

Persistence of a Rouse polymer chain under transverse shear flow

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We consider a single Rouse polymer chain in two dimensions in presence of a transverse shear flow along the x direction and calculate the persistence probability $P_0(t)$ that the x coordinate of a bead in the bulk of the chain does not return to its initial position up to time t . We show that the persistence decays at late times as a power law, $P_0(t) \sim t^{-\theta}$ with a nontrivial exponent θ . The analytical estimate of $\theta = 0.359\dots$ obtained using an independent interval approximation is in excellent agreement with the numerical value $\theta \approx 0.360 \pm 0.001$.

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I. INTRODUCTION

Polymer dynamics plays a central role in material science and biology. In particular, dynamics of an individual flexible or semi-flexible polymer under a suitable shear force has been of great interest [1, 2, 3, 4, 5, 6, 7]. Shear force comes into play when a fluid flows past a surface. Substantial effort has been undertaken to investigate the motion of polymers in shear field. Previously, studies were done on bulk samples using light-scattering and birefringence experiments. Recently, the dynamics of a single polymer has also been investigated using video-microscopy. Under a shear stress, such a polymer shows tumbling in addition to a longitudinal stretching [2, 3]. If one takes a tethered polymer, whose one point is made immobile, then tumbling leads to a cyclic motion of the spatially constrained polymer about a mean position [4]. Also statistics of polymer orientation angles has been of interest [6, 7]. These properties studied both experimentally and theoretically can be classified as long-time transport phenomena. In contrast, in this paper we explore the persistence or the survival probability behaviour of a flexible polymer chain under transverse shear flow within the paradigm of the simple Rouse model where the polymer chain consists of beads or monomers connected by harmonic springs [8]. We will show that even in this simple model, the persistence at late times decays as a power law characterized by a nontrivial exponent.

The survival/persistence probability $P_0(t)$ that a stochastic process $X(t)$ does not cross zero upto time t is a quantity of long standing interest in probability theory and with many practical applications [9]. The derivative $F(t) = -dP_0(t)/dt$ is the first-passage probability [10]. In many nonequilibrium many body systems, the persistence has been found to decay as a power law at late times, $P_0(t) \sim t^{-\theta}$. The exponent θ is called the persistence exponent and has been a subject of much theoretical, numerical and experimental studies in recent times [11]. The exponent θ is often nontrivial and is generally hard to calculate analytically even in sim-

ple systems such as the linear diffusion equation starting from random initial conditions [12]. The reason for this difficulty can be traced back to the fact that the spatial interactions in these extended systems makes the local stochastic field $X(t)$ a ‘non-Markovian’ process in time [11].

In this paper we study the persistence properties of a Rouse chain in 2-dimensions in presence of a transverse shear velocity field which is non-random. We show that the persistence probability in this system decays at late times as a power law with a nontrivial persistence exponent $\theta \approx 0.36$ that we compute numerically as well as analytically within an independent interval approximation (IIA). We note, that the current problem is in contrast to similar problems considered in ‘‘random’’ flow fields earlier. For example, for a Rouse chain [8] of infinite length, the transport properties [13, 14, 15] and the persistence properties [16] in a quenched random velocity flow field have been studied.

The paper is organized as follows. In Section II, we define the model precisely and summarize our main results. In Section-III we present exact calculations of the two-time correlation functions in our model. These results are used next in Section IV to calculate the persistence exponent analytically within the IIA. Sections V and VI describe details of the numerical methods and finally we conclude in Section VII.

II. THE MODEL AND MAIN RESULTS

We consider a Rouse polymer chain embedded in a 2-dimensional plane. The chain consists of beads connected by harmonic springs [8]. In addition, the chain is advected by shear velocity flow field. Let $[x_n(t), y_n(t)]$ denote the coordinates of the n -th bead at time t which evolve with time according to the following equations of motion

$$\frac{dy_n}{dt} = \Gamma(y_{n+1} + y_{n-1} - 2y_n) + \eta_1(n, t) \quad (1)$$

$$\frac{dx_n}{dt} = \Gamma(x_{n+1} + x_{n-1} - 2x_n) + v(y_n(t)) + \eta_2(n, t) \quad (2)$$

where Γ denotes the strength of the harmonic interaction between nearest neighbour beads, $\eta_1(n, t)$ and $\eta_2(n, t)$ represent the thermal white noises along the y and x directions respectively that are uncorrelated. The transverse shear velocity field $v(y)$ is linear

$$v(y) = y. \quad (3)$$

For a finite chain with N beads, Eqs. (1) and (2) are valid only for the $(N - 2)$ interior beads. The two boundary beads will have slightly different equations of motion. However, for an infinitely large chain ($N \rightarrow \infty$), the translational invariance along the length of the chain is restored since the boundary conditions become irrelevant for late time dynamics. Since we are mostly interested in the late time properties, one can make further simplifications by replacing the discrete index n of the beads by a continuous variable s and subsequently replace the discrete Laplacian by a continuous second derivative along the s direction. The coarse grained versions of the evolution equations (2) then become

$$\frac{\partial y(s, t)}{\partial t} = \Gamma \frac{\partial^2 y(s, t)}{\partial s^2} + \eta_1(s, t), \quad (4)$$

$$\frac{\partial x(s, t)}{\partial t} = \Gamma \frac{\partial^2 x(s, t)}{\partial s^2} + y(s, t). \quad (5)$$

Note that we have also dropped the $\eta_2(s, t)$ term in the second equation. This is simply because one can easily show that the noise term $\eta_2(s, t)$ becomes insignificant compared to the shear force term $y(s, t)$ at late times. Hence for late time asymptotic properties we can ignore the noise $\eta_2(s, t)$.

In the absence of harmonic interactions ($\Gamma = 0$), the beads become independent and the coordinates of any (say the n -th) bead represents a two-dimensional Brownian walker in a shear flow[17]. Equivalently, in this limit, the x coordinate of the walker evolves as $d^2x_n/dt^2 = \eta_1(n, t)$, i.e., it represents a randomly accelerated particle. The persistence probability of the x -coordinate, i.e., the probability that the x coordinate does not cross zero up to time t is known to decay as $\sim t^{-1/4}$ [18]. Recently, the persistence of a single random walker for various other deterministic velocity functions $v(y)$ has also been studied [19, 20]. Interestingly it has been shown that for all odd functions $v(y)$ survival probability decays as $t^{-1/4}$ [19]. It turns out that the same $t^{-1/4}$ decay also holds in the case when $v(y)$ is not a deterministic function, but represents a quenched random transverse velocity field with short-range correlations [21, 22]. This model of a single random walker in presence of a random transverse velocity field is known as the Matheron-deMarsily model[23] whose transport properties had been studied earlier extensively[24], but the studies of persistence properties are relatively new[21, 22, 25].

In this paper we study the persistence probability of the x coordinate of the n -th bead in the presence of harmonic interaction $\Gamma \neq 0$. Due to the translational invariance along the length of the chain in the bulk, the persistence probability is independent of the label n of the

bead. We also absorb the factor Γ by properly rescaling the time. Note that the continuum equation (4) for the y coordinate is precisely the Edwards-Wilkinson equation of one dimensional interface [26] and its persistence properties are known, both theoretically [27, 28] and also experimentally [29]. Here we focus on the x coordinate and define the persistence as follows

$$P_0(t) = \text{Prob}[x(s, t') \neq x(s, 0) \text{ for all } t' : 0 \leq t' \leq t], \quad (6)$$

i.e., $P_0(t)$ is the probability that the x coordinate of any bead does not return to its initial position within the time interval $[0, t]$.

The initial conditions for the chain coordinates do not play any role in the persistence probability. This is due to the fact that the evolution equations are linear, so we can redefine the change in positions $x(s, t) - x(s, 0)$ and $y(s, t) - y(s, 0)$ as the relevant coordinates which satisfy the same evolution equations. Hence, for the evolution equations (4) and (5) we can set the initial conditions $x(s, 0) = 0$ and $y(s, 0) = 0$ without any loss of generalities.

Our main results can be summarized as follows. We show that $P_0(t) \sim t^{-\theta}$ at late times t where the persistence exponent θ has a nontrivial value. The numerical value $\theta \simeq 0.360 \pm 0.001$, is in excellent agreement with the analytical value $\theta = 0.359\dots$ obtained within the IIA method. Thus as one switches on the harmonic interaction $\Gamma \neq 0$ between the beads, the exponent $\theta \simeq 0.36$ increases from its value $\theta = 1/4$ for $\Gamma = 0$. Thus the x coordinate of a bead survives less in presence of harmonic interactions, i.e., the interaction enhances the return probability.

III. CALCULATION OF EXACT TWO-TIME CORRELATION FUNCTIONS

The stochastic processes $x(s, t)$ and $y(s, t)$ evolving via Eqs. (4) and (5) are both Gaussian at late times since the evolution equations are linear. A Gaussian process is completely specified by its two-time correlation function. More detailed quantities such as the persistence probability, in principle, is a complicated functional of the two-time correlation function. In this section we compute the two-time correlation functions exactly and use these functions later for computing the persistence probability in Section IV.

To begin with, we Fourier transform Eq. 4. We define $\tilde{y}(k, t) = \int_{-\infty}^{+\infty} y(s, t) \exp(-isk) ds$, and $\tilde{\eta}_1(k, t) = \int_{-\infty}^{+\infty} \eta_1(s, t) \exp(-isk) ds$. This implies,

$$\frac{\partial \tilde{y}(k, t)}{\partial t} = -k^2 \tilde{y}(k, t) + \tilde{\eta}_1(k, t) \quad (7)$$

Assuming flat initial condition (i.e., $y(s, 0) = 0$), Eq. (7)

gives

$$\tilde{y}(k, t) = \exp(-k^2 t) \int_0^t \tilde{\eta}_1(k, t') \exp(k^2 t') dt', \quad (8)$$

which in turn implies the correlation function

$$\begin{aligned} \langle \tilde{y}(k_1, t') \tilde{y}(k_2, t'') \rangle &= \\ \frac{\delta(k_1 + k_2)}{2k_1^2} &[\exp(-k_1^2 |t' - t''|) - \exp(-k_1^2 (t' + t''))]. \end{aligned} \quad (9)$$

For Eq. (5), defining $\tilde{x}(k, t) = \int_{-\infty}^{+\infty} x(s, t) \exp(-isk) ds$ and again considering flat initial condition (i.e., $x(s, 0) = 0$), we get

$$\tilde{x}(k, t) = \exp(-k^2 t) \int_0^t \tilde{y}(k, t') \exp(k^2 t') dt', \quad (10)$$

which further implies,

$$\begin{aligned} \langle \tilde{x}(k_1, t_1) \tilde{x}(k_2, t_2) \rangle &= \exp(-k_1^2 t_1 - k_2^2 t_2) \times \\ &\int_0^{t_1} dt' \int_0^{t_2} dt'' \langle \tilde{y}(k_1, t') \tilde{y}(k_2, t'') \rangle \exp(k_1^2 t' + k_2^2 t''). \end{aligned} \quad (11)$$

Substituting Eq. (9) in Eq. (11), we get

$$\begin{aligned} &\langle \tilde{x}(k_1, t_1) \tilde{x}(k_2, t_2) \rangle \\ &= \delta(k_1 + k_2) \int_0^{t_1} dt' \int_0^{t_2} dt'' \times \\ &\frac{\exp(-k_1^2 (t_1 + t_2 - 2 \min(t', t''))) - \exp(-k_1^2 (t_1 + t_2))}{2k_1^2}. \end{aligned} \quad (12)$$

By inverting the Fourier transform above, we obtain the correlation function

$$\begin{aligned} C(t_1, t_2) &= \langle x(s, t_1) x(s, t_2) \rangle \\ &= \int_0^{t_1} dt' \int_0^{t_2} dt'' \int_{-\infty}^{+\infty} dk_1 \int_{-\infty}^{+\infty} dk_2 \\ &\exp(i(k_1 + k_2)s) \langle \tilde{x}(k_1, t') \tilde{x}(k_2, t'') \rangle \\ &= \int_0^{t_1} dt' \int_0^{t_2} dt'' \int_{-\infty}^{+\infty} dk_1 \\ &\left[\frac{1 - \exp(-k_1^2 (t_1 + t_2))}{2k_1^2} - \frac{1 - \exp(-k_1^2 (t_1 + t_2 - \tilde{t}))}{2k_1^2} \right] \end{aligned} \quad (13)$$

where $\tilde{t} = 2 \min(t', t'')$. After some algebra, Eq. (13) leads to,

$$\begin{aligned} C(t_1, t_2) &= \\ B \left[t_1 t_2 \sqrt{t_1 + t_2} - \frac{1}{5} \{ (t_1 + t_2)^{5/2} + |t_2 - t_1|^{5/2} \} \right], \end{aligned} \quad (14)$$

where B is an unimportant constant.

Note that due to the translational invariance in the bulk, the correlator of the process $x(s, t)$ does not depend on the location s of the bead along the chain. Thus, for simplicity of notations, we can now drop the label s and consider $x(t)$ as the relevant Gaussian process with the correlator $C(t_1, t_2) = \langle x(t_1) x(t_2) \rangle$ as given in Eq. (14). Clearly the process $x(t)$ is non-stationary since its two-time correlator in Eq. (14) depends on both t_1 and t_2 and not just on their difference. One can however define a logarithmic time $T = \ln t$ and consider the normalized process $X(T) = x(t) / \sqrt{\langle x(t)^2 \rangle}$ in T [31]. The survival or no zero crossing probability is clearly the same for both the normalized process $X(T)$ and the original unnormalized process $x(t)$. It then follows from Eq. (14) that the autocorrelation function of this normalized Gaussian process $X(T)$ is stationary in the T variable and is given by

$$\begin{aligned} A(T) &= \frac{C(t_1, t_2)}{\sqrt{C(t_1, t_1) C(t_2, t_2)}}, \\ &= \frac{5}{\sqrt{2}} \exp\left(\frac{5}{4} T\right) [\exp(-T) \sqrt{1 + \exp(-T)} \\ &\quad - \frac{1}{5} (1 + \exp(-T))^{5/2} + \frac{1}{5} (1 - \exp(-T))^{5/2}]. \end{aligned} \quad (15)$$

This form of the stationary autocorrelator will be used in the next section to compute the persistence probability.

IV. CALCULATION OF THE PERSISTENCE EXPONENT θ

We have thus mapped our problem to a Gaussian stationary process in $T = \ln t$ variable with a prescribed correlator $A(T)$ and we want to calculate the probability $P_0(T)$ that the process does not cross zero up to time T . For a general correlator $A(T)$, the computation of $P_0(T)$ is very hard [9, 11, 32]. However, some general results are known for the late time behavior of $P_0(T)$. For example, it is known [9, 11, 32] that when $A(T)$ decays faster than $1/T$ for large T , the persistence probability $P_0(T)$ decays exponentially, $P_0(T) \sim \exp(-\theta T)$. Since, in our case, $A(T)$ is Eq. (15) decays faster than $1/T$ for large T , we expect $P_0(T) \sim \exp(-\theta T)$. In terms of the original time variable, $t = e^T$, this would signify a power law decay of the persistence $P_0(t) \sim t^{-\theta}$ for large t . Thus (13) the inverse decay rate θ in the T variable is precisely the exponent of the algebraic decay in the real time t .

While we were not able to compute the exponent θ exactly, one can obtain a very accurate analytical estimate of θ using the IIA method that was first used in the context of persistence in diffusion equation [12]. This method works reasonably well only for smooth Gaussian stationary processes. A process is smooth if $A(T) = 1 - aT^2 + \dots$ for small T . In that case, the process has

a finite mean density $\rho = \sqrt{-A''(0)}/\pi$ [33] of zero crossings. For our process, the correlator in Eq. (15) can be expanded for small T

$$A(T \rightarrow 0) = 1 - \frac{15}{16}T^2 + \frac{1}{\sqrt{2}}T^{5/2}, \quad (16)$$

indicating $a = 15/16$ and thus proving that the process is smooth.

In the IIA, applicable only to smooth processes, one assumes that the intervals between successive zero crossings of a Gaussian stationary process are statistically independent. Within this approximation, one can then express the distribution $P(T)$ of the intervals between successive zero crossings in terms of the correlation function $A(T)$ in the Laplace space [12]

$$\tilde{P}(s) = \frac{1 - (\langle T \rangle / 2)s[1 - s\tilde{A}(s)]}{1 + (\langle T \rangle / 2)s[1 - s\tilde{A}(s)]}. \quad (17)$$

Here $\tilde{P}(s)$ and $\tilde{A}(s)$ are the Laplace transforms of $P(T)$ and $A(T)$ respectively and $\langle T \rangle = 1/\rho = \pi/\sqrt{-A''(0)}$ is the mean interval size.

Using the exact expression of $A(T)$ from Eq. (15), we can find $P(T)$ from the above formula. The persistence probability $P_0(T)$ is simply related to the interval distribution [12], $d^2P_0(T)/dT^2 = P(T)/\langle T \rangle$. Since we expect $P_0(T)$ to decay exponentially at late times T , i.e. $P_0(T) \sim \exp(-\theta T)$, it follows that the interval distribution $P(T)$ will also have the same late time decay, $P(T) \sim \exp(-\theta T)$ with identical exponent θ . This means that the Laplace transform $\tilde{P}(s)$ must have a simple pole at $s = -\theta$. In other words the denominator in Eq. (17) must have a root at $s = -\theta$. Substituting $s = -\theta$, the denominator reads

$$G(\theta) = 1 - (\theta/2)\left(\frac{\pi}{\sqrt{2a}}\right) \left[1 + \theta \tilde{A}(-\theta)\right], \quad (18)$$

where we have put $\langle T \rangle = \pi/\sqrt{2a}$ with $a = 15/16$ and θ is given by the smallest positive root of $G(\theta) = 0$.

To determine the root of $G(\theta) = 0$ accurately, it is convenient to switch variables and define $x = \exp(-T)$, such that

$$A(x) = \frac{x^{3/4}}{\sqrt{2(1+x)}} \left[2 + \frac{2x-1}{1+\sqrt{1-x^2}} - x + \sqrt{1-x^2}\right], \quad (19)$$

and then Eq. (18) becomes,

$$G(\theta) = \frac{1}{\sqrt{2}} \int_0^1 dx \frac{x^{-(\theta+1/4)}}{1+x} \times \left[2 - x + \sqrt{1-x^2} + \frac{2x-1}{1+\sqrt{1-x^2}}\right] = 0. \quad (20)$$

Solving Eq. (20) numerically gives

$$\theta_{\text{IIA}} = 0.359\dots \quad (21)$$

Thus the persistence probability $P_0(t) \sim t^{-\theta}$ decays algebraically for large time t with a nontrivial exponent, whose analytical value within the IIA is $\theta_{\text{IIA}} = 0.359\dots$

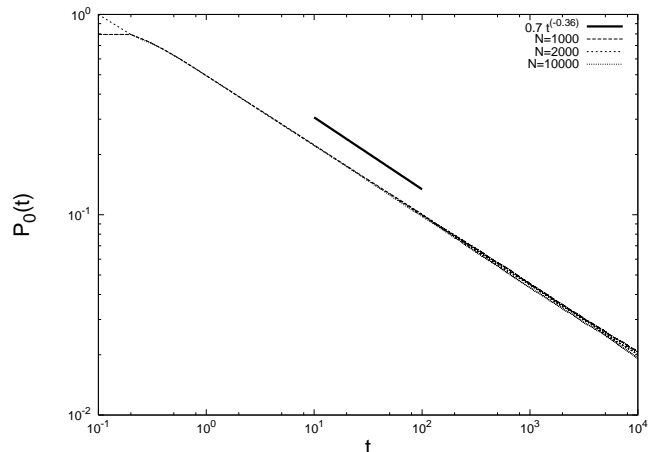


FIG. 1: Persistence probability $P_0(t)$ versus t , simulated for the polymer chain length $N = 1000, 2000$ and 10000 . The fitted power law $t^{-0.360}$ is shown by plotting a thick line above the data.

V. SIMULATION OF DISCRETISED LANGEVIN EQUATIONS

In this section we describe simulation of the Rouse chain evolving via Eqs. (1) and (2) and further discretised in time t as

$$y_n(t_{m+1}) = y_n(t_m) + \Delta t [y_{n+1}(t_m) + y_{n-1}(t_m) - 2y_n(t_m)] + \sqrt{\Delta t} \zeta_1(n, t_m), \quad (22)$$

$$x_n(t_{m+1}) = x_n(t_m) + \Delta t [x_{n+1}(t_m) + x_{n-1}(t_m) - 2x_n(t_m)] + \Delta t y_n(t_m), \quad (23)$$

where $t_m = m\Delta t$. For the boundary points $n = 1$ and $n = N$, we use free boundary conditions, i.e., we hold $x_0 = x_1$, $y_0 = y_1$, $x_N = x_{N+1}$ and $y_N = y_{N+1}$ for all times t_m . We choose $\Delta t = 0.1$ in our simulations [27], and used chain lengths of size $N = 1000 - 10000$. The variable $\zeta_1(n, t_m)$ is an independent Gaussian variable for all n and t_m and distributed with zero mean and unit variance.

The persistence probability for x_n upto time t_m was obtained by keeping track of the fraction of x_n 's that have $\text{sgn}[x_n(t_m)]$ same as $\text{sgn}[x_n(1)]$ for all times starting from 1 to t_m . The data are shown in fig. 1. Typically each data curve in fig. 1 was obtained by averaging over 500 thermal histories. We find that $P_0(t)$ decays as a power law $\sim t^{-\theta}$ with $\theta \simeq 0.360 \pm 0.001$. The latter value is in good agreement with the IIA estimate in Eq. (21).

VI. SIMULATION OF THE GAUSSIAN PROCESS

Since a Gaussian stationary process $X(T)$ is completely specified by its stationary correlator $A(T)$, one can simulate the process by constructing a time-series with the same correlator. In the frequency do-

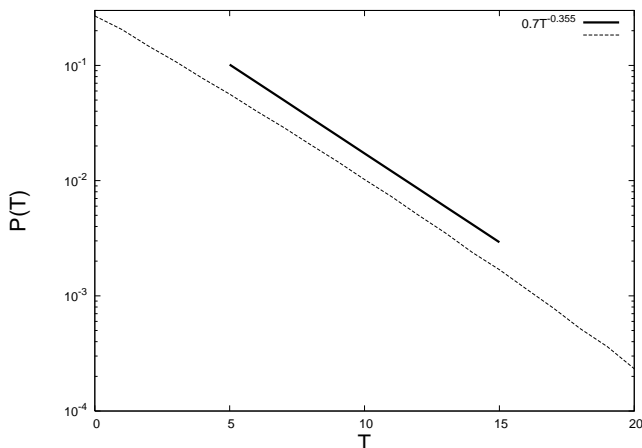


FIG. 2: The graph (dashed line) shows $P(T)$ vs. T from the simulation of the Gaussian process $X(T)$. The upper short thick line goes as $0.7 \exp(-0.355T)$.

main (Fourier space) the corresponding correlator is $\langle \tilde{X}(\omega_1) \tilde{X}(\omega_2) \rangle = 2\pi \tilde{A}(\omega_1) \delta(\omega_1 + \omega_2)$, where $\tilde{A}(\omega) = \int dt e^{i\omega T} A(T)$ is the Fourier transform of $A(T)$. The latter formula allows us to easily generate stochastic processes

$$\tilde{X}(\omega) = \tilde{\eta}(\omega) \sqrt{\tilde{A}_{S_0}(\omega)}, \quad (24)$$

where $\tilde{\eta}(\omega)$ is a Gaussian white noise with $\langle \tilde{\eta}(\omega_1) \tilde{\eta}(\omega_2) \rangle = 2\pi \delta(\omega_1 + \omega_2)$.

We performed simulations following the above route by first constructing random functions $\tilde{X}(\omega)$ as per Eq. (24) for discrete ω 's. Then we did a discrete inverse Fourier transform to obtain the time series $X(T)$ [27]. After generating 10^6 such random time-series of $X(T)$, we used them to calculate the probability density function $P(T)$ of intervals between two consecutive zero-crossings. In the calculation, the time-step size used was $\delta T = 1$, and

$T_{max} = 50$ as we found that $A(T)$ almost vanishes for $T > 50$. As stated earlier, in terms of the variable T , both $P(T)$ and $P_0(T)$ decay as $\sim \exp(-\theta T)$. Hence, from the decay of $P(T) \sim \exp(-\theta T)$, we estimated θ . In Fig. 2, we have shown $P(T)$ versus T , and we find the decay constant $\theta \approx 0.355$. The latter value is slightly smaller than the θ obtained from IIA and the Langevin simulation, because the step-size $\delta T = 1$ was a bit large and we missed some intervals smaller than that.

VII. CONCLUSION

In summary, we have studied the persistence probability of the x coordinate of a bead in the bulk of a Rouse polymer chain advected by a shear flow field. We have shown that the persistence probability decays as a power law in time at late times and the associated persistence exponent $\theta \approx 0.36$ is nontrivial. We have computed this exponent analytically within an independent interval approximation and also determined it numerically by two different methods. The analytical result is in excellent agreement with the numerical simulations.

There are several directions in which our work can be extended. Here we have considered the Rouse chain embedded in two spatial dimensions. It should be relatively straightforward to extend our method to calculate the persistence properties of the Rouse chain in higher dimensions in presence of a transverse shear flow. It would also be of interest to study the persistence properties of the polymer chain in a more realistic setting going beyond the simple Rouse model, e.g. in presence of excluded volume interactions.

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