability per unit time p_a, see Fig. 1(a).

(ii) If the particle is located at the end of the chain and its nearest site is empty, the end particle jumps with a probability per unit time p_b, see Fig. 1(b).

(iii) If the particle is not an end particle (i.e., it is a middle particle) and one of its nearest site is occupied and the other one is empty, the middle particle jumps to the empty site with a probability per unit time p_c, see Fig. 1(c).

(iv) If the particle is a middle particle with both nearest sites occupied, or both nearest sites empty, the middle particle does not jump and remains at its original position, see Figs. 1(d) and 1(e).

Hence, p_a, p_b, and p_c are the free parameters of the model. Every time a particle jumps, the center of mass of the chain

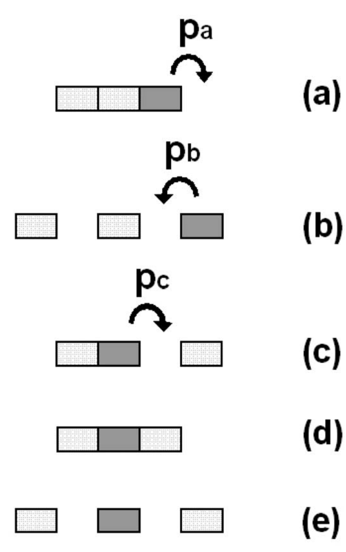

FIG. 1. Jumping probabilities per unit time for end [(a), (b)] and middle [(c), (d), (e)] particles. In cases (d) and (e) the middle particle, the shaded one, cannot jump.

moves $1/N$ of the distance a between adjacent lattice sites. In the following we use $a=1$.

An empty site in the chain is named a hole. A hole is created or annihilated every time an end particle jumps moving away from the chain or towards the chain. With no external fields, an end particle jumping attempt that creates a hole is successful with frequency $p_a(1-P_h)$, where P_h is the hole probability. Similarly, an end particle jumping attempt that annihilates a hole succeeds with frequency $p_b P_h$. In equilibrium we expect the same frequency for creation and annihilation. Then, P_h can be expressed as

$$P_h = \frac{p_a}{p_a + p_b}. \quad (1)$$

Note that P_h is independent of p_c.

When a force is applied to a particle, say to the right, the jumping frequencies per unit time of the particle to the right and to the left will be considered to be $(1+\delta)k$ and k, respectively. k is the jumping frequency, to the right or to the left when no field is applied (i.e., $k=p_a$, p_b, p_c) and $\delta>0$. In what follows we will refer to δ as the applied "force" to a particle of the chain.

We will start considering the case named the *uniform force case* when a force δ to the right is applied to every particle of the chain. We discuss next the case when a force δ to the right is only applied to the right end particle of the chain. This case will be called the *pull case*. Similarly, one can obtain the drift velocity for the case in which a force δ to the right is only applied on the left end particle of the chain (the *push case*).

III. RESULTS AND DISCUSSIONS

A. Uniform force case

Exact analytical expression for the drift velocity, in the uniform force case, for a chain with small values of N, can be derived as follows. We will focus on $N=3$. In Fig. 2 different configurations for a chain with three beads and its evolution are presented. The scheme also shows the probabilities for the possible transitions among configurations.

It is important to note that we consider that the system is formed by a large number of noninteracting chains. It is then assumed that, after some time, the system will be in steady state in which the number of chains n_i in every configuration "i" and the number of chains per unit time evolving among configurations remain constant. Possible configurations of the chains have been grouped together in cells that take into account the symmetry of the system, see Fig. 2. Note that in Fig. 2, $n_0=n_4$, $n_1=n_5$, $n_2=n_6$, and $n_3=n_7$. Therefore, we can write the following:

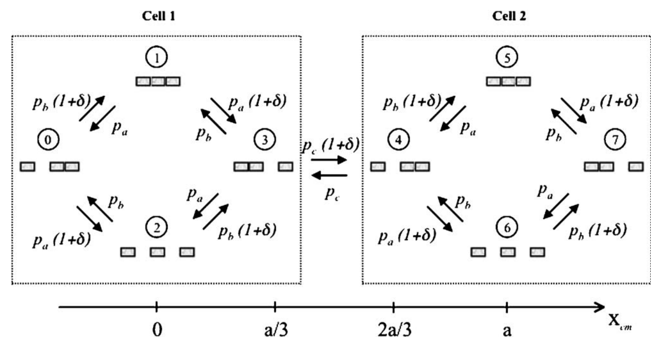

FIG. 2. Representation of the possible configurations for a chain with three beads, transitions among configurations, and jumping probabilities per unit time when a force δ to the right is applied to each particle of the chain. Different positions for the center of mass are indicated. In the analytical expressions the value $a=1$ was used.

$$[n_0(1+\delta)+n_3]p_b = n_1 p_a(2+\delta), \quad (2)$$

$$[n_0(1+\delta)+n_3]p_a = n_2 p_b(2+\delta), \quad (3)$$

$$(n_1p_a+n_2p_b)(1+\delta)+n_0p_c = n_3[p_a+p_b+p_c(1+\delta)], \quad (4)$$

$$n_1p_a+n_2p_b+n_3p_c(1+\delta) = n_0[(p_a+p_b)(1+\delta)+p_c]. \quad (5)$$

From this set of equations, the average number of chains n_i in each configuration i in cells 1 and 2 can be determined. From Eqs. (2)–(5), it follows

$$\frac{n_1}{n_0} = \frac{p_b}{p_a}\left[\frac{p_c(1+\delta)^3+(p_a+p_b+p_c)(1+\delta)(2+\delta)+p_c}{[p_a+p_b+p_c(1+\delta)(2+\delta)](2+\delta)}\right],$$

$$\frac{n_2}{n_0} = \frac{p_a}{p_b}\left[\frac{p_c(1+\delta)^3+(p_a+p_b+p_c)(1+\delta)(2+\delta)+p_c}{[p_a+p_b+p_c(1+\delta)(2+\delta)](2+\delta)}\right],$$

$$\frac{n_3}{n_0} = \frac{(p_a+p_b)(1+\delta)^2+p_c(2+\delta)}{p_a+p_b+p_c(1+\delta)(2+\delta)}. \quad (6)$$

We expect that, in presence of an external field, charged chains move with a drift velocity v. Then the resulting flux is $J_{drift}=cv$, where $c=n_0+n_1+n_2+n_3$ is the total number of chains per cell. Furthermore, the net flux of particles between cells 1 and 2 is given by [see Fig. 2]

$$J_{drift} = [n_3(1+\delta)-n_0]p_c. \quad (7)$$

From Eqs. (6) and (7), after some algebra, the drift velocity can be found to be

$$v_{N=3} = \frac{p_ap_bp_c}{(p_a+p_b)p_c + \dfrac{(p_a+p_b-p_c)}{(p_a+p_b)}\left[\dfrac{(p_a+p_b)^2(1+\delta)+p_ap_b\delta^2}{3+3\delta+\delta^2}\right]}\delta. \quad (8)$$

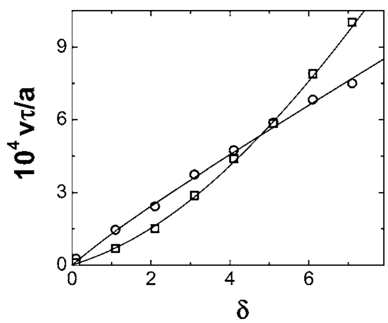

FIG. 3. Drift velocity of chains consisting of three beads as a function of the "external force" δ applied to every bead. The Monte Carlo results were obtained using $p_a\tau=0.05$ and $p_b\tau=p_c\tau=0.001$ (open squares), and $p_a\tau=0.0001$, $p_b\tau=0.001$, and $p_c\tau=0.1$ (open circles), where τ is the unit time. Lines correspond to theoretical results according to Eq. (8).

This result is valid for all values of δ. In Fig. 3, numerically calculated drift velocity and theoretical results, using Eq. (8) are shown. Note that for $p_a+p_b=p_c$ the drift velocity adopts the value $p_a p_b \delta/(p_a+p_b)$. Under this condition, the jumping probability per unit time is the same for every particle of the chain (i.e., the mobilities of all beads are the same, see Ref. [16]).

Using the same procedure as the one used above, the drift velocity for a chain of two particles can be obtained to be

$$v_{N=2} = \frac{p_a p_b}{(p_a+p_b)}\delta, \tag{9}$$

which is also valid for all δ.

We will analyze now the correlations between holes in a chain with three particles. For example, we will show the calculations of the correlation for the configuration named "0" in Fig. 2. Remember that n_i is the average number of chains in the configuration i. Let P be the probability of finding a hole between the right end and the central particle. Similarly, let Q be the probability of finding a hole between the central and the left end particle. Then, with no force applied, P and Q adopt the value given by Eq. (1).

The probability of finding the chain in the 0 configuration is $\mathrm{Prob}(0)=n_0/(n_0+n_1+n_2+n_3)$. Then, the correlation C can be expressed as

$$C = \mathrm{Prob}(0) - Q(1-P), \tag{10}$$

where

$$P = \frac{n_2+n_3}{n_0+n_1+n_2+n_3}, \tag{11}$$

$$Q = \frac{n_0+n_2}{n_0+n_1+n_2+n_3}. \tag{12}$$

Then, with the help of Eqs. (6), the correlation can be found to be

$$C = (p_a+p_b-p_c)\frac{p_a^2 p_b^2 p_c(3\delta^2+3\delta^3+\delta^4)}{F^2}, \tag{13}$$

where

$$F = (p_a^2+p_b^2)p_c + [(p_a^2+p_b^2)(p_a+p_b) + 2p_a p_b p_c](1+\delta) + [(p_a^2+p_b^2)p_c + p_a p_b(p_a+p_b+p_c)](1+\delta)^2. \tag{14}$$

Equation (13) shows, first, that for all values of p_a, p_b, and p_c, the correlation vanishes at order δ, and second, for $p_a+p_b=p_c$ the correlation vanishes for all values of δ. We expect that both properties, verified for $N=3$, are also valid for all values of N.

When $p_a+p_b=p_c$, we found that the mobilities of all the beads for a chain of any length are the same. Thus, chains are dragged without deforming, the Einstein relation is always valid (for any N and δ), and no correlation is found (see Ref. [16] for details). Assuming that the above-mentioned first property is valid for all N, one can use the mean field approach and write a set of equations corresponding to the average velocity of each bead of a chain. Then, one can obtain the following diffusion coefficient valid for $N\geq 2$ that was derived through a different method and also numerically verified in Ref. [16]

$$D_N = \frac{p_a p_b p_c}{(p_a+p_b)[(N-2)(p_a+p_b)+2p_c]}. \tag{15}$$

Using the second property, if $p_a+p_b=p_c$, one can obtain

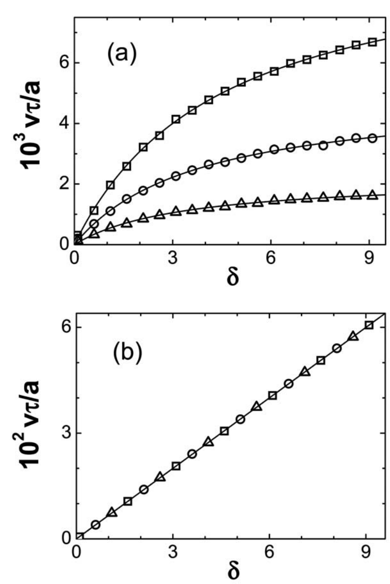

FIG. 4. (a) Drift velocity of chains with N particles as a function of the external force δ, when a force δ to the right is only applied on the right end particle of the chain (i.e., the pull case). (b) Linear dependence between drift velocity and the applied force δ for different N, in the uniform force case when $p_a+p_b=p_c$. The parameters of the model are $p_a\tau=0.01$, $p_b\tau=0.02$, and $p_c\tau=0.03$, where τ is the unit time. Open squares correspond to $N=3$, open circles to $N=5$, and open triangles to $N=10$. Numerical results were obtained using Monte Carlo simulations. Lines correspond to theoretical results of Eqs. (16) and (24).

$$v_N = \frac{p_a p_b}{(p_a + p_b)}\delta, \tag{16}$$

for $N \geq 2$ and all values of δ. Figure 4 (b) illustrates the linear dependence between drift velocity and the applied force δ, for different N, when $p_a + p_b = p_c$. The numerical results are obtained from Monte Carlo simulations.

B. Pull and push cases

We will study now the pull case for a chain of three beads. Using the same argument that in the uniform force case, we analyze the four configurations shown in Fig. 2 but considering that the force δ to the right is only applied on the right end particle. Then, we can write the following set of equations:

$$(n_0 + n_3)p_b = n_1 p_a(2 + \delta), \tag{17}$$

$$[n_0(1 + \delta) + n_3]p_a = 2n_2 p_b, \tag{18}$$

$$n_1 p_a(1 + \delta) + n_2 p_b + n_0 p_c = n_3(p_a + p_b + p_c), \tag{19}$$

$$n_1 p_a + n_2 p_b + n_3 p_c = n_0[p_a(1 + \delta) + p_b + p_c]. \tag{20}$$

Note that the flux is given by $J_{drift} = cv$, where $c = n_0 + n_1 + n_2 + n_3$. Furthermore, the net flux between cells can be written as

$$J_{drift} = (n_3 - n_0)p_c. \tag{21}$$

Using the same procedure as those used for the uniform force case, we can obtain

$$v_{N=3} = \frac{p_a p_b p_c}{[p_a(2 + \delta) + 2p_b]p_c + (p_a + p_b)[p_a(1 + \delta) + p_b]}\delta, \tag{22}$$

valid for all δ. Similarly, for $N=2$ we can easily deduce

$$v_{N=2} = \frac{p_a p_b}{p_a(2 + \delta) + 2p_b}\delta. \tag{23}$$

By comparing these last two equations, the general expression for any N can be proposed to be

$$v_N = \frac{p_a p_b p_c}{[p_a(2 + \delta) + 2p_b]p_c + (N - 2)\{(p_a + p_b)[p_a(1 + \delta) + p_b]\}}\delta, \tag{24}$$

which is valid for all δ.

Let us consider now the push case. Using the same method as above, the expression for the drift velocity for a chain with $N=3$ and $N=2$ can be obtained as

$$v_{N=3} = \frac{p_a p_b p_c}{[2p_a + p_b(2 + \delta)]p_c + (p_a + p_b)[p_a + p_b(1 + \delta)]}\delta, \tag{25}$$

and

$$v_{N=2} = \frac{p_a p_b}{2p_a + p_b(2 + \delta)}\delta. \tag{26}$$

Note that exchanging p_a by p_b, Eqs. (22) and (23) become Eqs. (25) and (26), respectively. Then, for the push case one infers that

$$v_N = \frac{p_a p_b p_c}{[2p_a + p_b(2 + \delta)]p_c + (N - 2)\{(p_a + p_b)[p_a + p_b(1 + \delta)]\}}\delta. \tag{27}$$

The validity of Eqs. (24) and (27) has been extensively verified using Monte Carlo simulations for different values of N and δ. In Fig. 4(a) numerically calculated drift velocity for the pull case, for different N, are presented. These results are in full agreement with Eq. (24).

It is interesting to note that, depending on the values of p_a and p_b, the drift velocity might result larger for the pull case than for push case or vice versa. This can be explained as follows. As seen in describing the model, see Fig. 1, particles of a chain need holes to move. However, if the number of holes is very large, internal particles become immobile most of the time. We conclude that chains with a very large (or very small) number of holes present a low mobility. When we deal with a large P_h ($p_a \gg p_b$ [see Eq. (1)]), by pulling from an end the average number of holes increases what does not favor mobility. Conversely, if we push one end the number of holes is reduced and the mobility is favored. Similarly, the behavior of a chain with a low P_h can be understood.

C. Einstein relation

One expects that, in the limit $\delta \to 0$, the Einstein relation will hold for all cases. Indeed, in this limit, from Eqs. (8) and

(9) (i.e., the uniform force case) one can verify that (for $N = 2,3$)

$$v_N = N\delta D_N, \tag{28}$$

where $N\delta$ is the total force applied to the chain and D_N is the diffusion coefficient presented in Eq. (15). Similarly, from Eqs. (24) and (27) (the pull and push cases, respectively) it can be found for $N \geq 2$ that

$$v_N = \delta D_N, \tag{29}$$

where δ is the total force applied to the chain.

D. The large field limit

Finally, we will consider the limit of very large fields ($\delta \to \infty$). In the uniform force case, from Eqs. (8) and (9), the drift velocity takes the form

$$v_{N=2} = \frac{p_a p_b}{(p_a + p_b)}\delta, \tag{30}$$

$$v_{N=3} = \frac{p_a p_b p_c}{(p_a + p_b)p_c + (p_a + p_b - p_c)\dfrac{p_a p_b}{(p_a + p_b)}}\delta. \tag{31}$$

In order to derive the drift velocity for a chain with four particles, in the limit $\delta \to \infty$, we can use the same method used to obtain Eq. (8). For large fields, some frequencies become negligible and then the algebra simplifies significantly. Thus,

$$v_{N=4} = \frac{p_a p_b p_c}{(p_a + p_b)p_c + \dfrac{p_a p_b (p_a + p_b - p_c)}{(p_a + p_b)} + \dfrac{(p_a p_b)^2[(p_a + p_b)^2 - p_c^2]}{(p_a + p_b)^2\left[(p_a + p_b)p_c + \dfrac{p_a p_b}{(p_a + p_b)}(p_a + p_b - p_c)\right]}}\delta. \tag{32}$$

With $N > 4$ this method is intractable even for large fields.

From the Eqs. (24) and (27) (the pull and push cases, respectively), it is easily obtained

$$v_N = \frac{p_b p_c}{p_c + (N-2)(p_a + p_b)}, \quad \text{pull case} \tag{33}$$

$$v_N = \frac{p_a p_c}{p_c + (N-2)(p_a + p_b)}, \quad \text{push case}. \tag{34}$$

Note that in the pull and push cases the velocity (for $\delta \to \infty$) does not depend on the field. This behavior is also found in the Rubinstein-Duke model as described in Ref. [18].

IV. CONCLUSIONS

In this paper, we have analyzed a discretized model of a chain consisting of N particles, in the presence of an external field, in one dimension. Exact analytic results of drift velocity have been derived by means of an alternative approach not regularly used in the literature. With this method, the drift velocity is obtained solving a system of linear equations. This method was successfully used for different cases. If a force is applied to all particles of the chain, the drift velocity could be exactly determined for $N=2$ and $N=3$. For $p_a + p_b = p_c$, the mobility becomes independent of the chain length and the applied force, and the drift velocity is obtained for all δ. For the cases in which a force is applied only to one of the chain ends, an analytical expression for the drift velocity was proposed for all N and for any value of the applied force, results that were supported by simulations.

It is verified that the Einstein relation is valid in the limit of $\delta \to 0$. We also found that for fully charged chains under very large fields, the drift velocity becomes proportional to the field. Conversely, chains with a single end bead charged, the drift velocity for large fields presents an asymptotic value. All these findings were tested with the help of Monte Carlo simulations.

ACKNOWLEDGMENT

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