Anomalous diffusion with absorbing boundary

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In a very long Gaussian polymer on time scales shorter than the maximal relaxation time, the mean squared distance traveled by a tagged monomer grows as $\sim t^{1/2}$. We analyze such subdiffusive behavior in the presence of one or two absorbing boundaries and demonstrate the differences between this process and the subdiffusion described by the fractional Fokker-Planck equation. In particular, we show that the mean absorption time of diffuser between two absorbing boundaries is finite. Our results restrict the form of the effective dispersion equation that may describe such subdiffusive processes.

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I. INTRODUCTION

The stochastic fluctuations of a broad range of physical systems [1] exhibit a behavior commonly denoted as anomalous diffusion. The random motion is characterized by the scaling of a mean squared coordinate, which (when averaged over many realizations) scales as t^{α} in time t. For "normal" diffusion $\alpha=1$, while the cases of $\alpha\neq 1$ are referred to as "anomalous," with $\alpha<1$, corresponding to subdiffusion, while $\alpha>1$ describes superdiffusion. The physical origin of anomalous behavior is usually the coupling of the particle (or some other coordinate) to many other degrees of freedom, such that its dynamics is the superposition of numerous other modes with widely distributed time scales. In principle, there is no reason to expect any "universality" in such anomalous processes, and any two situations described by the same exponent α may have very different characteristics. Nevertheless, certain general considerations have motivated approaches that encompass a large variety of cases: for a review see Ref. [2].

Many problems related to the behavior of random walkers can be formulated in terms of first passage of a walker, or its absorption at a boundary [3–5]. The presence of the absorbing boundary may help to discriminate between different types of anomalous random walkers. Indeed, in the following subsections we shall demonstrate how the study of absorption can be used to gain better understanding of the complexity of anomalous behavior. The behavior of a normal diffuser confined by absorbing boundaries is well understood; in particular, for large times t the survival probability $S(t)$ of such a diffuser decays exponentially. Consequently, the probability density function (PDF) of the diffuser to be absorbed at a particular time $Q(t)=-dS(t)/dt$ also exhibits an exponential decay, leading to a finite mean absorption time. The corresponding result in the case of subdiffusion is less clear. Only recently it was established [6] (while building on previously known expressions [2,7]) that for one-dimensional (1D) subdiffusion between two absorbing boundaries which is described by a particular (fractional) diffusion equation [2], the PDF of absorption $Q(t)$ decays as a small power of t, leading to an infinite mean absorption time. The fractional diffusion equation used in this analysis [6] applies to continuous time random walks, which at each step have a waiting time distribution with a long tail.

A relatively simple and practically important case of subdiffusion is the motion of a tagged monomer in a long polymer, whose anomalous dynamics was deduced and (numerically) observed by Kremer *et al.* [8]. A polymer consisting of a large number N of monomers has processes happening on multiple length scales, ranging from the microscopic distance, such as separation between adjacent monomers a to the size of the polymer. (A measure of the latter is the radius of gyration R_g. In a good solvent $R_g\approx aN^{\nu}$ [9], with the exponent $\nu\approx 0.59$ in space dimension $d=3$. The "$\approx$" sign indicates omission of a dimensionless prefactor of order unity. In the absence of intermonomer repulsion $\nu=1/2$ for any d.) To these length scales are associated times $\tau_{\rm micro}\approx a^2/D_o$, below which a selected monomer "does not feel" its surroundings, and $\tau_N\approx R_g^2/D_{\rm c.m.}\approx a^2N^{1+2\nu}/D_o$ for how long it takes the polymer to diffuse its own R_g. Here D_o denotes the diffusion constant of a single monomer, while the diffusion constant of the entire polymer, or its center of mass (c.m.), is D_o/N. (In this discussion we disregard hydrodynamic interactions.) Very short and very long times correspond to normal diffusion with different diffusion constants. It has been shown in Ref. [8] that for intermediate times $\tau_{\rm micro}<t<\tau_N$, the polymer undergoes anomalous diffusion with mean squared distance $\approx a^{2-2\alpha}(D_ot)^{\alpha}$, where $\alpha=2\nu/(1+2\nu)$. Note, that subdiffusion occurs even in the case of the ideal polymer with $\nu=1/2$.

In this work we analyze the subdiffusive motion of a tagged monomer which is part of an ideal (Gaussian) one-dimensional (1D) polymer. While the entire polymer performs diffusive (Monte Carlo) dynamics, we record the position of a single monomer at the midpoint of the chain. In the absence of absorption, this is a simple, analytically solvable problem, and the exact PDF of the monomer position is easily obtained. We could not extend these solutions in the presence of absorbing boundaries, and instead resorted to numerical studies. Indeed, with a single absorbing boundary, the PDF of the monomer position cannot be found using the standard method of images, which is the standard approach for normal diffusion and even some cases of subdiffusion.

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We show that when such a particle is placed between two absorbing boundaries, it has a finite mean absorption time, which scales (as expected) with the distance between the absorbing boundaries. Thus, the tagged monomer presents a simple example of subdiffusion whose survival probability differs drastically from that obtained by application of fractional diffusion.

To provide the basis of comparison with anomalous diffusion, in Sec. II we briefly review the behavior of a normal diffuser in the presence of absorbing boundaries. Our model of the tagged monomer, and the numerical procedure used, are presented in Sec. III. We also present some numerical results confirming the expected subdiffusive motion of a single monomer. In Secs. IV and V we study the behavior of the tagged monomer in the presence of a single and a pair of absorbing walls, respectively. We thereby demonstrate the similarities and distinctions between our anomalous diffuser and a normal random walk. Notably, we stress the differences between our case and the solution to the fractional diffusion equation. In the final Sec. VI, we discuss the possible applicability of our results to the translocation of a polymer through a membrane pore, which was in fact one of the motivations for this study.

II. NORMAL DIFFUSION WITH ABSORBING BOUNDARIES

The simplest model of a Brownian particle is a random walk (RW) on a discrete lattice, in which both the position of particle R and time (number of steps) t are integers. Exact expressions for the PDF $p(R,t)$, and many other properties, are readily available [10]. A continuum version is the Langevin equation for the motion (diffusion) of a single particle in a solvent (in the high friction limit), moving under the influence of thermal noise [11]

$$\zeta\frac{\partial R}{\partial t} = \eta(t). \tag{1}$$

Here ζ is the friction coefficient, and the thermal noise satisfies $\langle \eta(t)\rangle=0$ (no bias) and $\langle \eta(t)\eta(t')\rangle=2\zeta k_B T\delta(t-t')$. (The angular brackets, $\langle\cdots\rangle$, indicate averages over different realizations of the thermal noise.) Starting at $R=0$ at $t=0$, the PDF of particle position at a later time is

$$P(R,t) = \frac{1}{\sqrt{2\pi}\sigma}\exp\left(-\frac{R^2}{2\sigma^2}\right), \tag{2}$$

where $\sigma^2=2D_o t$ depends on the diffusion constant $D_o=k_B T/\zeta$. From the Langevin equation, one can also directly construct the Fokker-Planck (diffusion) equation [11,12] for the PDF as

$$\frac{\partial P(R,t)}{\partial t} = D_o\frac{\partial^2 P(R,t)}{\partial R^2}. \tag{3}$$

(Throughout this paper we consider one-dimensional motion; the generalization to higher dimensions is straightforward.)

Consider a diffusing particle starting at the origin and reaching position R at time t without ever touching an absorbing boundary at $R_a>0$. The solution of both continuous and discrete versions of this problem have been described in detail by Chandrasekhar [13]. It can be shown that the PDF for the random walker must vanish on the absorbing boundary. Since the diffusion equation is linear, this boundary condition can be satisfied by superposing the PDF of a free particle [Eq. (2)], and one starting at a reflected image as $\tilde{P}(R,t)=P(R,t)-P(R-2R_a,t)$. The survival probability $S(t)=\int_{-\infty}^{R_a}\tilde{P}(R,t)$ reduced by absorption [4], and for large times the absorption PDF decays as $Q(t)\propto t^{-3/2}$. This PDF has diverging mean, since the particle can drift infinitely far in the direction opposite the wall. It should be noted that the image method is specifically suited to random walkers performing independent unit steps; it fails for the subdiffusive walkers considered in this paper, and also for long-range hops of superdiffusive motion [14].

If the 1D diffusing particle is confined by two absorbing boundaries, one can still use superposition by the method of images to create a solution. However, in order to satisfy both boundary conditions, an infinite set of images is necessary. A more convenient answer is obtained by expanding the solution in terms of the eigenfunctions of the diffusion Eq. (3). For a particle enclosed by absorbing boundaries at $R_{a1}=0$ and $R_{a2}=L$, this gives

$$\tilde{P}(R,t) = \sum_{n=1}^{\infty} A_n \sin\left(\frac{n\pi R}{L}\right)\exp\left[-\left(\frac{n\pi}{L}\right)^2 D_o t\right], \tag{4}$$

where $\{A_n\}$ depend on the initial conditions. Note that at long times $\tilde{P}(R,t)\simeq A_1\sin(\pi R/L)e^{-(\pi/L)^2 D_o t}$, i.e., the PDF has a simple sinusoidal shape with zeroes on the boundaries. The survival probability is $S(t)\propto e^{-t/\tau}$, where the characteristic decay time $\tau=L^2/\pi^2 D_o$ is of the order of time the particle needs to diffuse over the length of the interval. The PDF for absorption $Q(t)$ also decays with the same time constant.

Anomalous diffusion can in principle have a myriad of distinct causes. An extensively studied case corresponds to the so-called continuous time random walks for which the waiting time between successive steps is taken from a broad distribution, with power law tails and a diverging mean. The interest in such processes originated in studies of diffusion in semiconductors [15], but they eventually became a prototype of anomalous diffusion. The fractional diffusion equation (which involves an integral operator) was developed to describe the evolution of the PDF for such walkers [16,17], and explicit solutions are now available [2,17–19]. Unlike Eq. (2) the solution to these equations is not smooth, but has a cusp at the origin. Another interesting feature is the behavior of the absorption PDF for anomalous diffusers between two absorbing boundaries: it has been shown [6], by careful analysis of the solutions [2,7], that for large times, $Q(t)$ decays as $t^{-(1+\alpha)}$, leading, for $\alpha<1$, to a diverging mean absorption time!

III. THE MODEL AND NUMERICAL PROCEDURE

A monomer in a polymer undergoes anomalous diffusion even in the trivial case of a phantom chain with no interactions, for which $\nu=1/2$ in any d. For this value of ν, monomer fluctuations are governed by an exponent $\alpha=1/2$, and thus exhibit subdiffusion. Since many properties of phantom polymers can be calculated exactly, this presents an excellent model for the study of subdiffusion. For simplicity, we shall restrict ourselves to the one-dimensional situation; generalization to higher dimensions is straightforward.

After coarse graining, a sufficiently long flexible polymer can be represented by effective monomers connected to their nearest neighbors by harmonic potentials (Gaussian springs) [9,20]. Thus, the Hamiltonian for a chain of N monomers is

$$H=\frac{K}{2}\sum_{n=1}^{N-1}(R_{n+1}-R_n)^2. \tag{5}$$

The distribution of the distance between two adjacent (along the chain) monomers at a temperature T is governed by the Boltzmann factor $\exp[-\beta K(R_{n+1}-R_n)^2/2]$, with $\beta=1/(k_BT)$ and k_B is the Boltzmann constant. The mean squared separation between adjacent monomers is $a^2=k_BT/K$, while the mean squared radius of gyration is $R_g^2=\frac{1}{6}N(1-1/N^2)k_BT/K \approx \frac{1}{6}Nk_BT/K$.

Theoretical treatment of the polymer described above requires solution of N coupled Langevin equations. However, the problem becomes particularly simple if we describe the configurations using Rouse modes [20]

$$U_q \equiv \frac{1}{N}\sum_{n=1}^{N} R_n \cos\left[q\left(n-\frac{1}{2}\right)\right], \tag{6}$$

where $q=p\pi/N$ and $p=0,1,\ldots,N-1$. In terms of U_q, Langevin equations decouple, and each Rouse mode can be viewed as an independent "particle" moving in a harmonic potential whose strength depends on q. The PDF of every U_q is Gaussian. Conversely, the position of each monomer can be viewed a linear combination of U_q's [inverse of Eq. (6)]. Since the linear combination of Gaussian variables is a Gaussian variable, we are assured that each monomer is described exactly by a Gaussian PDF, and the theoretical study is reduced to evaluation of the mean and variance of that distribution (see later). In the presence of absorption, such treatment is not possible.

We measured distances in dimensionless units, i.e., multiplied by $\sqrt{K/k_BT}$. In these units the root mean square separation of adjacent monomers is $a=1$, and $R_g^2 \approx N/6$. We used diffusive (Rouse) dynamics to evolve the system in time, i.e., the monomers were moved using standard Monte Carlo (MC) moves. An elementary MC move consists of randomly picking one monomer and attempting to increment its position by δR chosen uniformly from the interval $(-1,+1)$, in dimensionless units. The change in the Boltzmann weight factor controls the probabilistic decision of whether the move is accepted. N elementary move attempts are defined as one MC time unit. The mean squared displacement of a monomer in a single move determines the diffusion constant D_o; with the above choice of step size we had $D_o=0.10$.

For simulations we chose polymers of odd lengths $N=2^l+1$, with $l=1,2,\ldots,10$, i.e., $N=3,5,9,\ldots,1025$. While all the monomers moved during the simulation, we followed

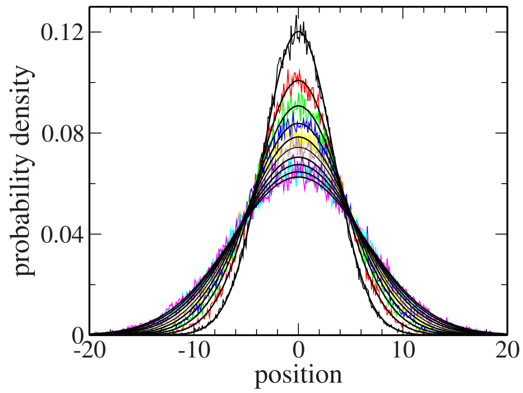

FIG. 1. (Color online) PDF for the position of the central monomer in a Gaussian chain of 129 monomers at times $t=2000,4000,\ldots,20\,000$ (from narrowest to the widest graph). The distributions were obtained from 100 000 runs using bin size $\Delta R=0.1$. The continuous lines represent normalized Gaussian fits to the distributions.

only the position of the central monomer numbered $c=2^{l-1}+1$. For each case, 100 000 independent simulations were performed to ensure reliable averages.

As an example, Fig. 1 depicts the PDF of the position of a central monomer ($c=65$) in a Gaussian polymer of $N=129$ monomers. At $t=0$ all monomers were located at the coordinate origin. As the configuration of the polymer evolved in time, the position of the 65th monomer was recorded. Repeating the process 100 000 times produced the distributions shown if Fig. 1. Note the excellent (single parameter) fit of the normalized Gaussian to the actual graphs. Indeed, as explained in the discussion following Eq. (6) the PDF of the monomer must be Gaussian at all times. It should be noted, that this shape is the same as in the case of the normal diffusion, and significantly differs from solutions of subdiffusive fractional diffusion equations which contain a cusp at the origin (see, Ref. [2]).

While the shapes of the graphs in Fig. 1 are not anomalous, the time dependence of their variance is. For times shorter than the longest relaxation time $\tau_N=R_g^2/2D_{\mathrm{c.m.}}=a^2N^2/12D_o$, which in the above case becomes $\tau_{129}=1.4\times10^4$, the variance of the distribution grows as $t^{1/2}$, while for times longer than τ_N it is linear in t. This result can be demonstrated analytically, since the variance of the particle position can be expressed as a sum of variances of Rouse modes. [Analogous calculation for a fluctuating line (or surface) can be found in Ref. [21].] Figure 2 depicts the dependence of the variance on t. While all the points are within a half decade from the crossover point, one can clearly discern the two types of behavior: the slope of the straight line through the first four points is 0.52, very close to the expected 1/2, and gradually increases to the right of the graph.

IV. A SINGLE ABSORBING BOUNDARY

Let us now introduce absorption into the problem. We assume that at $t=0$ all monomers are located at $R=0$, and an absorbing boundary is placed at $R_a=8$, i.e., when the central

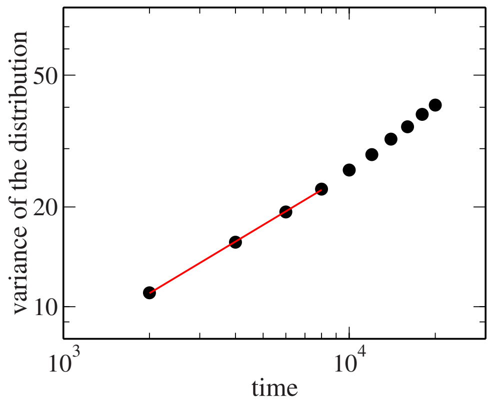

FIG. 2. (Color online) Logarithmic plot of the variance of the probability distributions depicted at Fig. 1 as a function of time.

particle reaches this point it is absorbed and the diffusion process ends. It should be stressed that other monomers of the polymer do not feel the absorbing boundary; their sole function is to generate anomalous diffusion of the tagged particle.

We begin with a very short polymer with $N=3$, whose radius of gyration is significantly shorter than R_a. More importantly, its maximal relaxation time $\tau_3 \approx 8$ is significantly shorter than the time (about 10^3) for the c.m. of the polymer to diffuse the distance from the origin to the absorbing boundary. Therefore, at the time scales at which the particle can be absorbed, the motion of the tagged monomer is indistinguishable from that of the c.m. of the polymer. Consequently, the problem of absorption of the central monomer should be indistinguishable from that of a normal diffuser with diffusion constant $D_o/3$.

Figure 3 depicts the observed PDF of the position of the central monomer of a polymer with $N=3$ at various times. The area under the graphs decreases with time due to absorption. The shapes are the same as expected for normal single particle diffusion: the solid lines are (single parameter) fits to

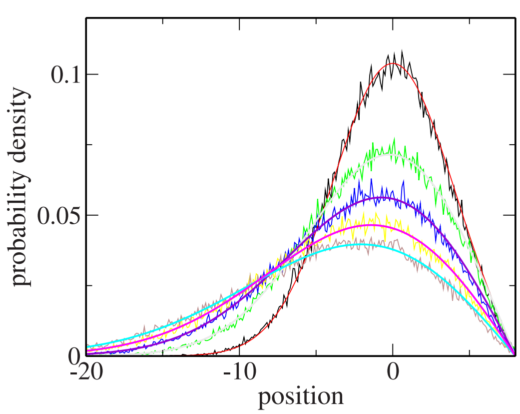

FIG. 3. (Color online) PDF of the position of the central particle in a polymer with $N=3$ monomers with an absorbing wall at $R_a=8$. The graphs correspond (narrow to broad) to $t=200,400,\ldots,1000$, and solid lines represent fits to the difference of two identical Gaussians centered at $R=0$ and $R=16$. The distributions are obtained from 100 000 runs, and the bin size is $\Delta R=0.1$.

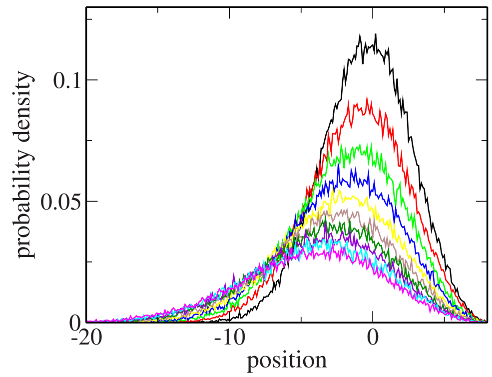

FIG. 4. (Color online) PDF of the position of central particle in a polymer with $N=129$ monomers with an absorbing wall at $R_a=8$. The graphs correspond (narrow to broad) to times $t=2000,4000,\ldots,20\,000$. The distributions were obtained from 100 000 runs using bin size $\Delta R=0.1$.

a difference between two Gaussians centered at image points $R=0$ and $R=2R_a$. The excellent fits demonstrate that normal diffusion well describes the absorption for such small N. Moreover, the variances of the Gaussians fits increase linearly with time, with a prefactor corresponding to $\sigma^2(t)=2D_{\text{c.m.}}t$, in which $D_{\text{c.m.}}$ was calculated independently.

This behavior changes radically when N becomes large. Already for $N=129$ all resemblance to regular diffusion vanishes. The maximal relaxation time $\tau_{129}=1.4\times10^4$ is of the same order as the time required for the c.m. of the polymer to diffuse the distance to the absorbing boundary (about 4×10^4), and R_g of the polymer is of the order of the distance to the absorbing boundary. The PDF depicted in Fig. 4 cannot be fitted by the difference between two Gaussians at image points. In particular, the PDF is not linear close to the boundary, but appears to vanish quadratically. Thus the qualitative behavior changes drastically on going from regular diffusion for small N to anomalous diffusion at large N.

V. TWO ABSORBING BOUNDARIES

We next consider absorption of the central monomer by two boundaries located at $R_a=\pm 8$, for N ranging from 3 to 1025. Figure 5 depicts on a semilogarithmic scale the PDF of the absorption $Q(t)$ for several N. For small polymers the curves are indistinguishable from that of a normal random walker with diffusion constant $D_{\text{c.m.}}=D_o/N$, which can be calculated from Eq. (4), with $\{A_n\}$ selected to correspond to the initial state $[P(R,0)=\delta(R)]$. After integrating $\widetilde{P}(R,t)$ over R to obtain $S(t)$, we get $Q(t)=-dS/dt$. As explained in Sec. II, for large times $Q(t)$ decays exponentially with a time constant $\tau \approx R_a^2/D_{\text{c.m.}}=NR_a^2/D_o$. The mean absorption time is of the same order of magnitude. The dependence of the mean time, and of the time constant for decay, is depicted by squares and circles, respectively, in Fig. 6. Note that when N becomes large enough, so that the longest relaxation time of the polymer exceeds the typical time it takes for a particle to travel the distance between the absorbing boundaries, $Q(t)$

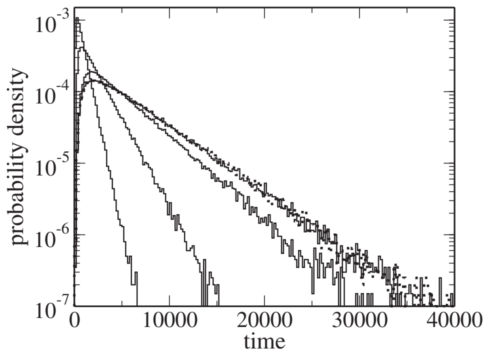

FIG. 5. PDF of the absorption time (in Monte Carlo time units) of the central monomer in a Gaussian polymer of length N. The tagged monomer can be absorbed at one of two boundaries at $R_a = \pm 8$. The plots (from left to right, solid lines) correspond to $N=3$, 9, 33, 129, and 513 (dots), and the histogram was calculated from 100 000 independent runs, with bin size $\Delta t=200$. The graphs for $N=257$, 1025 (not shown), and 129 are virtually indistinguishable.

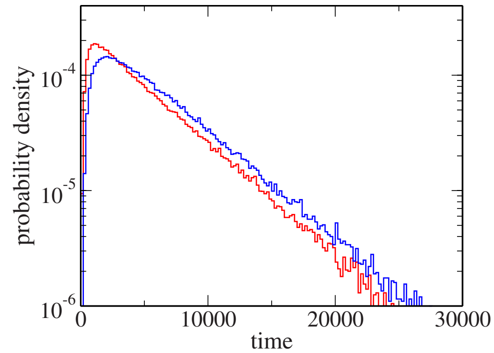

FIG. 7. (Color online) PDF of the central monomer of a 129-monomer Gaussian polymer absorbed at boundaries a distance 8 from the initial position on both sides. The curve with the larger mean corresponds to the case when at $t=0$ all $R_n=0$, while the other plot corresponds to starting configuration where $R_c=0$ while the remaining monomers are equilibrated. This plot (histogram) was calculated from 100 000 independent samples; bin size $\Delta t=200$.

becomes independent of N. Indeed all the graphs for $N = 129, 257, 513, 1025$ coincide with each other. The long time behavior remains an exponential decay, as can be seen from the straight lines on the semilogarithmic plot. These curves thus depict true anomalous diffusion in the "infinite-N limit," and the corresponding exponential decay time constant scales as the time it takes to cover the interval by subdiffusion, i.e., $\tau \approx R_a^4/(a^2 D_o)$.

So far, we reported on simulations in which at time $t=0$, the entire polymer is located at the origin, i.e., $R_n=0$ for all n. This is a particularly convenient choice for analytical calculations, since all Rouse modes vanish at $t=0$ and their mean values (averaged over realizations of the noise) remain zero at all times. In any case, we know that the initial value

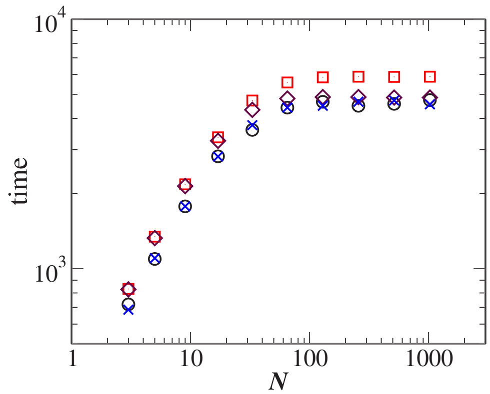

FIG. 6. (Color online) The mean first passage (absorption) time (square), and the decay time-constant of the absorption PDF (circle), as a function of polymer size N, when all monomers were located at the origin at $t=0$. Diamonds and crosses show the same quantities when at time $t=0$ only the central monomer is at the origin, while the remaining monomers are in a typical equilibrium position. The data are obtained from 100 000 independent runs. The statistical error bars in the mean times (approximately 0.3%), and the estimated systematic errors in the decay time constants (less than 5%) are much smaller than symbol sizes.

of each Rouse mode will be forgotten after one relaxation time of that mode. One may consider a different case, where at $t=0$ the polymer assumes a randomly selected equilibrium configuration. Thus, in addition to averaging our results over different realizations, we also need to average over the starting configurations. This initial condition appears more natural since the time $t=0$ is not special. In any case, we find that the differences between the two procedures are rather small. For small N we cannot expect much difference, because by the time the polymer reaches the absorbing boundary it is equilibrated in any case. The results for mean absorption time and decay time constant are depicted by diamonds and crosses, respectively, in Fig. 6. We see that the new procedure gives slightly shorter mean absorption times and essentially the same decay times. Figure 7 depicts the PDF of absorption times for $N=128$. It seems that at short times the random starting point diffuser moves slightly faster leading to shorter mean times, but for large times both cases are characterized by the same decay constant.

With its exponential decay the long time behavior of a particle between absorbing boundaries more resembles normal diffusion, although the time scales have to be determined using anomalous diffusion arguments. Nevertheless, the PDF of the unabsorbed monomer at long times does not resemble that of a normal diffuser. We studied the PDF of the positions of surviving particles in 100 000 independent runs for a polymer with $N=129$. Naturally, as the time increases the probability of not being absorbed decreases. (The decrease in probability also means that for large t the PDF was derived from samples significantly smaller than 100 000 and, consequently, the statistical accuracy of the results decreased.) To enable a convenient comparison between the PDFs at various times we normalized them to 1. In the results depicted in Fig. 8, the PDFs of the particle position were recorded at different times, all of the order of mean absorption time. Superficially these results resemble regular diffusion. In analogy to Eq. (4), it appears as if at very long times only a slowest "eigenmode" survives and the PDF decays as $\Psi(R/R_a)e^{-t/\tau}$, with an eigenvalue related to τ. The eigenfunction Ψ, depicted in

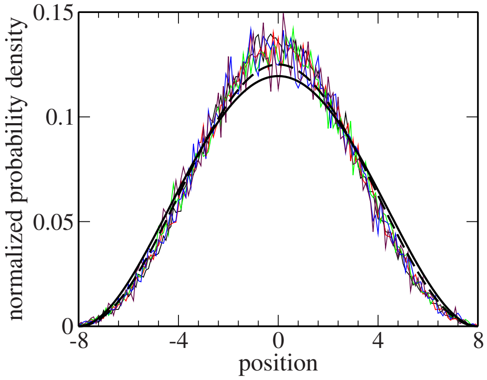

FIG. 8. (Color online) Probability density of the position of the central monomer of a 129-monomer polymer, between absorbing walls located at $R_a = \pm 8$. The curves are obtained at times $t = 2000, 4000, 6000, 8000, 10\,000$, and are the result of 100 000 independent simulations collected in bins of size $\Delta R = 0.1$. To remove the effect of absorption all curves have been normalized, such that their integral is unity. The $t=2000$ curve is relatively smooth, while that of $t=10000$ is very noisy because only in a small portion of runs the tagged particle was not absorbed, and consequently the sample size is small. Smooth lines represent two suggested eigenfunctions $\Psi(xR_a)/R_a$: the dashed line corresponds to $\Psi(x) = [1 + \cos(\pi x)]/2$ (see text), while the solid line represents the normalized eigenfunction given by Eq. (A4) in Ref. [14].

Fig. 8, appears to be universal, although specific to our form of subdiffusion, while τ scales as R_a^4 and is independent of N.

In the case of a regular diffusion (in the scaled variable $x = R/R_a$) we have $\Psi(x) \propto \cos(\pi x/2)$, i.e., the function vanishes at the boundaries ($x = \pm 1$) with a finite slope. By contrast, the results depicted in Fig. 8 suggest a vanishing slope at the boundary. In fact, an attempt to fit the function by a few terms of the Fourier series $b_0 + b_1 \cos(\pi x) + \cdots$ gives $b_0 \approx b_1$ while the coefficients of higher Fourier components are by an order of magnitude smaller. In Ref. [14] the fractional Laplacian operator was examined in a bounded domain. Their particular implementation of boundary conditions enabled calculation of the eigenfunction $\Psi(x)$ for various values of the fractional order. In particular, the explicit expression for the case corresponding to subdiffusion with $\alpha = 1/2$ in our notation is given in Eq. (A4) of Ref. [14] with $\alpha = 4$ in their notation. While this (normalized) function, depicted by a smooth solid line in Fig. 8, qualitatively resembles the numerical curves, it does not provide a quantitative fit. This makes the fractional Laplacian operator a somewhat unlikely candidate for describing the long-time behavior of our diffuser.

VI. DISCUSSION

In this work we concentrated on an extremely simple, and yet nontrivial model of subdiffusion. The Gaussian nature allows analytic calculation of some properties, such as the probability distribution of freely moving particles; but the absorption properties were studied numerically. We believe that similar results should apply to self-avoiding polymers, although separation into independent Rouse modes is no longer possible, and probably not much can be done beyond simple scaling arguments. Within our simple model, we find that the process of absorption is quite different from other simplified subdiffusive processes in the literature.

Anomalous diffusion of a monomer has several features resembling the translocation of a long polymer through a narrow pore in a membrane. This process has been extensively studied experimentally during the last decade [22–24]. In the theoretical description of translocation, a single variable s representing the monomer number at the pore [25–28] indicates how much of the polymer has passed to the other side. If the translocation process is very slow, the mean force acting on the monomer in the hole can be determined from a simple calculation of entropy, and the translocation problem is reduced to the escape of a "particle" (the translocation coordinate) over a potential barrier. Such theories produce qualitative understanding of experimental results [29]. However, if the process is not slow enough, compared to the relaxation times of Rouse modes, then its dynamics is more complicated. Successive steps of the reaction coordinate are then correlated in a manner closely resembling the correlations between steps of a tagged monomer in a polymer. In Ref. [30], it was numerically verified that s indeed undergoes anomalous diffusion in the 1D "space of monomer numbers." It was further argued that the relaxation of the polymer constrains the translocation process and consequently determines the translocation time. Such behavior closely relates the translocation process to the anomalous diffusion of a single monomer.

In the last few years significant progress has been made in the theoretical modeling of the translocation process. On one hand, short time behavior has been modeled in great detail [31], and on the other hand scaling consideration of the long time behavior have been extended to include hydrodynamic interactions [32,33]. Recently Grosberg *et al.* [34] developed an intuitive scaling picture of polymer translocation under the influence of a force. (See also Ref. [35].) A variety of scaling regimes with force applied to the end point or at the pore have been investigated numerically in some detail [36]. Some recent studies [37,38] suggest that the translocation process maybe even slower than dictated by the relaxation of the Rouse modes. If so, this would weaken the analogy between the translocation and the anomalous diffusion of a monomer. (The accuracy of these claims is questioned in further work [39].)

To the extent that one may draw an analogy between translocation and anomalous diffusion in the presence of absorbing boundaries, one may inquire whether the mean translocation time is finite. Reference [40] argues that translocation may be described by a fractional diffusion equation and, consequently, require an infinite mean time, as found in the solutions of such an equation [6]. A similar point is made in Ref. [38], where a detailed study of the PDF of translocation times is fitted to a slowly decaying function for large times. However, direct (experimental and numerical) measurements appear to indicate well defined average translocation times. Our results offer a model where absorption times of an anomalous diffuser are finite. Clearly more detailed studies of translocation are needed to resolve this question.

In this work we studied in detail the subdiffusion of a tagged monomer in a Gaussian polymer. In the absence of absorption all properties can be derived analytically. However, upon inclusion of absorbing walls, we had to resort to numerical simulations. While we can characterize all properties of the numerical results, we are still missing an equation that can describe the evolution of the PDF of the position of the tagged particle. In fact, the numerical results exclude several simple forms for such an equation.

Note added in proof. Ref. [41] was recently brought to our attention. This paper treats analytically a similar problem. However, its use of method of images leads to conclusions that are inconsistent with our results.

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