

PAPER

Finite-size scaling in unbiased translocation dynamics

To cite this article: Giovanni Brandani *et al* *J. Stat. Mech.* (2014) P05019

View the [article online](#) for updates and enhancements.

You may also like

- [Kinetic equations for systems with long-range interactions: a unified description](#)
Pierre-Henri Chavanis
- [A method to calculate the gamma ray detection efficiency of a cylindrical NaI \(TI\) crystal](#)
S. Ahmadi, S. Ashrafi and F. Yazdansetad
- [Versatile firmware for the Common Readout Unit \(CRU\) of the ALICE experiment at the LHC](#)
O. Bourrion, J. Bouvier, F. Costa et al.

Finite-size scaling in unbiased translocation dynamics

Giovanni Brandani¹, Fulvio Baldovin², Enzo Orlandini² and Attilio L Stella²

¹ SUPA, School of Physics, University of Edinburgh, Mayfield Road, EH9 3JZ, UK

² Dipartimento di Fisica e Astronomia and Sezione INFN, Università di Padova, Via Marzolo 8, I-35131 Padova, Italy
E-mail: s1246659@sms.ed.ac.uk, baldovin@pd.infn.it, orlandini@pd.infn.it and stella@pd.infn.it

Received 25 February 2014

Accepted for publication 4 April 2014

Published 22 May 2014

Online at stacks.iop.org/JSTAT/2014/P05019

doi:[10.1088/1742-5468/2014/05/P05019](https://doi.org/10.1088/1742-5468/2014/05/P05019)

Abstract. Finite-size scaling arguments naturally lead to the introduction of a coordinate-dependent diffusion coefficient in a Fokker–Planck description of the late-stage dynamics of unbiased polymer translocation through a membrane pore. The solution for the probability density function of the chemical coordinate matches the initial-stage subdiffusive regime and takes into account the equilibrium entropic drive. We find precise scaling relations connecting the subdiffusion exponent to the divergence with the polymer length of the translocation time, and also to the singularity of the probability density function at the absorbing boundaries. Quantitative comparisons with numerical simulation data in $d = 2$ strongly support the validity of the model and of the predicted scalings.

Keywords: stochastic particle dynamics (theory), polymer dynamics, dynamical processes (theory), stochastic processes (theory)

Contents

1. Introduction	2
2. Simulations and scaling relations	3
3. Survival and translocation probabilities	7
4. Conclusions	10
Acknowledgments	10
Appendix A	10
Appendix B	11
References	14

1. Introduction

Translocation of long polymers across a membrane is a basic biological process [1]–[3] and a fundamental problem in polymer dynamics. In the past fifteen years, a number of facts have been established and open issues pointed out [4]–[15]. Early attempts [4, 5] to study unbiased translocation on the basis of quasi-equilibrium assumptions and Fokker–Planck equations for the chemical-coordinate probability density function (PDF) were revealed to be inadequate for long chains [6]. There is now consensus [6, 12, 9] on the fact that, during the initial stages, the scaling with time of the mean square displacement of the chemical coordinate is subdiffusive, and clear evidence indicates that within this anomalous stage the process is reproduced well by a fractional Brownian motion. The precise value of the subdiffusive exponent still remains controversial [10, 6, 12, 13, 15] and could even depend on the viscosity of the solvent [16]. Most important, for finite lengths of the chain (which is a necessary condition for the translocation process to occur) the fractional Brownian motion description breaks down for times at which the translocation process has not yet occurred [9, 15]. The result is that, to the best of our knowledge, no theory is presently capable of quantitatively reproducing either the chemical-coordinate PDF, or the survival probability over the whole time span of the process. It is interesting to notice that, in spite of the breaking down of the initial subdiffusion behavior, signatures of it could remain in the late stages of the process. The singular behavior of the asymptotic PDFs of polymer displacements at the boundary values of the translocation coordinate could be such a candidate [12]. However, it is not clear how these singularities can be linked to the initial anomalous diffusion regime.

Here we show that the unbiased translocation process, in the time window following the initial anomalous diffusion, is in fact described by a Fokker–Planck equation with a displacement-dependent diffusion coefficient which neatly originates from a finite-size scaling analysis. Based on only two free parameters associated with microscopic details,

the Fokker–Planck equation quantitatively reproduces numerical results for both the translocation coordinate PDF and the survival probability. In addition, the finite-size scaling properties of the diffusion coefficient provide the mechanism for the appearance of singularities in the long-time PDF of the translocation regime. We are thus able to furnish a theoretical explanation of these singularities by linking them to the anomalous scaling exponent of the initial stages of the process. In section 2 we present the results of our simulations and the finite-size scaling analysis defining the displacement-dependent diffusion coefficient subsequently used in the effective Fokker–Planck description of the unbiased translocation process. Based on these developments we present in section 3 analytical results for the survival and the translocation probabilities of the process. In particular we find precise scaling relations connecting the subdiffusion exponent to the exponent that governs the singular behavior of the polymer probability density at the absorbing boundaries. Our conclusions are given in section 4. We further discuss the basis and the limits of validity of our approach in appendix A. In appendix B we report detailed calculations of the mean translocation time based on our Fokker–Planck equation and compare the analytical results with numerical data.

2. Simulations and scaling relations

Our numerical results are based on molecular dynamics simulations for the translocation dynamics of 2d self-avoiding linear chains made by $N + 1$ monomers of unit length and described by a finite extensible nonlinear elastic (FENE)-shifted Lennard-Jones interaction potential, in contact with a Langevin heat bath. By indicating with $0 \leq s(t) \leq N$ the number of monomers at one side of the pore at time t , the symbols in figure 1 refer to the (time-rescaled) mean square displacement $\langle \Delta s^2(t) \rangle \equiv \langle [s(t) - s_0]^2 \rangle$ for chains initially equilibrated with the monomer $s(0) = s_0$ at the pore. The first important feature to note in figure 1 is the existence of an initial anomalous regime, independent of both N and s_0 , during which $\langle \Delta s^2(t) \rangle = 2D_\alpha t^\alpha$, with $\alpha \simeq 0.81$ and D_α a generalized diffusion coefficient. The precise value of α , which is expected to be bound from below by $(1 + \nu)/(1 + 2\nu)$ [10] and from above by $2/(1 + 2\nu)$ [6], is still under debate [10, 6, 12, 13, 15]; recently, it has been claimed that α is also dependent on the viscosity [16]. For the system parameters and sizes analyzed here, we have found values of α close to the upper bound pointed out in [6]. In any case, our approach does not imply or require universality of this exponent. This N - and s_0 -independent initial stage can be ascribed to the scale-free, self-similar structure of the polymer, which is explored by the chemical coordinate during translocation. The finite size of the polymer implies a breakdown of the initial regime, which is followed by a stage in which the growth of $\langle \Delta s^2(t) \rangle$ is closer to linear in t , before dropping down as a consequence of the fact that with finite probability the translocation process has been completed. The times τ at which the breakdown of the initial anomalous scaling occurs, of course depend on both s_0 and N : $\tau = \tau(s_0, N)$.³ Thus, if one wishes to *match* the behavior of $\langle \Delta s^2(t) \rangle$ just after the breakdown with that of a normal diffusion starting at $t = 0$ with $s = s_0$, the normal-diffusion coefficient $D(s_0, N)$

³ $\tau(s_0, N)$, not to be confused with the mean translocation time, has been practically defined as the time at which we observe a variation of 5% with respect to the extrapolation of the initial anomalous behavior of $\Delta s^2(t)$.

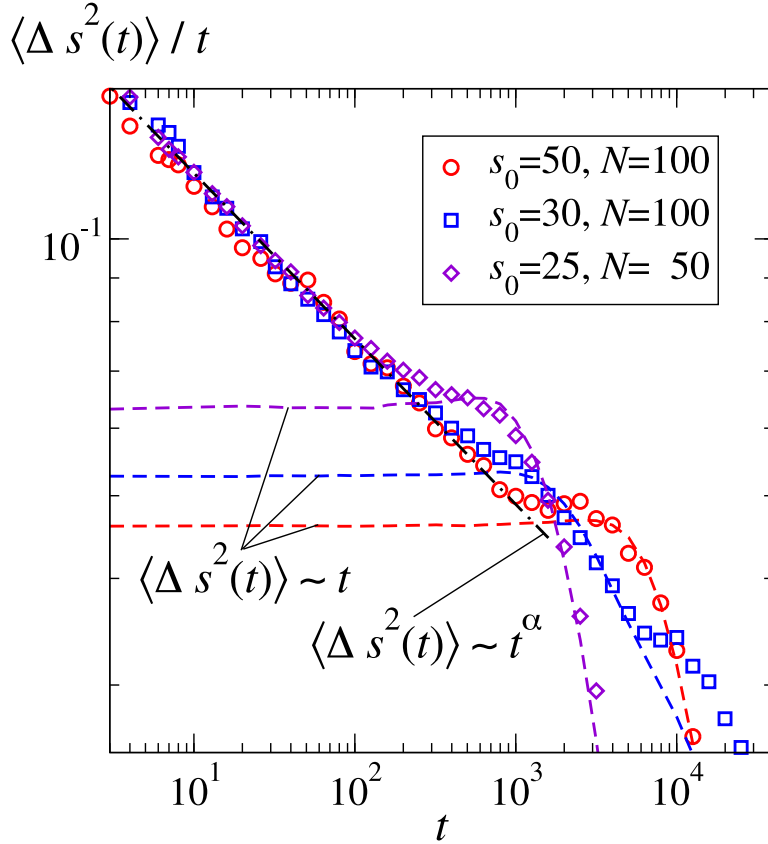


Figure 1. Symbols: Time-rescaled mean square displacement evolution for a translocating chain. At early stages, the dynamics follows a universal subdiffusive behavior $\langle \Delta s^2(t) \rangle \sim t^\alpha$, with $\alpha \simeq 0.81$ (dot-dashed line). This regime breaks down at a time τ depending on both s_0 and N . The dashed curves are obtained by numerically solving equation (2) with $D(s, N)$ given by equation (5), $A = 0.13$, and $s(0) = s_0$.

should satisfy the condition

$$2D_\alpha \tau^\alpha(s_0, N) = 2D(s_0, N)\tau(s_0, N). \quad (1)$$

Below, we argue that the idea of matching the evolution of the whole process for $t > \tau(N/2, N)$ with an effective Fokker–Planck description indeed works very well, provided one permits the diffusion coefficient $D(s_0, N)$ identified by equation (1) to enter, with its coordinate dependence, in the Fokker–Planck equation.

Treating s as a continuous coordinate, our goal is thus to develop an effective Fokker–Planck equation to be satisfied by the PDF $p(s, t|s_0, N)$ of having the monomer s at the pore at time t , given that the translocation process, for a polymer of size N , started at time zero with s_0 monomers at one side of the wall. The problem has natural absorbing boundaries at $s = 0$ and $s = N$, corresponding to the configurations in which the polymer completes the translocation process. We wish to profit from equation (1) and start to construct our model by first neglecting the entropic drive on the process. According to

Itô's rules for stochastic integration⁴, an over-damped Fokker–Planck equation with a position- and size-dependent diffusion coefficient, $D(s, N)$, reads

$$\partial_t p(s, t|s_0, N) = \partial_s^2 [D(s, N)p(s, t|s_0, N)]. \quad (2)$$

Multiplying equation (2) by $(s - s_0)^2$ and integrating over s , one easily obtains

$$\begin{aligned} \partial_t \mathbb{E} [(s - s_0)^2] &= \int_0^N ds 2D(s, N)p(s, t|s_0, N) \\ &\simeq 2D(s_0, N), \end{aligned} \quad (3)$$

where the approximation holds for times at which $p(s, t|s_0, N)$ is sufficiently concentrated around s_0 , or for $D(s_0, N)$ slowly varying in such a range. Below, we confirm *a posteriori* that these conditions are verified as long as the survival probability $S(t|s_0, N) \equiv \int_0^N ds p(s, t|s_0, N)$ is close to 1. Within this approximation, one is entitled to identify in figure 1 the ordinate at $t = \tau(s_0, N)$ as $2D(s_0, N)$.

To make further progress we have to clarify why we may expect $D(s_0, N)$ to satisfy a finite-size scaling symmetry. By equation (1) one gets $D(s_0, N) \propto \tau(s_0, N)^{\alpha-1}$ (see footnote 3). The quantity $\tau(s_0, N)$ is a measure of the time up to which the dynamics of the chemical coordinate is characterized by the cooperative motion of the polymer degrees of freedom determining anomalous dynamics. In this respect, τ can be regarded as the time beyond which the self-similar structure of the polymer ceases to be explored due to finite-size effects. In the related problem [6] of a tagged monomer diffusion with Rouse dynamics, the time taken by the central monomer to ‘feel’ the finite size of the polymer thus crossing over from sub- to normal-diffusion, scales as $N^{1+2\nu}$. Constraints imposed by the presence of the wall and the pore indicate that in general our $\tau(N/2, N)$ should be bounded from above by this time, but we here assume $\tau(N/2, N) \propto N^{1+2\nu}$ ($\nu = 3/4$ for 2d self-avoiding polymers [17]). More generally, we expect $\tau(s_0, N)$ to obey a scaling law both in s_0 and N of the form $\tau(s_0, N) \sim N^{1+2\nu} f(s_0/N)$ with $f(x) = f(1-x)$, or

$$D(s_0, N) \propto \left[\frac{1}{N^{1+2\nu}} \frac{1}{f(s_0/N)} \right]^{1-\alpha}. \quad (4)$$

A further condition can be found for $s_0 \ll N$. In this case, only the branch of the chain with length s_0 breaks the self-similarity sustaining the anomalous scaling (since the other branch becomes arbitrarily long). Thus, $\tau(s_0, N) \underset{s_0 \ll N}{\sim} s_0^{1+2\nu}$, implying $f(x) \underset{x \ll 1}{\sim} x^{1+2\nu}$. This behavior is again supported by the analogy with the Rouse dynamics, considering this time a tagged monomer close to the ends of the chain. By putting together this small-argument behavior with the symmetry $f(x) = f(1-x)$, it is reasonable to guess

$$D(s_0, N) = \frac{A}{N^\sigma} \left[\frac{1}{(s_0/N)^{1+2\nu}} + \frac{1}{(1-s_0/N)^{1+2\nu}} \right]^{1-\alpha}, \quad (5)$$

where A is a size-independent coefficient characterized by the microscopic details of the polymer's dynamics and $\sigma \equiv (1+2\nu)(1-\alpha)$. Notice that the maximum crossover time is

⁴ We use here Itô's prescriptions for multiplicative noise, in place of Stratonovich's ones; the latter being frequently used in classical transport equations. We have verified that this choice does not significantly affect our results.

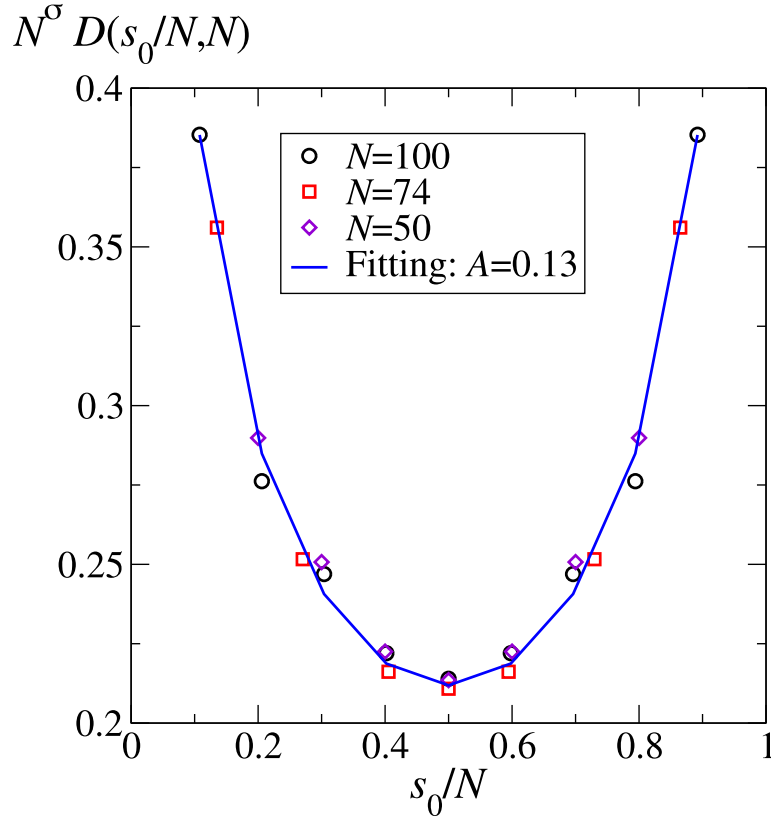


Figure 2. Data-collapse of $D(s_0, N)$ according to equation (5). Points are obtained from translocation simulations by averaging $\langle \Delta s^2(t) \rangle / 2t$ between $\tau(s_0, N)$ and the maximum time for which $S(t|s_0, N) \simeq 1$.

associated with the central monomer, $\tau(N/2, N) \sim N^{(1+2\nu)}$. On the other hand, as $s_0 \rightarrow 0$ (or $s_0 \rightarrow N$), $\tau(s_0, N) \rightarrow 0$ and correspondingly $D(s_0, N)$ in equation (5) diverges. We will see below that these divergences, which are hard to directly detect numerically, generate a singular behavior at the borders for $p(s, t|s_0, N)$.

As a first important check of the above deduction, we verify the finite-size scaling implied by equation (5). In figure 2 we data-collapse the numerical results of translocation dynamics obtained with various N and s_0 . Confirmation of equation (5) is remarkable, yielding a best-fitted $A \simeq 0.13$. Further validations of our approach are furnished by the comparison of the solution of equation (2) with the molecular dynamics simulations of the translocation process, as reported in figure 1 and specifically commented in appendix A. Such a comparison also indicates that our theory is expected to work well for $t > \tau(N/2, N)$ and $s_0 = N/2$, and to become less accurate as s_0 moves closer to the ends of the polymer chain.

Similarly to what has been done in the original approach by Sung and Park [4], equation (2) can be improved by considering the effect of an entropic force $-(D(s, N)/k_B T)$ ($dF(s, N)/ds$), where $F(s, N) = -k_B T \ln \Omega(s, N)$ is the free energy of the constrained polymer, and the validity of the Einstein relation has been assumed. Standard results [18]–[20] for the number of possible polymer configurations with the monomer s at the

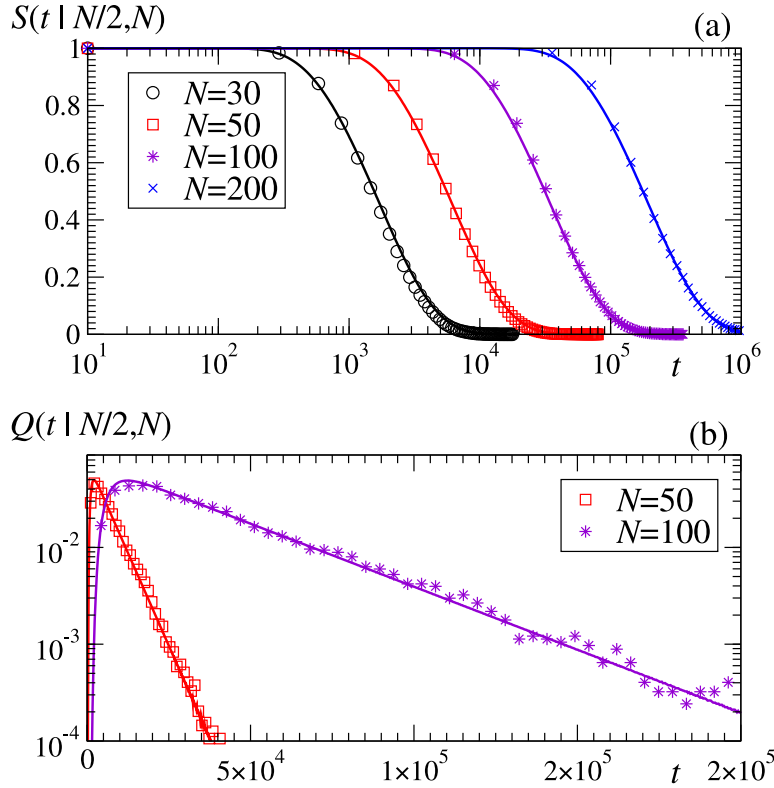


Figure 3. Survival (a) and translocation (b) probability for 2d linear polymers: MD simulations (symbols) versus theory (full lines).

pore, $\Omega(s, N)$, including scaling corrections, yield

$$\Omega(s, N) \propto [s(N-s)]^{(\gamma_1-1)} C(s) C(N-s), \quad (6)$$

where the surface entropic critical exponent is $\gamma_1 = 61/64 = 0.95$ for 2d linear polymers with self-avoidance [20], and

$$C(s) \simeq 1 + \frac{b_0}{s^{1/2}}, \quad (7)$$

with b_0 a parameter depending on the microscopic details of the model. Indeed, the inclusion of the entropic drive with a best-fitted $b_0 = 0.4$ (with $T = 1.2$ in natural dimensionless units) improves our overall results by about 5% (see figures 3(a), (b), 4(a)–(c)).

3. Survival and translocation probabilities

With the limitations mentioned in the previous paragraph, our complete description is thus given by the solution of the following equation:

$$\begin{aligned} \partial_t p(s, t | s_0, N) = -\partial_s \left\{ D(s, N) \frac{\partial_s \ln \Omega(s, N)}{\partial s} p(s, t | s_0, N) \right\} \\ + \partial_s^2 [D(s, N) p(s, t | s_0, N)], \end{aligned} \quad (8)$$

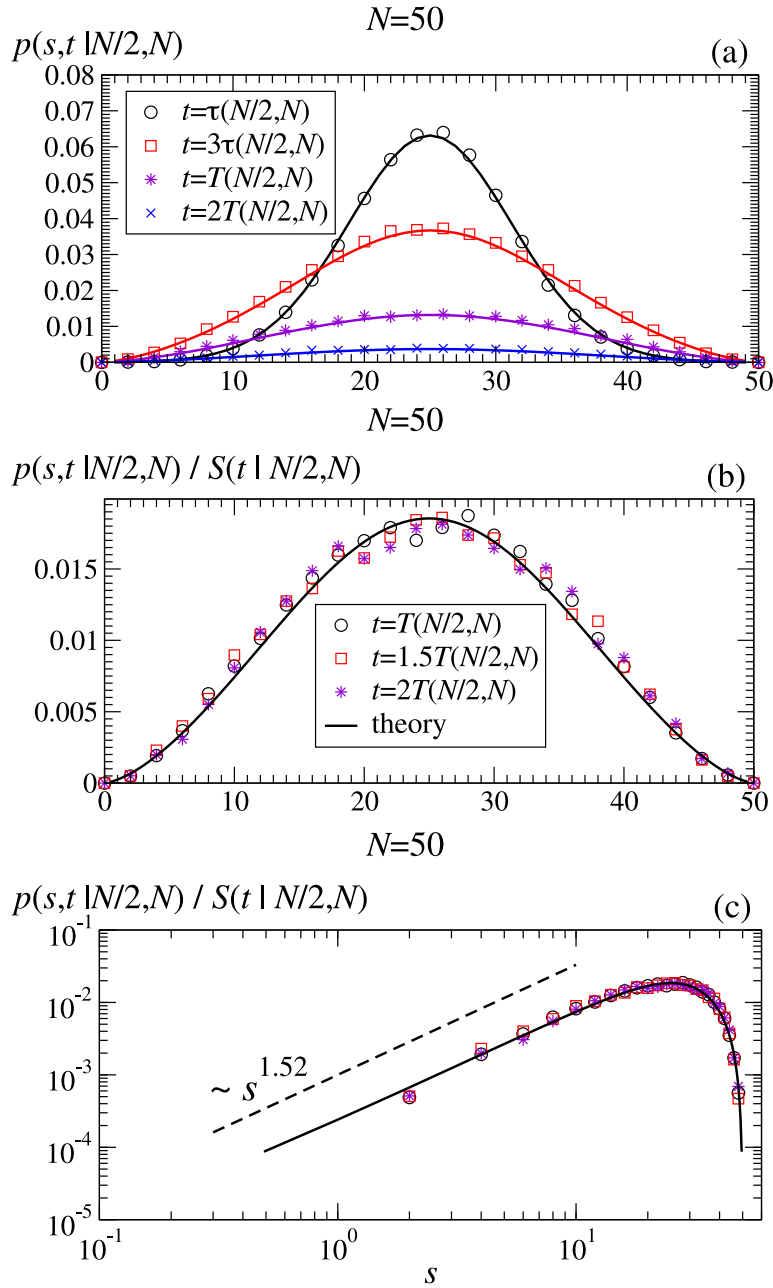


Figure 4. Time evolution of $p(s, t | N/2, N)$ (a) and PDF of the surviving polymers $p(s, t | N/2, N) / S(t | N/2, N)$ for large time (b): MD simulations (symbols) versus theory (full lines). (c) Same as (b) on a log–log scale, to appreciate the singular behavior at the boundary.

with $D(s, N)$ as in equation (5), $\Omega(s, N)$ as in equations (6) and (7), initial conditions $p(s, t | s_0, N) = \delta(s - s_0)$, and absorbing boundaries at $s = 0$ and $s = N$.

Equation (8) is separable, so that its general solution can be written in the form

$$p(s, t | s_0, N) = \sum_{m=1}^{\infty} A_m(s_0, N) X_m(s, N) e^{-\lambda_m^2 t}, \quad (9)$$

where X_m are the eigenfunctions corresponding to the eigenvalues λ_m ($0 < \lambda_1 < \lambda_2 < \dots$), and the amplitudes $A_m(s_0, N)$ are determined by the initial conditions. For large time, the behavior of the solution is dominated by the smallest eigenvalue λ_1 . This implies that both the survival probability $S(t|s_0, N)$ and the translocation probability $Q(t|s_0, N) = -\partial_t S(t|s_0, N)$ decay exponentially in the long-time limit. In addition, the PDF of the surviving polymers tends to the stable form

$$\frac{p(s, t|s_0, N)}{S(t|s_0, N)} \simeq A_1(s_0, N)X_1(s, N). \quad (10)$$

The eigenfunctions X_m and eigenvalues λ_m are numerically obtained discretizing the Liouvillian operator of the Fokker–Planck equation (see appendix B) into a matrix. Finding X_m and λ_m then reduces to computing the Schur decomposition of the matrix [21]. The solution for the first eigenfunction and eigenvalue is very stable with respect to the discretization procedure. Specifically, in our case we used 50 equally spaced points between 0 and N .

Recent simulations [12] indicated the long-time stability of $p(s, t|s_0, N)/S(t|s_0, N)$ and revealed a singular behavior at the boundaries as a specific anomalous signature of the translocation process (see also [22]). By using the Frobenius method (see, e.g., [23]) in equation (8), it can be proved that $X_1(s) \sim s^\phi$ for $s \rightarrow 0$ and $X_1(s) \sim (N-s)^\phi$ for $s \rightarrow N$, with

$$\phi = \sigma + 1 = (1 + 2\nu)(1 - \alpha) + 1. \quad (11)$$

Such a singular behavior is due only to the divergence of $D(s, N)$ and does not depend on the entropic drive. Putting $\alpha = 0.81$ and $\nu = 3/4$ in equation (11), we thus get $\phi = 1.52$, consistent with the simulation data (figure 4(c)) and very close to the value $\phi = 1.44$ numerically found in [12]. Using standard methods [24], from equation (8) one can also deduce ordinary differential equations for the survival probability $S(t|s_0, N)$ or for the mean translocation time $T(s_0, N) = \int_0^\infty dt S(t|s_0, N)$.

Our description performs extremely well for $s_0 = N/2$. Rescaling $s \mapsto s/N$ and $t \mapsto t/N^{\sigma+2}$ in equation (8), it is easily seen that the equation becomes independent of N as $N \gg 1$. This implies that the mean translocation time scales as

$$T(N/2, N) \sim N^{\sigma+2}. \quad (12)$$

With $\alpha \simeq 0.81$ for our 2d benchmark case, $\sigma + 2 \simeq 2.48$, which is consistent with what is observed in our simulations and also in previous studies [6, 13]. In appendix B, besides verifying the validity of equation (12), we show a very satisfactory quantitative comparison of the theoretical $T(N/2, N)$ with that estimated from the simulations. We stress, however, that different values of α lead to different scaling exponents for the mean translocation time. Taking $\alpha = 2/(1+2\nu)$ gives $T(N/2, N) \sim N^{1+2\nu}$, in agreement with [6]; taking $\alpha = (1+\nu)/(1+2\nu)$ gives $T(N/2, N) \sim N^{2+\nu}$, in agreement with [10]. This is an important versatility of the theory, especially in view of the fact that α has been recently claimed to be viscosity dependent [16]. Figures 3(a) and (b) display a very good agreement of the theory also with the numerical simulations of the process in terms of the survival and translocation probability, respectively. In particular, figure 3(b) highlights

the exponential decay of $Q(t|N/2, N)$ for large t . More stringently, even $p(s, t|N/2, N)$ is accurately reproduced by the theory for $t > \tau(N/2, N)$, as depicted in figure 4(a). In the long-time limit, the PDF of the surviving polymers collapses onto the predicted form $A_1(N/2, N)X_1(s, N)$, inclusive of the singular behavior at the borders (see figures 4(b) and (c)).

By considering s_0 closer to borders of the chain, the condition $S(\tau(N/2, N)|s_0, N) \simeq 1$ is violated. According to our arguments above, the analysis of the mean translocation time $T(s_0, N)$ as a function of s_0 reported in appendix B indeed shows that with s_0 becoming closer to the borders the mean translocation time becomes slightly smaller than that predicted by our effective theory.

4. Conclusions

We have shown that the late stages of unbiased polymer translocation can be described by an effective Fokker–Planck equation whose solution precisely reproduces the translocation PDF $p(s, t|s_0, N)$. The finite-size scaling characterizing the Fokker–Planck diffusion coefficient establishes a link with the anomalous diffusion at early times, providing a convincing explanation of all the features of $p(s, t|s_0, N)$, including the singular behavior at the border.

Acknowledgments

This work is supported by ‘Fondazione Cassa di Risparmio di Padova e Rovigo’ within the 2008–2009 ‘Progetti di Eccellenza’ program.

Appendix A

In this appendix we comment on the validity of our theory and corresponding limitations, based on figure 1.

Besides the results presented in figures 3 and 4, a further validation of our approach and an identification of its expected limits of validity comes from the comparison, given in figure 1, of the simulation results (symbols) with the numerical solutions of the Fokker–Planck equation

$$\partial_t p(s, t|s_0, N) = \partial_s^2 [D(s, N)p(s, t|s_0, N)] \quad (\text{A.1})$$

with $D(s, N)$ given by

$$D(s, N) = \frac{A}{N^\sigma} \left[\frac{1}{(s/N)^{1+2\nu}} + \frac{1}{(1-s/N)^{1+2\nu}} \right]^{1-\alpha}, \quad (\text{A.2})$$

and initial condition $p(s, 0|s_0, N) = \delta(s - s_0)$ (dashed curves).

The dashed curves in figure 1 confirm that the approximation reported in equation (3),

$$\begin{aligned} \partial_t \mathbb{E} [(s - s_0)^2] &= \int_0^N ds 2D(s, N)p(s, t|s_0, N) \\ &\simeq 2D(s_0, N), \end{aligned} \quad (\text{A.3})$$

is justified up to time t such that $S(t|s_0, N) \simeq 1$. In addition, with $s_0 = N/2$, simulations of equation (A.1) are shown to reproduce the time evolution of the mean square displacement well for $t > \tau(s_0, N)$, even when the effect of the absorbing boundaries becomes important and $S(t|s_0, N) < 1$. If we choose s_0 closer to the borders of the chain, deviations appear in the long-time behavior (see the $s_0 = 30, N = 100$ plot).

In our effective Fokker–Planck equation, different chemical coordinates are entailed with different diffusion coefficients $D(s, N)$. As can be appreciated through figure 1 and equation (A.3), during the initial anomalous stage, the mean square displacement of the translocation coordinate is larger than that effectively assumed in the Fokker–Planck description. Only for t larger than the maximum τ , i.e., $t > \tau(N/2, N)$, may the anomalous stage be considered ended and the effective diffusion coefficients $D(s, N)$ could be a faithful representation of the ‘diffusivity’ of the translocation coordinate for all s . This poses a first limitation to our theory. In addition, since we put as initial condition $p(s, 0|s_0, N) = \delta(s - s_0)$ in place of the PDF $p(s, \tau(N/2, N)|s_0, N)$ resulting from the initial anomalous stage, we also need to assume that at $t = \tau(N/2, N)$ only a negligible fraction of polymers have completed the translocation process, i.e., that $S(\tau(N/2, N)|s_0, N) \simeq 1$. This condition is satisfied for s_0 close to $N/2$. In view of the lower ‘diffusivity’ in our representation, as s_0 becomes close to the borders we expect our approach to provide an upper bound for the survival probability of a translocating polymer. This is illustrated in figure B.1 of appendix B.

Appendix B

In this appendix we detail derivation of the mean translocation time. Our Fokker–Planck equation, equation (8) of the main text, may be rewritten as

$$\partial_t p(s, t|s_0, N) = \mathcal{L}_s p(s, t|s_0, N), \quad (\text{B.1})$$

where the Liouvillian operator \mathcal{L}_s is given by

$$\mathcal{L}_s \equiv \left\{ \partial_s D(s, N) \frac{\partial \ln \Omega(s, N)}{\partial s} \right\} + \{ \partial_s^2 D(s, N) \}. \quad (\text{B.2})$$

Defining the survival probability $S(t|s_0, N)$ as

$$S(t|s_0, N) \equiv \int_0^N ds p(s, t|s_0, N), \quad (\text{B.3})$$

it follows [24] that $S(t|s_0, N)$ satisfies the equation:

$$\partial_t S(t|s_0, N) = \mathcal{L}_{s_0}^\dagger S(t|s_0, N), \quad (\text{B.4})$$

where the adjoint Liouvillian operator $\mathcal{L}_{s_0}^\dagger$ (acting now on the initial data s_0) is

$$\mathcal{L}_{s_0}^\dagger = \left\{ D(s_0, N) \frac{\partial \ln \Omega(s_0, N)}{\partial s_0} \partial_{s_0} \right\} + \{ D(s_0, N) \partial_{s_0}^2 \}. \quad (\text{B.5})$$

In terms of $S(t|s_0, N)$ the mean translocation time $T(s_0, N)$ is given by

$$T(s_0, N) = - \int_0^\infty dt t \partial_t S(t|s_0, N) \quad (\text{B.6})$$

$$= \int_0^\infty dt S(t|s_0, N), \quad (\text{B.7})$$

inheriting from equation (B.4) the ordinary differential equation

$$\mathcal{L}_{s_0}^\dagger T(s_0, N) = -1. \quad (\text{B.8})$$

Equation (B.8) has boundary conditions

$$T(0, N) = 0, \quad (\text{B.9})$$

$$T(N, N) = 0, \quad (\text{B.10})$$

and can be solved, for example, numerically for a generic s_0 . Numerical solutions for $N = 50$ are compared in figure B.1 with the results of molecular dynamics simulations of the translocation dynamics as described in section 2. Taking advantage of the symmetry with respect to the middle point, here we explicitly calculate the mean translocation time for $s_0 = N/2$. We first rewrite equation (B.8) as

$$\{\partial_{s_0} \Omega(s_0, N) \partial_{s_0}\} T(s_0, N) = - \frac{\Omega(s_0, N)}{D(s_0, N)}. \quad (\text{B.11})$$

Integrating between $N/2$ and s_0 we have

$$\Omega(s_0, N) \partial_{s_0} T(s_0, N) = - \int_{N/2}^{s_0} ds'_0 \frac{\Omega(s'_0, N)}{D(s'_0, N)}, \quad (\text{B.12})$$

where we have used that $\partial_{s_0} T(N/2, N)|_{s_0=N/2} = 0$, as implied by the symmetry of the problem around $s_0 = N/2$. Rearranging equation (B.12) and integrating between $N/2$ and N we finally obtain

$$T(N/2, N) = \int_{N/2}^N ds_0 \frac{1}{\Omega(s_0, N)} \int_{N/2}^{s_0} ds'_0 \frac{\Omega(s'_0, N)}{D(s'_0, N)}, \quad (\text{B.13})$$

where we have used the boundary condition $T(N, N) = 0$.

Equation (B.13) can be evaluated explicitly by using the expressions for $D(s_0, N)$ and $\Omega(s_0, N)$ given in the main text. Namely,

$$D(s_0, N) = \frac{A}{N^\sigma} \left[\frac{1}{(s_0/N)^{1+2\nu}} + \frac{1}{(1-s_0/N)^{1+2\nu}} \right]^{1-\alpha}, \quad (\text{B.14})$$

$$\Omega(s_0, N) \propto [s_0(N-s_0)]^{(\gamma-1)} C(s_0) C(N-s_0), \quad (\text{B.15})$$

with

$$C(s_0) \simeq 1 + \frac{b_0}{s_0^{1/2}}. \quad (\text{B.16})$$

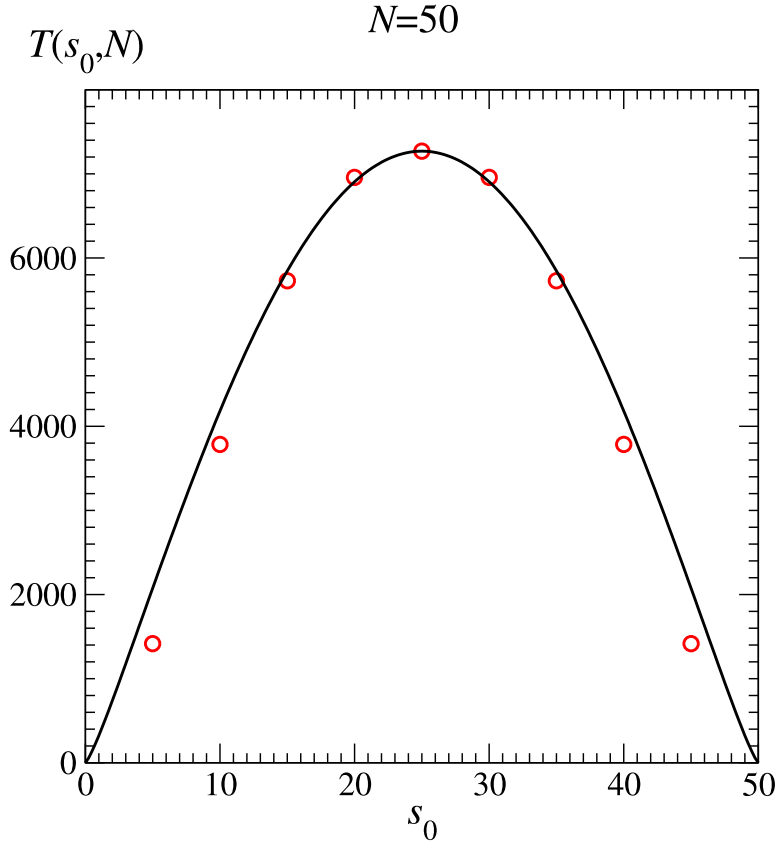


Figure B.1. Mean translocation time as a function of s_0 : MD simulations (symbols) versus theory (full lines).

The result is

$$T(N/2, N) = \frac{N^{\sigma+2}}{A} \int_{1/2}^1 dx \frac{1}{[x(1-x)]^{(\gamma_1-1)} [1 + b_0/N^{1/2}x^{1/2}] [1 + b_0/N^{1/2}(1-x)^{1/2}]} \times \int_{1/2}^1 dx' \frac{[x'(1-x')]^{(\gamma_1-1)} [1 + b_0/N^{1/2}x'^{1/2}] [1 + b_0/N^{1/2}(1-x')^{1/2}]}{[1/x'^{1+2\nu} + 1/(1-x')^{1+2\nu}]^{1-\alpha}}, \quad (\text{B.17})$$

where $\sigma = (1 + 2\nu)(1 - \alpha)$. As $N \gg 1$, the correction to scaling can be neglected, and the above expression simplifies to

$$T(N/2, N) = \frac{N^{\sigma+2}}{A} \int_{1/2}^1 dx \frac{1}{[x(1-x)]^{(\gamma_1-1)}} \int_{1/2}^1 dx' \frac{[x'(1-x')]^{(\gamma_1-1)}}{[1/x'^{1+2\nu} + 1/(1-x')^{1+2\nu}]^{1-\alpha}} \propto N^{\sigma+2}, \quad (\text{B.18})$$

yielding the expected scaling behavior. In figure B.2 we compare the analytical expression (B.17) with numerical data based on MD simulations: The agreement turns out to be extremely good.

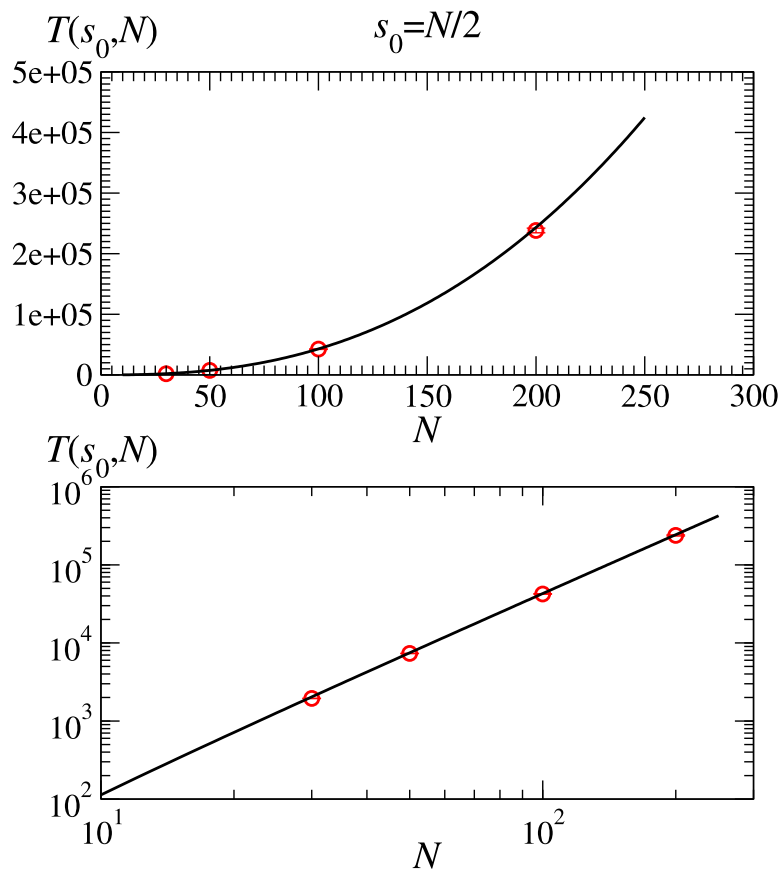


Figure B.2. N -dependence of the mean translocation time at $s_0 = N/2$ in linear and log–log scales: symbols refer to MD simulations while the full curves refer to equation (B.17) with $A = 0.13$, $b_0 = 0.4$, and $\sigma = (1 + 2\nu)(1 - \alpha)$ with $\nu = 3/4$, $\alpha = 0.81$.

References

- [1] Kasianowicz J J, Brandin E, Branton D and Deamer D W, 1996 *Proc. Nat. Acad. Sci. USA* **93** 13770
- [2] Meller A, Nivon L and Branton D, 2001 *Phys. Rev. Lett.* **86** 3435
- [3] Dekker C, 2007 *Nature Nanotechnol.* **2** 209
- [4] Sung W and Park P, 1996 *Phys. Rev. Lett.* **77** 783
- [5] Muthukumar M, 1999 *J. Chem. Phys.* **111** 10371
- [6] Chuang J, Kantor Y and Kardar M, 2001 *Phys. Rev. E* **65** 011802
- [7] Metzler R and Klafter J, 2003 *Biophys. J.* **85** 2776
- [8] Ali I and Yeomans J M, 2005 *J. Chem. Phys.* **123** 234903
- [9] Wolterink J, Barkema G and Panja D, 2006 *Phys. Rev. Lett.* **96** 208301
- [10] Panja D, Barkema G and Ball R, 2007 *J. Phys.: Condens. Matter* **19** 432202
- [11] Dubbeldam J, Milchev A, Rostiashvili V and Vilgis T, 2007 *Phys. Rev. E* **76** 010801
- [12] Chatelain C, Kantor Y and Kardar M, 2008 *Phys. Rev. E* **78** 021129
- [13] Luo K, Ollila S, Huopaniemi I, Ala-Nissila T, Pomorski P, Karttunen M, Ying S and Bhattacharya A, 2008 *Phys. Rev. E* **78** 050901
- [14] Zoia A, Rosso A and Majumdar S, 2009 *Phys. Rev. Lett.* **102** 120602
- [15] Panja D *et al.*, 2010 *J. Chem. Phys.* **132** 14902
- [16] de Haan H and Slater G, 2012 *J. Chem. Phys.* **136** 204902
- [17] Nienhuis B, 1982 *Phys. Rev. Lett.* **49** 1062

- [18] Vanderzande C, 1998 *Lattice Models of Polymers* (Cambridge: Cambridge University Press)
- [19] Li B, Madras N and Sokal A, 1995 *J. Stat. Phys.* **80** 661
- [20] Duplantier B and Saleur H, 1986 *Phys. Rev. Lett.* **57** 3179
- [21] Galassi M, Davies J, Theiler J, Gough B, Jungman G, Alken P, Booth M and Rossi F, 2009 *GNU Scientific Library Reference Manual-(v1.12)* (Bristol: Network Theory Ltd)
- [22] Amitai A, Kantor Y and Kardar M, 2010 *Phys. Rev. E* **81** 011107
- [23] Kusse B and Westwig E, 2006 *Mathematical Physics* (New York: Wiley-VCH)
- [24] Risken H, 1989 *The Fokker-Planck Equation* (Berlin: Springer)