

Universalities in a constrained motion of a particle with memory friction: A bead of a Rouse chain on a periodic wire

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In our previous work [Phys. Rev. E **110**, 034104 (2024)], we considered the mean-squared displacement (MSD) of particles whose free motion is subdiffusive and is described by a generalized Langevin equation (GLE) with power-law memory kernel under geometric constraints, e.g., when the particles are moving in channels of different shape. The MSD at long times was found to be independent of the channel's shape. Motivated by this finding, we discuss a simple physical model corresponding to such a situation. Here the particle is a tagged end monomer of a Rouse polymer chain, and the bath is represented by the rest of the chain and its surroundings. The constraints correspond to the motion of a monomer on a static, sinusoidally meandering wire. For the case of long chains we find the same independence of the long-time behavior on the wire's modulation as in the case of GLE: The MSD at longer times does not depend on the amplitude of the wire's modulation and is the same as for the straight wire. For shorter chains whose Rouse time lays in the observation domain, for moderate modulation, if the MSD already approached the one for a straight wire at times smaller or comparable to the Rouse time, the independence on the modulation is carried over to the final, diffusion regime at long times. In the case when constraints apply not only to the tagged monomer, but also to the rest of the chain (i.e., to the bath), the sensitivity to the wire's shape never disappears. A simple analytical approach based on homogenization gives a quite satisfactory description of our findings.

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I. INTRODUCTION

In our work [1] we considered a behavior of a particle in a contact with a non-Markovian equilibrium heat bath, when the motion of the particle is subjected to geometric constraints corresponding either to its motion in a corrugated channel (nonholonomic constraints) of infinite length oriented along the x axis or on a wire (holonomic constraint) corresponding to the case of a narrow meandering channel. The results of the work show that in the case when the motion of a particle is subdiffusive and is modeled by a generalized Langevin equation (GLE) with a power-law memory kernel, the constraints hardly play any role, and the long-time mean-squared displacement (MSD) of a particle is not influenced by the channel's shape. The result is in this sense similar to the one for the case when the particle moves in a one-dimensional periodic potential, as discussed by Goychuk [2], and differs from the case of Markovian dynamics, in which case the MSD

under homogenization does depend on the channel's or wire's shape.

In principle, GLEs can be derived from underlying physical models, but such derivation often involves approximations. An exact derivation is possible for the case of harmonic baths (Kac-Zwanzig bath), see Ref. [1] and references therein, but such a model may be considered as a mathematical exercise lacking important physics. This model does not answer the question regarding what happens if the constraints also apply to the bath particles. In what follows we consider a specific bath model, which has some physics behind, and allows us to discuss different situations behind homogenization of generalized Langevin dynamics. The discussion shows that care should be taken when simply putting additional conditions to a GLE.

The model discussed in the present work is as follows. We consider a polymer chain with a tagged monomer on its end, whose motion is followed. The whole system is in a contact with the external heat bath, with the chain serving as the “intermediate bath” for the tagged particle, providing memory effects which the outside bath lacks. Two cases are considered. The first one corresponds to the situation when only the motion of the tagged monomer is restricted, while these restrictions do not affect the rest of the chain. The second one corresponds to the situation, when the same restrictions apply to all monomers. In the present work we consider a beads-and-springs Rouse chain, and a holonomic situation,

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where one or all beads move on a sinusoidal wire (or in a narrow sinusoidal channel). Here the first situation is similar to the one we considered in Ref. [1] on the level of the GLE. The discussion of an explicit physical model of the bath allows us to somewhat “demystify” the findings and, moreover, leads to interesting observations in the case of relatively short chains, where terminal, long-time regime of motion of the tagged bead is diffusive. As we proceed to show, the long-time behavior of the MSD in the first case may or may not be sensitive to restrictions, and this depends on the parameters of the wire, and on the chain’s length, while in the second one it is always sensitive to constraints. Note that the second situation is remotely resembling the reptating polymer’s motion [3] but is considerably simpler due to its holonomic nature and periodicity.

In spite of simplicity of our model, it is a not-too-far relative of several quite realistic situations as observed when examining the mobility of biological macromolecules. One of the modern methods for genetic information readout from DNA corresponds to confining them in microfluidic nanochannels [4,5]. Since the DNA contour length in the elongated state greatly overcomes the typical nanochannel’s diameter, the geometric constrains matter. The Rouse model is used as one of the efficient tools to simulate the stochastic dynamics of such highly confined DNA molecules [6,7], although the results obtained up to now have been limited to the straight geometry. The domain of applicability of the Rouse model to diffusion of long polymer chains in long cylindrical channels has been discussed in Ref. [8]. The development of meandering microfluidic devices now also attracts attention from the experimental point of view since they enable optical treatment of a whole long chain molecule in a single field of view [5,9].

Another kind of confinement, when only a polymer’s head is confined by some surface and the rest of the chain is moving in the bulk, originates from the consideration of the diffusion of lipids constituting biological membranes in a quasiliquid state [10] and motion of mRNA penetrating the membrane [11], which combines the lateral diffusion of the head group on the membrane’s surface with the tail protruding into the membrane’s depth, and so on. It is worth noting that cellular surfaces can not be considered flat over reasonable areas. This has induced recent interest in how bulging, bending, and undulating may affect the lipid diffusion [12,13] as well as the behavior of membrane-bound bulky structured proteins attached to membranes [14].

Our interest to the problem is, however, mostly theoretical. The Rouse chain is a simple polymer model for which the memory kernel is well known, and an anomalous dynamics at intermediate times is a well-established fact. Using such a model of an (intermediate) bath allows us to understand the short-, intermediate-, and long-time dynamics of a system with memory friction, and to illustrate the effects which arise when the constraints are applied to a coordinate of interest only, and when they affect the bath as well. Although the corresponding effects could be qualitatively predicted from what we know about homogenization in generalized Langevin dynamics and about dynamics of polymers, we think that being able to see these effects in their full purity and to calculate them up to number constants is of a great value to sharpen

our intuition about different situations which may occur in systems with memory friction. Most of our new results are of numerical nature, but at the end of the work we consider a limiting case, for which analytical results can be provided as well. These results compare favorably with the ones of direct simulations even in the domain of parameters where our simple description based on the timescale separation could essentially be anticipated to lose its accuracy dramatically.

The work is structured as follows. In Sec. II we introduce the Rouse model and the dimensionless units used in the further work. To be able to clearly and easily identify the different regimes and the crossovers between them, we use an unusual, beyond-the-textbook approach to Rouse dynamics based on the Laplace representation of the polymer chain’s response function. This approach is used in the theoretical discussion following after presentation of our main numerical results in Sec. III. Section III starts from the presentation of our simulation approach and then turns to numerical results for the MSD of a tagged end bead of the chain for two different cases: when the motion of only this bead is constrained by the sinusoidal wire while all other beads move without external restrictions and when all beads of the chain can move on the wire only. Our model has a limiting case corresponding to a fast, small-amplitude modulation of the wire, in which case it is amenable to analytical treatment based on the results of Sec. II. The discussion of this analytical approach and the comparison of its results with numerical ones is a topic of Sec. IV. The conclusions are given in Sec. V. The details of some calculations and derivations are presented in Appendixes A–C.

II. THE ROUSE MODEL

A motion of a tagged monomer of a long polymeric molecule at intermediate times $\tau_0 < t < \tau_R$ often serves as a paradigmatic example of subdiffusion; see, e.g., Refs. [15,16]. Here we consider the Rouse (beads-and-springs) model of a molecule. Within the model, the molecule of N monomers (“beads”) is described by the set of Langevin equations,

$$\gamma \frac{d\mathbf{r}_n}{dt} = \mathbf{F}_n + \mathbf{f}_n, \quad (1)$$

for coordinates $\mathbf{r}_n$ of the beads, with $\mathbf{F}_n$ being the total deterministic force acting on the bead, $\mathbf{f}_n$ being the random force (noise), and γ being the friction coefficient. The total deterministic force includes the elastic interactions between neighboring beads along the chain via Hookean springs and may contain an additional external force $\mathbf{F}_a(t)$ applied to the first bead, which is used to probe the chain’s response to an external perturbation. Explicitly, the equations in the absence of the additional force look as follows:

$$\gamma \frac{d\mathbf{r}_n}{dt} = -k(2\mathbf{r}_n - \mathbf{r}_{n+1} - \mathbf{r}_{n-1}) + \mathbf{f}_n \quad (2)$$

for the internal beads of the chain ($n = 2, 3, \dots, N-1$) and

$$\gamma \frac{d\mathbf{r}_1}{dt} = -k(\mathbf{r}_1 - \mathbf{r}_2) + \mathbf{f}_1, \quad (3)$$

and

$$\gamma \frac{d\mathbf{r}_N}{dt} = -k(\mathbf{r}_N - \mathbf{r}_{N-1}) + \mathbf{f}_N \quad (4)$$

for the end ones [3]. The random forces satisfy the relations

$$\begin{aligned}\langle \mathbf{f}_n(t) \rangle &= 0, \\ \langle f_{n,\alpha}(t) f_{m,\beta}(t') \rangle &= 2\gamma k_B T \delta_{n,m} \delta_{\alpha,\beta} \delta(t - t')\end{aligned}\quad (5)$$

with α, β numbering the Cartesian coordinates, and the spring constant k is chosen to be

$$k = \frac{dk_B T}{b^2} \quad (6)$$

with d being the dimension of space and b being the actual size of the repeated unit (i.e., the Kuhn's length of the polymer). Although the Rouse model fully neglects the hydrodynamic interaction between monomers and therefore does not quantitatively describe the dynamics of polymers in a dilute solution, it is of high conceptual value, and it is sufficient for a qualitative discussion of the situation we want to conduct here.

In what follows, we consider a tagged bead at end of the molecule ($n = 1$), whose coordinate is $\mathbf{r} = \mathbf{r}_1$. The work [15] considers exactly the same situation, but for the middle monomer of the chain, so that the results differ in numerical factors. For a tagged monomer, the rest of the chain constitutes an “intermediate bath” leading to the effectively nonwhite noise and memory friction. The dynamics of a tagged bead can be described by the GLE [15,16] which in the overdamped limit reads:

$$\int_0^t dt' K(t - t') \dot{\mathbf{r}}(t') = \zeta(t) + \mathbf{F}_a(t), \quad (7)$$

with $\mathbf{F}_a(t)$ being an additional deterministic force (if any) acting at the tagged bead, and with the memory kernel and the noise $\zeta(t)$ satisfying the fluctuation-dissipation relation (FDR) of the second kind $k_B T K(|t - t'|) = \langle \zeta_\alpha(t') \zeta_\alpha(t) \rangle$ for any Cartesian component of ζ . The memory kernel $K(t)$ follows a power law with an exponential cutoff at a characteristic time,

$$\tau_c \sim \tau_R = \frac{\gamma N^2 b^2}{d\pi^2 k_B T} \equiv \frac{\gamma}{k\pi^2} N^2,$$

with τ_R being the Rouse time [3]. The Rouse time is, up to a prefactor, the time during which the center of mass of the chain (diffusing with the diffusion coefficient $D_N = D_1/N$ with $D_1 = k_B T/\gamma$ being the diffusion coefficient of a single monomer) acquires mean-squared displacement $\langle \mathbf{R}^2 \rangle = 2dD_N t$ of the order of the chain's mean-squared end-to-end distance $R_0^2 = b^2 N$, namely

$$\tau_R \sim \frac{b^2 N}{2dD_N} = \frac{\gamma N^2 b^2}{2dk_B T}.$$

The dynamics of the tagged bead on times

$$t_{\min} < t < \tau_R$$

(with $t_{\min} \sim b^2/D_1$) is subdiffusive, $\langle \mathbf{r}^2(t) \rangle \propto t^\alpha$ with subdiffusion exponent $\alpha = 1/2$. Outside of this interval, the dynamics is diffusive. The dimension of space d enters as a parameter. Since our simulations will be performed for a two-dimensional case, $d = 2$ in what follows.

The system of Eqs. (2), (3), and (4) separates into sets of independent equations for each of d coordinates. For example,

for x coordinate we get

$$\begin{aligned}\gamma \frac{dx_1}{dt} &= -\frac{dk_B T}{b^2} (x_1 - x_2) + f_1(t) + F_a(t), \\ \gamma \frac{dx_N}{dt} &= -\frac{dk_B T}{b^2} (x_N - x_{N-1}) + f_N(t), \\ \gamma \frac{dx_n}{dt} &= -\frac{dk_B T}{b^2} (2x_n - x_{n-1} - x_{n+1}) + f_n(t)\end{aligned}\quad (8)$$

(for $1 < n < N$), where $F_a(t)$ is the x component of the additional force applied to the first bead. Similarly, the components in the GLE, Eq. (7), decouple.

The additional force $F_a(t)$ will be used in what follows to define the response of the chain to the external perturbation which allows to analytically determine the memory kernel, which, in turn, determines the MSD of the tagged bead in a force-free situation. This MSD, on the other hand, is the main object of our further numerical investigation.

Units. The the overdamped beads' motion with the spring strength set by the actual Kuhn's length of the chain assumes a slightly unusual system of natural units for its description. The system of Eqs. (2), (3), and (4) with the noise correlation function given by Eq. (5), or the corresponding equations (8) for a single coordinate contain, apart from N , three free parameters, γ with dimension $[\gamma] = \frac{M}{T}$, k with dimension $[k] = \frac{M}{T^2}$, and $k_B T$ with dimension $[k_B T] = \frac{ML^2}{T^2}$, whose dimensions are not independent and do not allow to define the unit of mass, since the equations of the overdamped motion do not depend on the beads' masses. Dividing all equations by γ , we get a system of equations of the type

$$\frac{dx_n}{dt} = -\frac{1}{\tau_0} (2x_n - x_{n-1} - x_{n+1}) + \tilde{f}_n(t)$$

(and the corresponding equations for the first and the last bead), with

$$\tau_0 = \frac{\gamma}{k} = \frac{\gamma b^2}{dk_B T} \equiv \frac{b^2}{dD_1}, \quad (9)$$

and

$$\langle \tilde{f}_m(t) \tilde{f}_n(t') \rangle = \frac{2k_B T}{\gamma} \delta_{m,n} \delta(t - t') \equiv 2D_1 \delta_{m,n} \delta(t - t'),$$

with $D_1 = k_B T/\gamma$ being the diffusion coefficient of a single bead. Therefore, the Rouse model has, apart from N , only two free parameters: τ_0 (with dimension of time) and D_1 with dimension $[D_1] = L^2 T^{-1}$. The combination $\lambda_0 = \sqrt{D_1 \tau_0} \equiv b/\sqrt{d}$ then sets the length scale of the problem. In what follows, it will be convenient to choose τ_0 and λ_0 as units of length and time, i.e., to put $\tau_0 = 1$ and $\lambda_0 = 1$. This corresponds to fixing $\tau_0 = D_1 = 1$, and is convenient for the following theoretical discussion leading to concise expressions without superfluous number coefficients. In simulations, this is equivalent to taking $\gamma = k = k_B T = 1$. This choice of units does not put any restrictions since the dynamics of a chain with N beads, possessing the Kuhn's length b , in a solvent with friction coefficient for a single bead γ at temperature $k_B T$ can be recalculated from the master dynamics for $\tau_0 = D_1 = 1$ by change of lengths and timescales by the factors $b/\sqrt{d}$ and $\gamma b^2/(d k_B T)$, respectively. Up to the units, the dynamics of the chain only depends on N .

A. Memory friction kernel and MSD for the Rouse model

The memory friction (response) function of the Rouse model can be calculated from the mode picture [3], not only in the continuous limit, as is done in Refs. [15,16], but also for a finite, relatively short chain, where the relaxation times of the modes are known as well [17]. Due to the linearity of the model, it is enough to consider the deterministic response only. Moreover, due to the separation of different coordinates in the Rouse model, it is fully sufficient to consider its one-dimensional variant, Eqs. (8). Here we present an alternative approach to this calculation which simplifies the discussion of the intermediate and the terminal asymptotics of the behavior. The results will be also used in the discussion of the behavior of a constrained system.

Let us consider Eq. (7) and look at the mean response of the first bead to a force $F_a(t)$ applied to this bead. For the mean displacement, the contribution of the noise averages out, so that this displacement is governed by a deterministic equation:

$$\int_0^t dt' K(t-t') \dot{x}(t') = F_a(t), \quad (10)$$

with $x(t) \equiv x_1(t)$. This displacement will be compared to the response of the chain given by the set of ODEs, Eq. (8). In our system of units $\tau_0 = D_1 = 1$, making all quantities dimensionless, this system of equations reads:

$$\begin{aligned} \frac{dx}{dt} &= -(x - x_2) + F_a(t), \\ \frac{dx_N}{dt} &= -(x_N - x_{N-1}) \end{aligned} \quad (11)$$

for the end beads [note again that $x(t) \equiv x_1(t)$] and

$$\frac{dx_n}{dt} = -(2x_n - x_{n-1} - x_{n+1}), \quad (12)$$

$1 < n < N$, for the intermediate ones. Passing to the Laplace domain, we get from Eq. (10)

$$K(s)[sx(s) - x(t=0)] = F_a(s).$$

Here we can take $x(t=0) = 0$, which leaves us with $K(s) = F_a(s)/[sx(s)]$, so that

$$K^{-1}(s) = s \frac{x(s)}{F_a(s)}. \quad (13)$$

On the other hand, the equations of motion, Eqs. (11) and (12), give

$$\begin{aligned} sx(s) - x(t=0) &= -[x(s) - x_2(s)] + F_a(s), \\ sx_n(s) - x_n(t=0) &= -[2x_n(s) - x_{n-1}(s) - x_{n+1}(s)], \\ sx_N(s) - x_N(t=0) &= -[x_N(s) - x_{N-1}(s)], \end{aligned}$$

where the intermediate equation applies for $1 < n < N$. The last system of equations can be rewritten in a matrix form,

$$\hat{T} \vec{x}(s) = \vec{F}(s) + \vec{x}(t=0),$$

where

$$\vec{F}(s) = (F_a(s), 0, \dots, 0)^T,$$

$$\vec{x}(t=0) = (x(t), x_2(t), \dots, x_N(t))^T \Big|_{t=0}$$

is the vector of initial conditions and $\hat{T}$ reads:

$$\hat{T} = \begin{bmatrix} s+1 & -1 & \dots & 0 & 0 \\ -1 & s+2 & \dots & 0 & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & \dots & s+2 & -1 \\ 0 & 0 & \dots & -1 & s+1 \end{bmatrix} \quad (14)$$

with diagonal entries $a_{11} = a_{NN} = s+1$ and $a_{ii} = s+2$ for $1 < i < N$, and the entries of the two adjacent diagonals equal -1 .

The matrix $\hat{T}$ is a tridiagonal symmetric nearly Toeplitz matrix, see, e.g., Refs. [18–20]. The solution to our equation is then given by

$$\vec{x}(s) = \hat{T}^{-1}[\vec{F}(s) + \vec{x}(t=0)].$$

Since we are interested only in $x = x_1$, we only have to know the first line of the matrix $\hat{T}^{-1}$. Moreover, since the first element of $\vec{x}(t=0)$ can be put to zero, and we are interested only in the response averaged over the equilibrium initial conditions, we essentially need only the matrix element $E(s) = \{\hat{T}^{-1}\}_{11}(s)$ [since in equilibrium $\langle x_i(t=0) \rangle = x_1(t=0) = 0$] and get $x(s) = E(s)F_a(s)$. Applying Eq. (13) we get $K^{-1}(s) = sE(s)$, so that

$$K(s) = \frac{1}{sE(s)}. \quad (15)$$

To obtain $E(s)$ we use the results of Ref. [18]. The final expression reads:

$$E(s) = \frac{\sqrt{s(4+s)}[(2+s+\sqrt{s(4+s)})^N + (2+s-\sqrt{s(4+s)})^N] - 1}{2s[(2+s+\sqrt{s(4+s)})^N - (2+s-\sqrt{s(4+s)})^N]} \quad (16)$$

The intermediate steps of calculations based on the results of Corollary 2 in Ref. [18] are given in Appendix A. Note that $E(s)$ is essentially a rational function (in spite of all square roots present) but has a square root intermediate asymptotics. To see what happens, we apply binomial formula for powers. In the numerator this leads to vanishing of all terms containing odd powers of the square root, so that the square bracket is a polynomial in s , while in the denominator all even powers of square root $\sqrt{s(4+s)}$ vanish, so that the square bracket

contains only odd powers of this root. Being divided by the square root in the numerator, this leaves us with a polynomial in s . The inverse Laplace transform of a rational function (with numerator being an order N polynomial starting with the zero-order term, and denominator the order $N+1$ polynomial starting with the first order term) is a sum of a constant and N exponential functions, so that the whole behavior corresponds to multiexponential relaxation to a constant. Another way to see this (and an alternative way to obtain expressions for $E(s)$)

for polymers of different lengths) is based on the recurrence relation for $E_N(s) \equiv E(s)$ for polymers of different lengths N discussed in Appendix B.

To investigate the asymptotic behavior of Eq. (16) in the asymptotics of very large and very small s , as well as the intermediate asymptotics of moderately small s , we note that

For $s \gg 1$ and $N > 1$ we have

$$[2 + s + \sqrt{s(4+s)}]^N \gg [2 + s - \sqrt{s(4+s)}]^N,$$

$$\text{so that } E(s) \simeq \frac{\sqrt{s(4+s)}}{2s} - \frac{1}{2} \simeq \frac{1}{s}.$$

For $s \ll 1$ we can safely neglect s compared to constant contributions and write:

$$E(s) \simeq \frac{1}{\sqrt{s}} \frac{(1 + \sqrt{s})^N + (1 - \sqrt{s})^N}{(1 + \sqrt{s})^N - (1 - \sqrt{s})^N} - \frac{1}{2}. \quad (17)$$

This expression applies to both intermediate and terminal asymptotic regimes. In the intermediate domain $1/N^2 \ll s \ll 1$, we have $(1 - \sqrt{s})^N \ll (1 + \sqrt{s})^N$ so that $E(s) \approx 1/\sqrt{s}$, while in the final asymptotic domain $s \ll 1/N^2$ we can expand the binomials and get $E(s) \simeq 1/Ns$. Note that in this domain, a constant contribution $-1/2$ in Eq. (17) can be safely neglected. Thus, we can separate three domains of s corresponding to three distinct types of behavior,

$$E(s) = \begin{cases} 1/s & \text{for } s \gg 1 \\ 1/\sqrt{s} & \text{for } 1/N^2 \ll s \ll 1 \\ 1/Ns & \text{for } s \ll 1/N^2. \end{cases} \quad (18)$$

From this, the corresponding asymptotics for the memory kernel K follow by Eq. (15).

B. The mean-squared displacement of an end bead

In our work we concentrate on the diffusion properties of the end bead. For a free chain we can use the results of Ref. [21] based on Ref. [22], with

$$\langle x^2(t) \rangle = 2k_B T \int_0^t H(t') dt', \quad (19)$$

with $H(t)$ given by its Laplace transform. For a massive bead of mass M one has [21]

$$H(s) = \frac{1}{s[K(s) + Ms]}.$$

Adapted to our overdamped situation corresponding to the limit $M \rightarrow 0$ we have in our special units

$$H(s) = \frac{1}{sK(s)} \equiv E(s),$$

see Eq. (15), and essentially do not need K in our further calculations [some discussion of $K(t)$ is, however, given in the Appendix A for the sake of completeness], so that

$$\langle x^2 \rangle(s) = 2 \frac{E(s)}{s}. \quad (20)$$

For the sake of completeness, we will derive the result, Eq. (20), independently of our limiting transition from the overdamped situation in Appendix C.

Now we can perform the Laplace inversion and get (first, in our special system of units)

$$\langle x^2(t) \rangle = 2 \begin{cases} t & \text{for } t \ll 1 \\ 2\sqrt{t}/\sqrt{\pi} & \text{for } 1 \ll t \ll N^2 \\ t/N & \text{for } t \gg N^2. \end{cases}$$

At this stage we can restore the units, note that s is measured in units of τ_0^{-1} and $E(s)$ in units of γ^{-1} , and see that in natural units all MSDs can be expressed in terms of the diffusion coefficient $D = D_1$ of a single bead and τ_0 only, so that in x direction

$$\langle x^2(t) \rangle = \begin{cases} 2Dt & \text{for } t \ll \tau_0 \\ 4D\sqrt{\tau_0 t}/\sqrt{\pi} & \text{for } \tau_0 \ll t \ll N^2 \tau_0 \\ 2Dt/N & \text{for } t \gg N^2 \tau_0. \end{cases} \quad (21)$$

The corresponding time domains will be referred as domains I, II, and III in what follows, respectively. The expression for intermediate times can be rewritten as

$$4D\sqrt{\tau_0 t}/\sqrt{\pi} = \frac{4}{\sqrt{\pi}} D \tau_0 \sqrt{\frac{t}{\tau_0}} \equiv \frac{4b^2}{d\sqrt{\pi}} \sqrt{\frac{t}{\tau_0}}.$$

III. SIMULATIONS

In what follows, we compare two situations:

- (i) only one bead on a sinusoidal wire (parameterized by its length l), all other beads in a free space, and
- (ii) all beads on the wire.

We are looking at the MSD of the tagged bead in projection on the x axis and return to natural units. For a bead on a sinusoidal wire at position x the coordinate y is $y = A \sin(\frac{2\pi x}{L})$, with L being the period of the modulation and A its amplitude. The position of the bead can be parameterized by its position l along the wire,

$$l = \int_0^x \sqrt{1 + y'^2} dx \quad (22)$$

with $y' = \frac{dy}{dx} = \frac{2\pi A}{L} \cos(\frac{2\pi x}{L})$, i.e., by the length of the wire l from the origin to the actual position of the bead (x, y) .

The motion along the wire is governed by the overdamped Langevin equation

$$\gamma \frac{ds}{dt} = F_l + f_l, \quad (23)$$

where F_l and f_l are the projections of the elastic force and random force onto the l direction tangential to the wire. A parameter important for the following discussion will be the relative length of the wire, defined via the length l at position x for $x \gg L$: $\kappa = \lim_{x \rightarrow \infty} \frac{l(x)}{x}$. This length is given by

$$\kappa(m) = \frac{2}{\pi} \sqrt{1 + m^2} E\left(\frac{m^2}{m^2 + 1}\right),$$

with $m = 2\pi A/L$. Here $E(z)$ is a complete elliptic integral of the second kind [23]; see Ref. [1] for the discussion. For the further reference, the values of κ are given in the Table I for the values of A and L used in simulations below.

TABLE I. The relative lengths.

A	L	κ
0	—	1
0.1	1	1.09
0.25	1	1.46
0.5	1	2.30
1.0	1	4.19

A. Implementation

We start from the discussion of the first situation. Here the equations of motion for all beads except for the first one are the ones of the genuine Rouse model [Eqs. (2) and (4)].

Let bead 1 be at position $[x, A \sin(\frac{2\pi x}{L})]$ and bead 2 at position $\mathbf{r}_2 = (x_2, y_2)$. At the position x of the first bead the wire makes an angle $\phi = \arctan y'(x)$ with the x axis. For our sinusoidal wires with finite amplitude of modulation the angles ϕ lay strictly in the domain $-\frac{\pi}{2} < \phi < \frac{\pi}{2}$, so that $\cos \phi > 0$. Then the projection of the force (F_x, F_y) [or (f_x, f_y)] on the wire is

$$F_l = F_x \cos \phi + F_y \sin \phi$$

with $\cos \phi = \frac{1}{\sqrt{1+y'^2}}$, $\sin \phi = \frac{y'}{\sqrt{1+y'^2}}$. Since $\frac{dl}{dt} = \frac{dl}{dx} \cdot \frac{dx}{dt}$, we can rewrite Eq. (23) as

$$\gamma \frac{dx}{dt} = \frac{1}{(dl/dx)} [F_x \cos \phi + F_y \sin \phi + f_x \cos \phi + f_y \sin \phi].$$

Now we note that f_x and f_y are two independent statistical copies of the same Gaussian white noise, and therefore the sum $f_l = f_x \cos \phi + f_y \sin \phi$ is a single white noise with the same correlation function as f_x or f_y . Therefore,

$$\gamma \frac{dx}{dt} = \frac{1}{(dl/dx)} [F_x \cos \phi + F_y \sin \phi + f_l]$$

with $dl/dx = \sqrt{1+y'^2}$. Therefore, the equation we have to integrate is

$$\gamma \frac{dx}{dt} = \frac{1}{1+y'^2} F_x + \frac{y'}{1+y'^2} F_y + \frac{1}{\sqrt{1+y'^2}} f_l, \quad (24)$$

with $F_x = k(x_2 - x)$, $F_y = k(y_2 - y(x))$. The noise f_l has a zero mean and the correlation function $\langle f_l(t) f_l(t') \rangle = 2k_B T \delta(t - t')$. The equations of motion for all other beads are the same as for the free chain, i.e., are given by Eq. (2) for intermediate beads and by Eq. (4) for the N th bead. The overall geometry of the situation is made clear in Fig. 1, where we plot three snapshots of the chain with the single bid on a wire for three different instants of time.

Since Eq. (24) follows from Eq. (23) with the additive noise by the continuous coordinate transformation, the correct interpretation of the stochastic integral for this case is the Stratonovich one, and the Heun algorithm is used for its numerical integration. We start with $x(0) \equiv x_1(0) = 0$, $y(0) \equiv y_1(0) = 0$ and then initialize the positions of all other beads iteratively according to the rules:

$$\begin{aligned} x_k(0) &= x_{k-1}(0) + \Xi_x \\ y_k(0) &= y_{k-1}(0) + \Xi_y \end{aligned} \quad (25)$$

with Ξ_x, Ξ_y being normal variables, $\mathcal{N}(0, b/\sqrt{d})$.

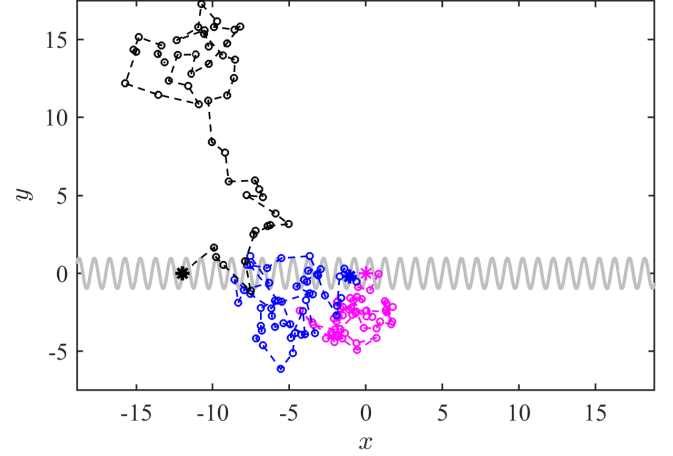


FIG. 1. The configurations of the Rouse chain of $N = 50$ beads at different instants of time $t = 0, 10^4$, and 10^5 . The position of the confined bead is indicated by an asterisk, and the positions of all other beads by circles. The position of the tagged bead is the rightmost for $t = 0$ and the leftmost for $t = 10^5$.

For the case of all beads on the wire, equations similar to Eq. (24) are used also for all other beads:

$$\gamma \frac{dx_i}{dt} = \frac{1}{1+y'^2} F_{x,i} + \frac{y'}{1+y'^2} F_{y,i} + \frac{1}{\sqrt{1+y'^2}} f_{l,i},$$

with $y' = \frac{2\pi}{L} \cos(\frac{2\pi x_i}{L})$, and with $F_{x,i} = k(x_{i+1} + x_{i-1} - 2x_i)$, $F_{y,i} = k(y_{i+1} + y_{i-1} - 2y_i)$ for $1 < i < N$ and $F_{x,N} = k(x_{N-1} - x_N)$, $F_{y,N} = k(y_{N-1} - y_N)$. The initial distribution of x coordinates of the beads is generated according to Eq. (25), after which their initial y coordinates were calculated as $y_k(0) = A \sin(\frac{2\pi x_k(0)}{L})$. This choice of initial coordinates may not correspond to an equilibrium distribution of the beads on the wire. To check the validity of the results, we carried out an additional test by fixing the tagged bead and letting the rest of the chain evolve according to the Rouse dynamics up to $t = 10$, corresponding to equilibration of the interbead distances. Then the tagged bead is released, and the initial time interval censored. The results do not differ statistically from ones obtained using Eq. (25) within the range of computational uncertainty.

B. Results

The results of our simulations are shown in Figs. 2–5 below. The simulations are performed in our special units which formally correspond to taking $\gamma = k = k_B T = 1$. To reproduce the generic results for a particle in a bath with long-range time correlations, we first present the results for a relatively long chain of 100 beads, up to dimensionless time $t = 10^4$ below the second crossover. For each of these simulations, an ensemble of $n = 10^4$ independent realizations was used. Heun's method with the time step of $dt = 10^{-2}$ was applied to integrate the equations of motion.

The upper curve in Fig. 2 corresponds to the straight wire and reproduces the regimes I and II discussed at the end of Sec. II A, with a crossover around the time $\tau_0 \sim 1$. The lower curves correspond to modulations of different amplitudes. All curves except for the one with the largest amplitude of the

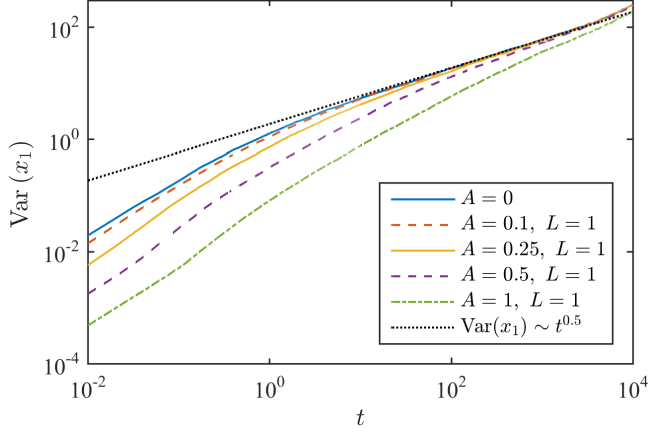


FIG. 2. The MSD $\langle x^2(t) \rangle$ of a bead on a wire for the Rouse chain of $N = 100$ beads. The values of other simulation parameters are given in the text.

modulation converge at longer times to the curve for the straight wire (unperturbed one-dimensional Rouse dynamics).

Figure 3 shows the same as Fig. 2 but for a shorter chain of $N = 50$ monomers, with 4 times smaller Rouse time. Here all three regimes, I, II, and III are seen for the unperturbed chain, with crossovers around τ_0 and $\tau_N \sim N^2\tau_0$. We see that if $\langle x^2(t) \rangle$ approaches the behavior for a straight wire at $t < \tau_N$ (i.e., the bath has already won), then all curves correspond to the same final regime (same coefficient of normal diffusion) for $t > \tau_N$. This finding is not surprising, since if we discretize the time in units of τ_N , the trajectory of the motion will correspond to a random walk with the MSD per step equal to $\lambda^2 = \langle x^2(\tau_N) \rangle$ which is practically the same for $A = 0, 0.1, 0.25$, and 0.5 , and the correlation between the subsequent steps of duration τ_N is negligible due to the exponential cutoff of the memory function (see Appendix A). An important finding is that even if no convergence to the common behavior took

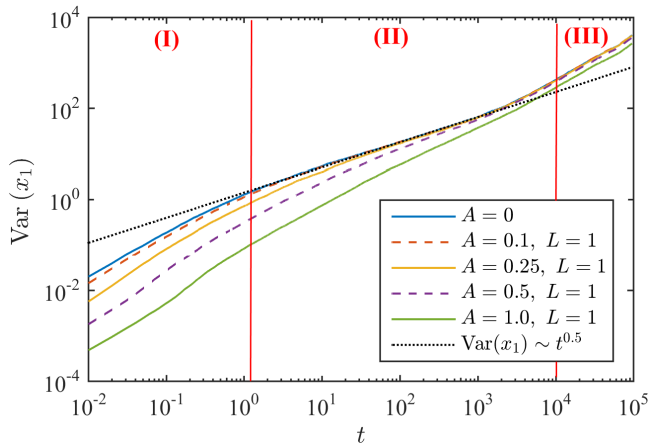


FIG. 3. The MSD $\langle x^2(t) \rangle$ of a bead on a wire for a shorter bath chain of $N = 50$ monomers and for longer overall simulation time than in Fig. 2. All other simulation parameters are the same as in Fig. 2. Here all three regimes and both crossovers for a free chain are visible. The corresponding time domains for a free chain are indicated as (I), (II), and (III).

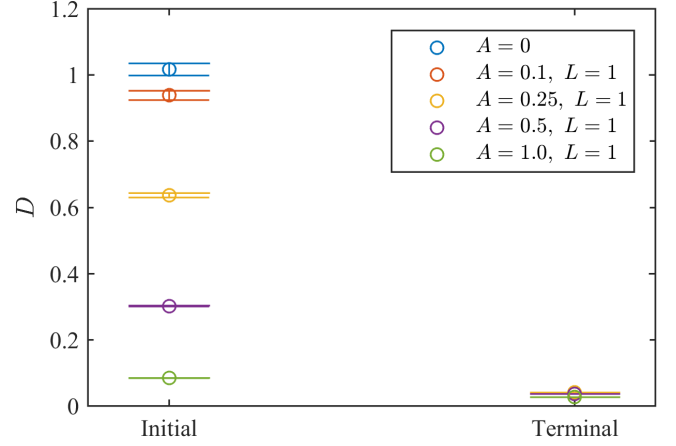


FIG. 4. The values of the diffusion coefficients obtained by a linear fit $\langle x^2(t) \rangle = 2Dt$ for a tagged bead of a chain with $N = 50$ beads. The initial domain corresponds to a fit for $0 < t < 1.8$, and the terminal domain to the fit in the domain $10^4 < t < 10^5$. The error bars show the uncertainty of the fit within 95% confidence interval.

place up to τ_N , the relative difference in the terminal diffusion coefficients is much smaller than the difference in the short-time ones. To corroborate the finding we calculated the values of diffusion coefficients by performing simple linear fits $\langle x^2(t) \rangle \simeq 2Dt$ for the initial and terminal time domains $0 < t < 1.8$ and $10^4 < t < 10^5$, i.e., in the domains I and III in Fig. 3. These results are shown in Fig. 4.

Figures 2 and 3 were pertinent to the case when the constraint only affected the tagged bead and did not affect the bath. Figure 5 shows the results for the case when the constraint affected the bath as well: All beads of the Rouse chain are now on the wire. The figure corresponds to $N = 100$: We again use the longer chain and see the regimes I and II for the unmodulated case. However, in the case of modulation, the behavior for subdiffusive regime II changes. The explanation for this follows.

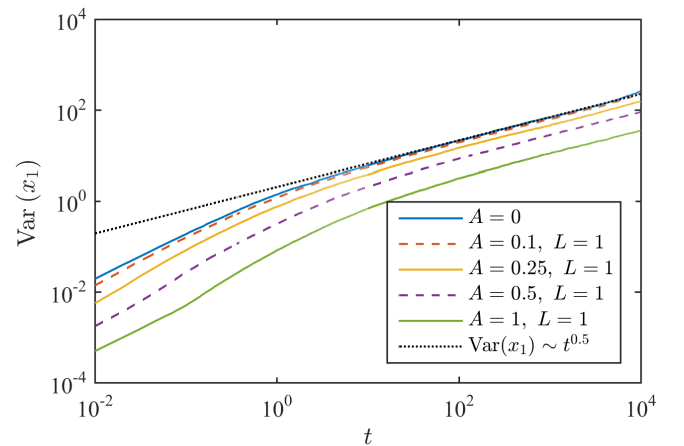


FIG. 5. The MSD $\langle x^2(t) \rangle$ for a tagged bead in the case when all $N = 100$ beads are confined to the wire. The values of parameters are the same as for the previous simulations.

IV. ANALYTICALLY TREATABLE LIMIT

Let us discuss our results and demystify somewhat the situation. Although we are not able to provide a full analytical description for the behavior observed in simulations, we can consider a specific limiting case which proposes an explanation of these findings. This explanation moreover leads to semiquantitative predictions, which are checked with our simulations.

We start from our first setup and consider the following situation: A particle on a wire (or in an external potential) coupled to a free chain showing slow dynamics with a cutoff, i.e., to a bath having nontrivial correlation properties. If we assume the timescale separation between the characteristic cutoff time and the homogenization time for a diffusion of a single bead on a wire, then the motion of this bead can be considered as following a standard Langevin equation with the renormalized friction coefficient $\tilde{\gamma}$ (renormalized mobility $\tilde{\mu} = 1/\tilde{\gamma}$) and renormalized diffusion coefficient $\tilde{D} = k_B T \tilde{\mu}$. This bead is coupled to the rest of the chain, a Rouse chain of $N - 1$ beads, characterized by the memory kernel $K(t)$, by a spring with elastic constant k . We start the general discussion in natural units and pass to special ones in final calculations.

The timescale separation essentially ensues in the limit when the modulation of the wire is very fast, $L \ll b$, in which case on the characteristic scale of motion the mean-squared displacement $\langle l^2 \rangle$ along the chain is translated into the MSD $\langle x^2 \rangle = \kappa^{-2} \langle l^2 \rangle$, so that the diffusion coefficient $\tilde{D}$ of the first bead is $\tilde{D} = \kappa^{-2} D$ and $\tilde{\gamma} = \kappa^2 \gamma$.

The effective equations of motion for this situation are

$$\tilde{\gamma} \dot{x} = -k(x - X) + \sqrt{2\tilde{\gamma}k_B T} \xi(t) \quad (26)$$

$$\int_0^t K(t - t') \dot{X}(t') dt' = -k(X - x) + \zeta(t), \quad (27)$$

This solution is now inserted into the Eq. (26) written in the Laplace domain with $x_0 = 0$,

$$\begin{aligned} \tilde{\gamma} s x(s) + k x(s) &= \sqrt{2\tilde{\gamma}k_B T} \xi(s) + k X(s) \\ &= \sqrt{2\tilde{\gamma}k_B T} \xi(s) + k \left\{ \frac{k}{sK(s) + k} x(s) + \frac{K(s)}{sK(s) + k} X_0 + \frac{\zeta(s)}{sK(s) + k} \right\}. \end{aligned}$$

Now we collect the terms,

$$x(s) \left[\tilde{\gamma} s + k - \frac{k^2}{sK(s) + k} \right] = \sqrt{\tilde{\gamma}k_B T} \xi(s) + k \frac{kK(s)}{sK(s) + k} X_0 + k \frac{\zeta(s)}{sK(s) + k},$$

note that the left-hand side of the equation represents $s\Phi(s)x(s)$ and read out the Laplace transform of the kernel Φ :

$$\Phi(s) = \tilde{\gamma} + \frac{kK(s)}{sK(s) + k}, \quad (30)$$

consisting of the renormalized Stokes friction and an additional memory term. The MSD given by Eq. (19) has then the Laplace representation,

$$\langle x^2(s) \rangle = 2k_B T \frac{\tilde{H}(s)}{s},$$

with X being the coordinate of the bead of the bath chain attached to the tagged one, with the noise $\zeta(t)$ fulfilling the FDR of the second kind, and $\xi(t)$ being the standard Gaussian white noise. Our next step will be excluding the variable X , putting the system of Eqs. (26) and (27) as a single generalized Langevin equation for x only,

$$\int_0^t \Phi(t - t') \dot{x}(t') dt' = Z(t), \quad (28)$$

and looking at the properties of its memory friction function $\Phi(t)$ and noise $Z(t)$. Note that due to the overall equilibrium setting, the FDR would be satisfied for this equation as well. Once we have determined the memory friction kernel $\Phi(t - t')$, we can proceed as before.

To obtain the new kernel, we pass to the Laplace domain, in which Eq. (28) reads:

$$\Phi(s)[sx(s) - x_0] = Z(s), \quad (29)$$

and the initial conditions correspond to $x_0 = 0$. Now we pass to the Laplace domain in Eqs. (26) and (27).

We start by solving the linear equation Eq. (27) for given $x(t)$ and given realization of the noise $\zeta(t)$ which in the Laplace domain reads

$$K(s)[sX(s) - X_0] = -kX(s) + kx(s) + \zeta(s),$$

and get

$$X(s) = \frac{k}{sK(s) + k} x(s) + \frac{K(s)}{sK(s) + k} X_0 + \frac{\zeta(s)}{sK(s) + k}.$$

with $\tilde{H}(s) = \frac{1}{s\Phi(s)}$. Representing $K(s)$ via $E(s)$ (which here has to be taken in natural units) we rewrite this result as

$$\langle x^2(s) \rangle = \frac{2k_B T}{s^2} \frac{1}{\tilde{\gamma} + k/[s + kE(s)]}. \quad (31)$$

For s large (which corresponds to the short-time domain) we get

$$\langle x^2(s) \rangle = \frac{2k_B T}{\tilde{\gamma} s^2},$$

i.e., $\langle x^2(t) \rangle = \frac{2k_B T}{\tilde{\gamma}} t$, by a factor of κ^2 slower than for a free bead on an unmodulated wire. This behavior terminates at times corresponding to the inverse values of s at which the

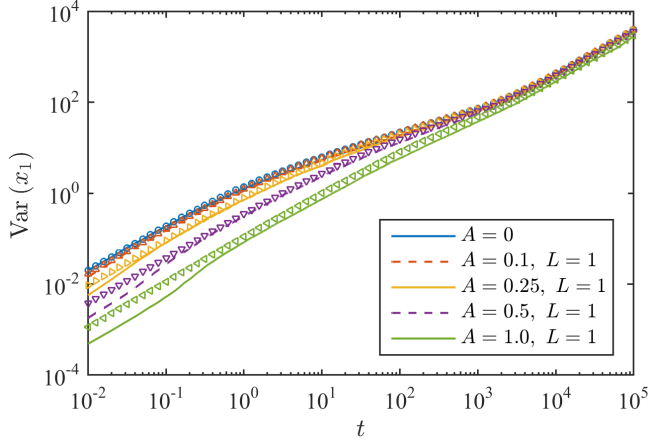


FIG. 6. The results for a chain of $N = 50$ beads, with only the first bead on the wire (lines) compared with the results of numerical inversion of Eq. (31) (symbols). The values of parameters are the same as for the previous simulations.

second term in the denominator of Eq. (31) gets of the order of $\tilde{\gamma}$.

For the further analysis, it is convenient to return to our dimensionless units and take $\gamma = k = k_B T = 1$. Now $\tilde{\gamma} = \kappa^2$. Equation (31) now reads

$$\langle x^2(s) \rangle = \frac{2}{s^2} \frac{1}{\kappa^2 + 1/[s + sE(s)]}.$$

For small $s \ll 1$ we have $E(s) \simeq 1/\sqrt{s}$ for $1 \gg s \gg 1/N^2$ and $E(s) \simeq 1/(Ns)$ for $s \ll 1/N^2$, so that

$$\langle x^2(s) \rangle \simeq \frac{2}{s^2} \frac{1}{\kappa^2 + 1/[sE(s)]}.$$

In the terminal domain $s \ll 1/N^2$ we have

$$\langle x^2(s) \rangle \simeq \frac{2}{s^2} \frac{1}{\kappa^2 + N},$$

so that the dependence of $\langle x^2(t) \rangle$ on κ gets very weak in the limit $\kappa^2 \ll N$. Such practical independence takes place for moderate modulation ($A = 0.1, 0.25$, and 0.5) in our Fig. 3 but does not hold anymore for the strongest modulation case, where $\kappa^2 \approx 18$ and $N = 50$. In the intermediate domain $1/sE(s) \sim 1/\sqrt{s}$, so that the transition between the initial, κ -dependent domain takes place at $s \sim \kappa^{-4}$ (corresponding to $t \sim \kappa^4$). If such a transition is allowed for by a position of the terminal crossover, then the behavior at all (dimensionless) times $t > \kappa^4$ is universal and the same as in the absence of the modulation.

In Fig. 6 we show the same simulation results as in Fig. 3 for a chain of $N = 50$ beads compared with the results of the numerical inversion of Eq. (31) with $E(s)$ given by Eq. (16) with $N = 49$. The numerical Laplace inversion is performed using the Gaver-Stehfest algorithm which is best suited for the cases when the original [in our case, $\langle x^2(t) \rangle$] does not oscillate; see, e.g., Ref. [24]. Note that our, relatively naive, homogenization approach is in a very good agreement with the numerical simulation data in the time domains II (intermediate time behavior) and III (long times). A poorer agreement is seen in the short-time domain. This is not astonishing, since

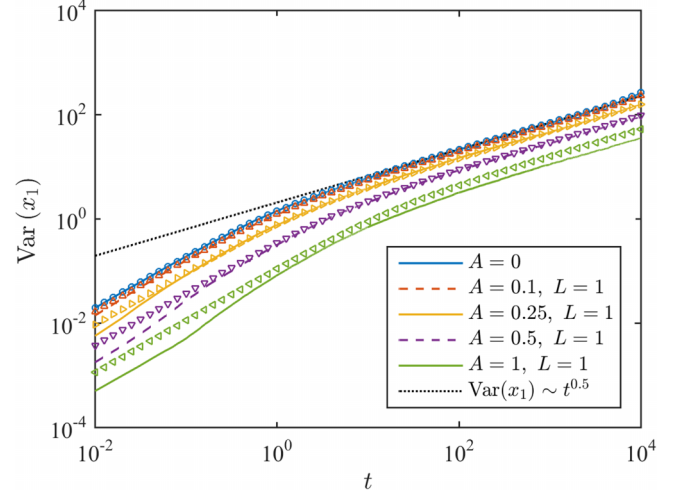


FIG. 7. The results for a chain of $N = 100$ beads, which all are confined to the wire (lines) compared with the results calculated via Eq. (32) (symbols).

the times up to $t \sim 1$ correspond to displacements smaller than the period of modulation, at which times no homogenization could be expected. Note that our “small parameter” which should guarantee the homogenization (something like L/b) is of the order of unity, i.e., essentially not small. Thus, at best only semiquantitative description could be anticipated, while in reality the quality of approximation (for long times) is very good for small modulation amplitudes and does not deteriorate too strongly for large ones ($A \sim 1$). This stresses that the time- or length-scale separation *ansatz* works better than expected. Note that this approach is similar in spirit but still different from the discussion in Ref. [2], since it does not assume separation of modes into slow and fast ones, which for a scale-free process is quite arbitrary.

A similar discussion can be applied to the case of all beads on a wire. In this case *all* values of γ are renormalized by the factor of κ^2 . This leads to renormalization of τ_0 by a factor of κ^2 , so that the diffusion in domains I and III are κ^2 times slower than for a bead on a straight wire, while the subdiffusion in the domain II is κ time slower than in the case when the modulation is absent. The renormalization of γ does not change the length unit, so that considering the homogenized situation for modulation with parameter κ simply corresponds to plotting

$$\langle x_\kappa^2(t) \rangle = \left\langle x_r^2\left(\frac{t}{\kappa^2}\right) \right\rangle, \quad (32)$$

where $x_r(t)$ is the displacement for an end bead of a Rouse chain on the straight wire following by the numerical Laplace inversion of Eq. (20) with $E(s)$ given by Eq. (16).

In Fig. 7 we show the whole dependence $\langle x^2(t) \rangle$ on the parameter κ . Here, our chain has the length of $N = 100$ monomers. Our homogenization approach predicts that the only changes with respect to unmodulated wire correspond to changing τ_0 as it is actually seen in the figure. Note that in this case again the intermediate- and long-time behavior is very well reproduced by the homogenization approach for all modulation amplitudes A but the largest one.

V. CONCLUSIONS

Motivated by a very unusual behavior of the mean-squared displacement of particles subjected to constraints in contact with a non-Markovian bath which in the case of a free particle would lead to a subdiffusive behavior, we considered a simple, physically motivated model where the particle is a tagged end monomer of a Rouse polymer chain, and the bath is represented by the rest of the chain and its surroundings. Two situations are considered: In the first case, the constraint, corresponding to moving on a sinusoidal wire, only applies to a tagged particle. In the second case, the same constraint is applied to all monomers of the chain. In the first case, for long chains, the long-time behavior of the MSD of the tagged monomer is not sensitive to the modulation of the wire, parallel to the previous findings for subdiffusive motions as described by GLEs with the power-law kernel: The MSD $\langle x^2(t) \rangle$ for modulated wire is the same as in the case of a straight wire (and the same as for the end monomer of a free Rouse chain). For shorter chains, whose Rouse time lays in the observation domain, new, interesting findings emerge. For moderate modulation, if $\langle x^2(t) \rangle$ already approached the one for a free chain for times smaller than or comparable to the Rouse time, the independence on the modulation is carried over to the final, diffusion regime of $t \gg \tau_R$. If such approach have not yet taken place, the relative difference of the terminal diffusion coefficients is still much smaller than the difference of short-time ones. If the constraints apply to all monomers (i.e., to the bath as well), then the sensitivity to the modulation never disappears. A simple approach based on homogenization explains the findings on a semiquantitative level.

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DATA AVAILABILITY

The data that support the findings of this article are not publicly available. The data are available from the authors upon reasonable request.

APPENDIX A: THE MEMORY KERNEL FOR THE ROUSE MODEL

We are looking for the upper left element $E(s) = \{\hat{T}\}_{11}^{-1}(s)$ of the inverse of a nearly Toeplitz matrix given by Eq. (14); see e.g., Refs. [18–20]. As stated in the main text, we use the results of Ref. [18] (see Corollary 2) to obtain $E(s)$. In the notation of Ref. [18] we have the following parameters defining $\hat{T}$: $b = -1$ (we note that b here does not have the meaning of the mean distance between the beads), $c = s + 2$, $d = s + 1$ (which is now not the dimension of space), and $\lambda = c - d = 1$.

In the notation of this work, the result reads

$$E = u_1 v_1$$

with $u_1 = 1$ and $v_1 = \frac{\kappa_{N-1}}{\tilde{\kappa}}$, where

$$\tilde{\kappa} = \phi_+^2 r_+^{N-1} - \phi_-^2 r_-^{N-1}, \quad \kappa_{N-1} = \phi_+ r_+^{N-1} - \phi_- r_-^{N-1}$$

with

$$r_{\pm} = (c \pm \sqrt{c^2 - 4})/2 = \frac{1}{2}(s \pm \sqrt{s^2 + 4s}) + 1,$$

$$\phi_{\pm} = r_{\pm} - \lambda = \frac{1}{2}(s \pm \sqrt{s^2 + 4s}),$$

so that

$$E(s) = 2 \frac{(s + \sqrt{s^2 + 4s})[1 + \frac{1}{2}(s + \sqrt{s^2 + 4s})]^{N-1} - (s - \sqrt{s^2 + 4s})[1 + \frac{1}{2}(s - \sqrt{s^2 + 4s})]^{N-1}}{(s + \sqrt{s^2 + 4s})^2[1 + \frac{1}{2}(s + \sqrt{s^2 + 4s})]^{N-1} - (s - \sqrt{s^2 + 4s})^2[1 + \frac{1}{2}(s - \sqrt{s^2 + 4s})]^{N-1}}.$$

This lengthy expression can be somewhat simplified, leading to

$$E(s) = \frac{\sqrt{s(4+s)}[(2+s+\sqrt{s(4+s)})^N + (2+s-\sqrt{s(4+s)})^N] - 1}{2s[(2+s+\sqrt{s(4+s)})^N - (2+s-\sqrt{s(4+s)})^N]} - \frac{1}{2}, \quad (\text{A1})$$

which is Eq. (16) of the main text. Then, the memory kernel $K(s)$ in Laplace domain is given by Eq. (15) of the main text,

$$K(s) = \frac{1}{sE(s)}.$$

For small Laplace frequencies $s \ll 1$ Eq. (A1) further simplifies to

$$E(s) \simeq \frac{1}{\sqrt{s}} \frac{(1 + \sqrt{s})^N + (1 - \sqrt{s})^N}{(1 + \sqrt{s})^N - (1 - \sqrt{s})^N} - \frac{1}{2}, \quad (\text{A2})$$

which is Eq. (17) of the main text, and

$$K(s) \simeq \frac{1}{\sqrt{s}} \frac{(1 + \sqrt{s})^N - (1 - \sqrt{s})^N}{(1 + \sqrt{s})^N + (1 - \sqrt{s})^N}. \quad (\text{A3})$$

This expression corresponds to the time domains II and III in our discussion.

For the sake of completeness, we discuss here the properties of $K(t)$ as following from Eq. (A2) [i.e., Eq. (17) of the main text] in the dimensionless units used in Sec. II A. In the intermediate time domain corresponding to $s \ll N^{-2}$ we have

$$K(s) \simeq \frac{1}{\sqrt{s}},$$

crossing over to $K(s) = N$ for $s \ll N^{-2}$. To describe the crossover, we use Eq. (A3) and note that writing $(1 \pm \sqrt{s})^N = \exp[N \ln(1 \pm \sqrt{s})] \approx \exp(\pm N\sqrt{s})$ one can approximate $K(s)$ in the domain $s \ll 1$ by

$$K(s) \simeq \frac{\tanh N\sqrt{s}}{\sqrt{s}}, \quad (\text{A4})$$

a function whose inverse Laplace transform is given by the Jacoby elliptic θ function

$$K(t) = \frac{1}{N} \theta_2(0, e^{-\frac{\pi^2 t}{N^2}}) \quad (\text{A5})$$

with

$$\theta_2(0, q) = \sum_{n=-\infty}^{\infty} q^{(n+\frac{1}{2})^2}, \quad (\text{A6})$$

leading to the same expression as following from the continuous approximation in terms of Rouse modes, similar to the one used in Ref. [15]. MATHEMATICA readily gives the inverse transform, Eq. (A5). To check the inversion, one can use the partial fractions expansion of $\tanh(z)$ (for $z = N\sqrt{s} \geq 0$) in the numerator of Eq. (A4), as following from the identity, Eq. (5.1.26.1) of Ref. [25], i.e., to write

$$\tanh(z) = \sum_{k=0}^{\infty} \frac{8z}{\pi^2(2k+1)^2 + 4z^2},$$

substitute z , and perform the inversion term by term.

For $t \ll N^2$ the series in Eq. (A6) can be changed for an integral leading to

$$K(t) \simeq \frac{1}{N} \int_{-\infty}^{\infty} e^{-\frac{\pi^2 t}{N^2}(n+\frac{1}{2})^2} dn = \frac{1}{\sqrt{\pi t}},$$

while for $t \gg N^2$ the series is dominated by the largest term (with $n = 0$), so that

$$K(t) \simeq \frac{1}{N} e^{-\frac{\pi^2 t}{4N^2}}. \quad (\text{A7})$$

Note that at long times $K(s)$ is not given by

$$K(t) \approx \frac{1}{\sqrt{\pi t}} e^{-\frac{\pi^2 t}{4N^2}}, \quad (\text{A8})$$

where the existence of a power-law correction to an exponential at long times is the artifact of the approximation done in Ref. [15].

APPENDIX B: RECURRENCE RELATION FOR RESPONSE FUNCTIONS

Let us return to Eq. (30) and rewrite it in our special system of units $\gamma = k = k_B T = 1$, considering the friction coefficient

for the first bead to be the same as for all other ones. In this case $\Phi(s)$ corresponds to the memory friction kernel of a chain with $N + 1$ beads, $\Phi(s) \equiv K_{N+1}(s)$, while $K(s) \equiv K_N(s)$ is the memory friction kernel for a chain of N beads. We thus get

$$K_{N+1}(s) = 1 + \frac{K_N(s)}{sK_N(s) + 1}.$$

Putting $K_N(s) = 1/sE_N(s)$ and performing transformations we get the recurrence equation for the response function $E_N(s)$:

$$E_{N+1}(s) = \frac{1 + E_N(s)}{s[1 + E_N(s)] + 1}, \quad (\text{B1})$$

which can be checked by direct substitution of the expressions for $E(s)$, Eq. (16), for the corresponding values of N . The series of $E_N(s)$ starts with a single bead, for which the matrix $\hat{T}$ is a scalar, $T = s$ and $E_1(s) = s^{-1}$. For a dimer of two beads connected by a single spring with

$$\hat{T} = \begin{bmatrix} s+1 & -1 \\ -1 & s+1 \end{bmatrix}$$

we get

$$E_2(s) = \{\hat{T}^{-1}\}_{11} = \frac{1+s}{2s+s^2},$$

which coincides with the result of Eq. (B1), and so on. Note that $E_1(s)$ is a rational function and that E_{N+1} is a rational function of $E_N(s)$. Therefore, by induction, $E_{N+1}(s)$ is a rational function.

APPENDIX C: MEAN-SQUARED DISPLACEMENT UNDER OVERDAMPED DYNAMICS

Let us start from the overdamped version of the GLE put down in our special units,

$$\int_0^t dt' K(t-t') \dot{x}(t') = \zeta(t)$$

with the noise having zero mean, $\langle \zeta(t) \rangle = 0$, and satisfying the FDR of second kind

$$\langle \zeta(t) \zeta(t') \rangle = K(|t-t'|)$$

(note that in our units $k_B T = 1$). We pass to the Laplace domain, getting

$$K(s)[sx(s) - x_0] = \zeta(s)$$

and take the initial condition $x(0) = 0$. We get

$$x(s) = \frac{1}{sK(s)} \zeta(s) \equiv E(s) \zeta(s).$$

Therefore, in time domain

$$x(t) = \int_0^t E(t-t') \zeta(t') dt'.$$

Now we square this expression, use the standard representation of a square of the integral via the double one, and average

it over the realizations of the noise:

$$\begin{aligned}\langle x^2(t) \rangle &= \left\langle \int_0^t \int_0^t E(t-t')E(t-t'')\zeta(t')\zeta(t'')dt'dt'' \right\rangle \\ &= \int_0^t \int_0^t E(t-t')E(t-t'')\langle \zeta(t')\zeta(t'') \rangle dt'dt'' \\ &= \int_0^t \int_0^t E(t-t')E(t-t'')K(|t'-t''|)dt'dt''.\end{aligned}$$

Now we pass to new variables of integration $\eta = t - t'$, $\xi = t - t''$ and separate the domain of integration into upper and lower triangles giving equal contributions, getting

$$\langle x^2(t) \rangle = 2 \int_0^t d\xi E(\xi) \int_0^\xi K(\xi - \eta)E(\eta)d\eta$$

(with all functions considered in the time domain). The inner integral $I(\xi) = \int_0^\xi K(\xi - \eta)E(\eta)d\eta$ in the last expression has a form of convolution. Its expression in the Laplace domain reads

$$I(s) = K(s)E(s) = K(s)\frac{1}{sK(s)} = \frac{1}{s},$$

so that the integral $I(\xi)$ is essentially equal to unity. Therefore,

$$\langle x^2(t) \rangle = 2 \int_0^t E(\xi)d\xi,$$

which in the Laplace domain corresponds to

$$\langle x^2 \rangle(s) = 2 \frac{E(s)}{s}.$$

This is our Eq. (20).

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