Anomalous diffusion of distinguished particles in bead-spring networks

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Abstract

We consider the anomalous sub-diffusion of a class of Gaussian processes that can be expressed in terms of sums of Ornstein-Uhlenbeck processes. As a generic class of processes, we introduce a single parameter such that for any $\nu \in (0, 1)$ the process can be tuned to produce a mean-squared displacement with $E[x^2(t)] \sim t^{\nu}$ for large $t$.

The motivation for the specific structure of these sums of OU processes comes from the Rouse chain model from polymer kinetic theory. We generalize the model by studying the general dynamics of individual particles in networks of thermally fluctuating beads connected by Hookean springs. Such a set-up is similar to the study of Kac-Zwanzig heat bath models. Whereas the existing heat bath literature places its assumptions on the spectrum of the Laplacian matrix associated to the spring connection graph, we study explicit graph structures. In this setting we prove a notion of universality for the Rouse chain’s well-known $E[x^2(t)] \sim t^{\frac{1}{2}}$ scaling behavior. Subsequently we demonstrate the existence of other anomalous behavior by changing the dimension of the connection graph or by allowing repulsive forces among the beads.

1 Introduction

Due to recent and compelling experimental observations using advanced microscopy [1, 2, 3] there is theoretical interest [4, 5, 6, 7, 8, 9, 10] in anomalous diffusion – stochastic processes whose long-term mean-squared displacement (MSD) satisfies $E[x^2(t)] \sim t^{\nu}$ where $\nu \neq 1$. In each of the cited references,
the observed behavior is sub-diffusive, where $\nu \in (0, 1)$. The canonical example of a sub-diffusive process is fractional Brownian motion \cite{8}, but in this paper, we focus on a model from polymer kinetic theory and natural generalizations.

The Rouse chain model of a polymer is a series of thermally fluctuating beads $\{x_n(t)\}_{t \geq 0}$, $n \in \{1, \ldots, N\}$ that interact with nearest neighbors through linear spring forces. It is a standard observation in the physics literature \cite{11, 12, 13} that while the center-of-mass of the chain is a diffusive process, there exist positive times $\tau_1$ and $\tau_N$ such that individual beads roughly exhibit the following MSD profile:

$$E[x^2_n(t)] \sim \begin{cases} 
  t, & t \ll \tau_1 \\
  t^2, & \tau_1 \ll t \ll \tau_N \\
  t, & t \gg \tau_N
\end{cases} \quad (1.1)$$

The times $\tau_1$ and $\tau_N$ are called the first and last relaxation times respectively. Two of the primary projects in the present paper are to give precise mathematical meaning to a profile such as (1.1) and to show that the anomalous exponent $\nu = \frac{1}{2}$ in the intermediate timescale is determined by the geometric structure of the graph of connections among the beads.

The observation that the dynamics of an individual particle in a network, a so-called distinguished particle process, can exhibit anomalous diffusion is not restricted to polymer kinetics. In a series of papers \cite{14, 5, 15} the authors studied the behavior of a distinguished particle in a Kac-Zwanzig heat bath, a model used in molecular dynamics theory to study the force exerted on a particle by a randomly fluctuating environment. Of present interest are the articles \cite{5} and \cite{8} wherein the authors showed that in an appropriately constructed large-$N$ limit, a family of distinguished particle processes can converge weakly to a sub-diffusive limiting process. In \cite{8}, this process is fractional Brownian motion, while in \cite{5} the limiting process is the so-called generalized Langevin equation (see also \cite{16}) with a power law memory kernel. It is worth noting that in each of the above cases, the results followed from assumptions that were placed on the spectrum of the weighted spring connection graph, rather than directly on its weights and geometric structure, which is the goal of the present paper.

In \cite{10}, the authors introduce a common mathematical framework to address the sub-diffusion seen in these models: a class of Gaussian processes expressible in terms of a Brownian motion plus a sum of Ornstein-Uhlenbeck
processes,
\[ x(t) = c_0 B_0(t) + \sum_{k=1}^{N-1} c_k z_k(t) \]  
(1.2)
where each \( z_k \) satisfies the SDE
\[ dz_k(t) = -\lambda_k z_k(t) + dB_k(t) \]  
(1.3)
The collection of standard Brownian motions \( \{B_{k,N}\}_{k \leq N-1} \) are assumed to be independent. The positive constants \( \{\lambda_k\}_{k \leq N-1} \) will be called the diffusive spectrum and the constants \( \{c_k\}_{k \leq N-1} \) will be called the coefficient family. The inverses of the elements of the diffusive spectrum \( \tau_k := \lambda_k^{-1} \) are called the relaxation times of the process. Henceforth we will refer to processes defined by (1.2) and (1.3) as \( \Sigma \text{OU} \) processes.

One can think of an \( \Sigma \text{OU} \) process as a diffusing particle that is free to explore all of space, but is subject to a sequence of linear mechanical responses from its environment. The central notion of this paper is that anomalous diffusion can arise from the structure of timing of this cascade of responses. One can directly show (see Section 1.2) that when the beads in a network interact through linear spring forces, the associated distinguished particle process is exactly expressible in terms of equations (1.2) and (1.3).

In [10], the authors laid out the general relationship between the diffusive spectrum \( \{\lambda_k\}_{k=1}^{N-1} \) and the intermediate timescale anomalous exponent for \( \Sigma \text{OU} \) processes. Generalizing the Rouse spectrum \( \lambda_k = \sin^2(k\pi/2N) \) from the polymer kinetic theory [11, 13] by defining the diffusive spectrum to be
\[ \lambda_{k,N} = \left(\frac{k}{N}\right)^\rho \tau_i^{-1}, \]  
(1.4)
we find that \( \Sigma \text{OU} \) processes can exhibit any desired anomalous exponent between 0 and 1. Indeed, the full MSD profile of an \( \Sigma \text{OU} \) process with generalized Rouse spectrum is given by
\[ \mathbb{E}[x^2(t)] \sim \begin{cases} t_i, & t \ll \tau_i \\ t^{1-\frac{1}{\rho}}, & \tau_0 \ll t \ll \tau_N \\ t, & t \gg \tau_N \end{cases} \]  
(1.5)
for any \( \rho > 1 \). The actual exponents observed in experiments vary widely, and so the existence of stochastic processes that exhibit robust and varied anomalous behavior is appealing to experimentalists and engineers. At present, this community still lacks effective statistical inference tools for these sub-diffusive processes as well as the ability to conduct simulated experiments that are not computationally prohibitive.
1.1 Summary of Results

In this paper, we seek to give a rigorous interpretation to the claims made in the companion work [10]. In Theorem 2.1 we give precise meaning to the MSD profile (1.1). The key observation, independently noted in [8], is that for these models, the largest relaxation time $\tau_N$ tends to infinity with the number of modes $N$. The family of processes is tight, with a sequence of autocorrelation (ACF) functions that converge uniformly on compact sets. Therefore, demonstrating anomalous diffusion for large $t$ in the limiting process is tantamount to proving it for the intermediate timescale of the finite $N$ processes.

There is a robust sense in which the anomalous exponent is determined by the diffusive spectrum rather than the coefficient family. This fact is vital if one hopes to perform statistical inference on an $\SigmaOU$ process, see [10] for further discussion. In Proposition 2.2 we show that setting the coefficients to be i.i.d. random variables with mild restrictions, the exponent $\nu$ remains the same.

While the generic $\SigmaOU$ structure can support all anomalous sub-diffusive exponents it turns out that the behavior of distinguished particle processes is not so varied. It is conjectured in the physics literature [11] that the Rouse model is a universality class that captures the qualitative behavior of a wide variety of bead-spring networks. The main result of Section 3 is that this is indeed true in some rigorous sense (Theorem 3.2). The only exponent seen for a wide class of models is $\nu = \frac{1}{2}$. However, it is possible to construct weighted networks that produce different behavior by 1) changing the dimension of the underlying spring connection graph, Section 3.3; and 2) by allowing for repulsive forces among the beads, Section 3.5. Ultimately, such modifications cannot account for the wide behavior seen experimentally. One will likely need to account for some combination of hydrodynamic self-interaction [17] [18] and excluded volume effects [11], but rigorous study of these effects without pre-averaging approximations remains an unsolved problem.

1.2 Distinguished particles in bead-spring networks

We demonstrate the connection between distinguished particle processes and $\SigmaOU$ processes. Let $x(t) = (x_1(t), x_1(t), \ldots, x_2(t), \ldots, x_N(t))$ denote the locations in $\mathbb{R}^d$ of a set of particles at time $t \geq 0$. For the sake of simplicity we take $d = 1$, although this is not essential (see Section 3.1.2). Following the development of flexible polymer kinetics [11][13], the particles are subject
to random thermal fluctuations while interacting through a given quadratic configuration potential

$$\Psi(x) = \frac{1}{2} \sum_{n \neq m} \kappa_{nm} |x_n - x_m|^2.$$ 

The set of pairs $E := \{(x_n, x_m) : \kappa_{nm} > 0\}$ constitutes the set of edges of the graph $G$ associated with network.

Particle dynamics are formally set by a balance of forces through the Langevin equation,

$$m \ddot{x} = -\eta \dot{x}(t) - \nabla \Psi(x(t)) + \sigma \dot{W}(t)$$

where $\eta$ is the viscosity of the fluid in which the particles are immersed, and the strength of the noise $\sigma$ is related to the viscosity through the fluctuation dissipation theorem: $\sigma = \sqrt{2k_B T \eta}$. The constant $T$ is the temperature of the fluid and $k_B$ is Boltzmann’s constant. For simplicity we will renormalize the dynamics so that $\eta = 1$.

The common mass $m$ of the particles is considered to be small. In the companion paper [10], we observe that the zero-mass limit is singular and non-trivial to analyze. Here we restrict our attention to the weak (over-damped) zero-mass limit, as described in [10], which amounts to setting $m = 0$ and heretofore taking the stochastic forcing term $W(t)$ to be an i.i.d vector of standard Brownian motions.

The force exerted by the configuration potential on the $n$-th bead is

$$-\nabla_{x_n} \Psi(x) = \sum_{m \neq n} \kappa_{nm} (x_m - x_m)$$

leading to the linear system of SDEs

$$d\dot{x}(t) = Lx(t)dt + \sigma dW(t) \quad (1.6)$$

where $L$ is the so-called Laplacian matrix for the spring connection graph $G$. The Laplacian matrix is sometimes written $L = A - D$ where $A$ is the weighted adjacency matrix for $G$ and $D$ is a diagonal matrix whose entries are the sums of spring constants $D_{nn} = \sum_m \kappa_{nm}$.

We note that $L$ is symmetric and negative definite. As such it can be diagonalized in the form

$$L = Q \Lambda Q^{-1} \quad (1.7)$$

where $\Lambda$ is a diagonal matrix with the eigenvalues of $L$ as its entries, and $Q$ is an orthogonal matrix with the eigenvectors of $L$ as its columns. We make
use of a few standard observations. First, 0 is always an eigenvalue of $L$ and if $G$ is connected, then 0 has multiplicity 1. The eigenvector associated to 0 has the form $(1, 1, \ldots, 1)'$. Second, all non-zero eigenvalues of $L$ are strictly negative. These will be denoted $\{-\lambda_k\}$ with $k = 1, \ldots, N - 1$.

One may work with the system (1.6) by taking a discrete Fourier transform, however we will use the eigendecomposition (1.7) to define the so-called normal modes: $z := Q^{-1}x$. We readily see that these modes satisfy a non-interacting system of SDEs,

$$dz(t) = \Lambda z(t)dt + \sigma dB(t)$$  \hfill (1.8)$$

where $B = Q^{-1}W$. Since $Q$ is a orthogonal, the rows of $Q^{-1}$ form an orthonormal family of vectors and it follows that $B$ is a vector of independent standard Brownian motions.

We observe that the mode $z_0$, associated to the eigenvalue 0, is simply a standard Brownian motion. Recalling that the form of the eigenvector associated with the eigenvalue 0 is $(1, 1, 1, \ldots, 1)'$, it immediately follows that the “center of mass” of the bead-spring network $\bar{x}(t) := \frac{1}{N} \sum_{n=1}^{N} x_n(t) = \frac{1}{N} z_0(t)$ is also a standard Brownian motion with diffusion coefficient $\sigma/\sqrt{N}$.

However, we will see that individual particles are sub-diffusive processes with an exponent that depends on the details of the network. We transform back into real coordinates by multiplying (1.8) on the left by $Q$. This recovers the $\SigmaOU$ process form of each particle:

$$x_n(t) = \frac{\sigma}{\sqrt{N}} B_0(t) + \sum_{k=1}^{N-1} q_{k+1,n+1} z_k(t)$$  \hfill (1.9)$$

where the coefficients $\{q_{kn}\}_{k,n \leq N}$ are the entries of $Q$ and the $\{z_k\}_{k \leq N-1}$ are defined by the system of SDEs

$$dz_k(t) = -\lambda_k z_k(t)dt + \sigma dB_k(t).$$  \hfill (1.10)$$

1.3 Touchstone example: the Rouse chain

We may now discuss the Rouse chain model in the context of $\SigmaOU$ processes. The graph $G_R$ associated with this model consists of edges $x_n \leftrightarrow x_{n+1}$ for all $n = 1, \ldots, N$, each with spring constant $\kappa$. We also include the edge $x_1 \leftrightarrow x_N$ so that the particles in the system are exchangeable. This yields the system of SDEs

$$dx_n(t) = \kappa[x_{n-1}(t) - x_n(t)] + \kappa[x_{n+1}(t) - x_n(t)]dt + \sigma dW_n(t),$$  \hfill (1.11)$$
which can be summarized by the vector equation
\[
\dot{x}(t) = \kappa L x(t) + \sigma dW(t)
\]
where \(L\) is the tridiagonal matrix
\[
L = \begin{pmatrix}
-2 & 1 & 0 & 0 & 0 & \ldots & 0 & 0 & 1 \\
1 & -2 & 1 & 0 & 0 & \ldots & 0 & 0 & 0 \\
0 & 1 & -2 & 1 & 0 & \ldots & 0 & 0 & 0 \\
& & \vdots \\
0 & 0 & 0 & 0 & 0 & \ldots & 1 & -2 & 1 \\
1 & 0 & 0 & 0 & 0 & \ldots & 0 & 1 & -2
\end{pmatrix}
\]
The eigenvalues of the matrix \(L\) are given by
\[
-\lambda_k = -4 \sin^2 \left( \frac{k\pi}{N} \right).
\]
for \(k = 0, \ldots, N - 1\) (see Section 3.4). The fact that the eigenvalues are selected from what we shall call a spectral shape function
\[
\varphi(x) = 4 \sin^2 (\pi x)
\]
is an essential feature to all the models studied in this paper (see Assumption 1 in Section 2).

The well known observation \[11, 12, 13\] that distinguished particles in Rouse chains are sub-diffusive with exponent \(\nu = \frac{1}{2}\) follows from noting that for small values of \(x\), the shape function \(\varphi(x)\) behaves essentially like \(x^2\), a notion that is generalized by Assumption 2. Then one can apply Laplace’s method to the MSD to determine the asymptotic behavior, see proof of Theorem 2.1.

2 Sums of Ornstein-Uhlenbeck processes

Define the family of processes
\[
x_N(t) = c_{0,N} B_{0,N} + \sum_{k=1}^{N-1} c_{k,N} z_{k,N}(t) \tag{2.12}
\]
where for each \((k, N)\) the Ornstein-Uhlenbeck processes \(\{z_{k,N}\}_{k=1}^{N-1}\) satisfy the SDEs
\[
dz_{k,N}(t) = -\lambda_{k,N} z_{k,N}(t) dt + dB_{k,N}(t). \tag{2.13}
\]
Dependence on $N$ will be suppressed wherever there is no chance of ambiguity.

Our focus will be on systems, such as the Rouse model, for which the diffusive spectrum can be analyzed asymptotically in $N$. The eigenvalues of the Laplacian matrix associated to the Rouse connection graph $G_R$ converged to the continuous shape function $4 \sin^2(\pi x)$ and we generalize the notion as follows.

**Assumption 1** (Diffusive spectrum shape function). There exists a non-negative continuous function $\varphi \in L_1([0,1])$, that is strictly positive for all $x \in (0,1)$ with $\varphi(0) = 0$ such that

$$
\lim_{N \to \infty} \sup_{k \in \{1, \ldots, N-1\}} \left\{ \left| \lambda_{k,N} - \varphi\left(\frac{k}{N}\right) \right| \right\} = 0
$$

Continuity of $\varphi$ along with the specification of the value $\varphi(0) = 0$ assures that the longest relaxation time $\tau_N$, which is the inverse of the smallest spectral value, tends to infinity with $N$. As is mentioned in the Discussion section at the end of this paper, there are natural generalizations such as subdiffusion in a quadratic potential where this will not be the case.

We will see that the behavior of the shape function near zero determines the most important qualitative dynamics of ΣOU processes.

**Assumption 2** (Spectral parameter $\rho$). The shape function $\varphi$ has a Frobenius expansion [19]

$$
\varphi(x) \sim x^\rho \sum_{n=0}^\infty a_n x^n \quad \text{for small } x
$$

for some $\rho > 0$ in the sense that for each fixed $N$,

$$
\lim_{x \to 0} x^{-N} \left( \varphi(t) - x^\rho \sum_{n=0}^N a_n x^n \right) = 0.
$$

We will see (Proposition 2.2) that the effect of perturbations to the coefficient family is subdominant to the shape of the diffusive spectrum. In applications of interest this happens due to averaging of the coefficients, which we may characterize in terms of weak convergence of measures. Define for $x \in [0, 1]$ the sequence of coefficient measures,

$$
\mu_N(dx) := \sum_{k=0}^{N-1} \delta \left( x - \frac{k}{N} \right) c_{k,N}^2
$$

(2.14)

where $\delta(x)$ is the Dirac $\delta$-distribution.
Assumption 3 (Convergence of coefficients). There exists a nonnegative finite Radon measure $\mu$ on the interval $[0,1]$ such that $\mu_N \to \mu$ weakly.

At this point, we make a note about initial conditions. The anomalous behavior in the limiting process is actually the infinite extension of the transient dynamics of the finite $N$ processes. In order for the sequence of processes $\{x_N(t)\}$ to be tight, it must be true that the sequence of initial conditions $\{x_N(0)\}$ must also be tight. It is natural to choose $x_N(0) = 0$ for all $N$, but we will further simplify by choosing vanishing initial condition for each of the OU processes: $z_{k,N}(0) = 0$. We note that in most relevant cases it is not appropriate to simply choose each $z_{k,N}$ from its respective stationary distribution. With such a choice, as $N \to \infty$ the sum of samples from stationary distributions will not converge.

2.1 Asymptotic behavior of $\Sigma$OU processes

We seek to relate the structure of the shape function near zero to the asymptotic anomalous diffusive exponent of an $\Sigma$OU process. As mentioned in the Introduction, for any fixed, finite $N$, it is expected that the MSD profile will have the form $1/\nu/1$ over the three timescale regimes. Before stating a rigorous description of the dynamics in Theorem 2.1, we include some intuitive discussion.

The short-timescale diffusive regime has both a mathematical and a physical interpretation. The mathematical intuition is that Ornstein-Uhlenbeck processes are locally like Brownian motions. Therefore for $t \leq \tau_1 := \lambda_{\text{max}}^{-1}$, the process $x_N(t)$ is essentially a finite sum of Brownian motions. Physically, in the context of distinguished particle dynamics, the initial diffusive regime results from the fact that for a short period the beads are able to diffuse independent of the constraints from the network.

To explain the diffusive behavior on the largest timescale, we first note that the sum $\sum_{k=1}^{N-1} c_k z_k$ converges to a stationary distribution which is normal with mean zero and variance $\sum_{k=1}^{N-1} c_k^2/(2\lambda_k)$. The timescale of the approach to stationarity is dictated by the longest relaxation time $\tau_N = \lambda_{\text{min}}^{-1}$. For $t > \tau_N$, the process $x_N(t)$ is a Brownian motion plus a stationary correction and so the MSD must satisfy $\lim_{t \to \infty} \mathbb{E}[x_N^2(t)]/t = c_0^2$.

We cannot analyze the intermediate regime exactly, but suppose that Assumption 2 holds for $\rho > 0$. Then $\lambda_{\text{min}}$ will be roughly $(k/N)^\rho$, which means that the longest relaxation time $\tau_N = N^\rho$ approaches infinity as $N$ increases. As a result, the anomalous stage of the diffusion is increasingly prolonged, and is infinite in extent in the large $N$ limit. In Theorem 2.1 we
show that this limit exists and in the course of the proof demonstrate that the MSD of the \(x_N(t)\) processes converge uniformly on compact sets. By performing an asymptotic analysis on the limiting process we discover the anomalous exponent and from the uniform convergence of the MSDs, we see that this is indeed the anomalous exponent seen in the intermediate phase of the finite \(N\) processes.

We are ready to state the main theorem for \(\Sigma\Omega\) processes. For the large-\(t\) asymptotic statements, we say that \(f(t) \sim t^\nu\) if \(\lim_{t \to \infty} f(t)/t^\nu = C\) for some nonnegative constant \(C\).

**Theorem 2.1.** Let the sets of processes \(\{x_N(t)\}\) and \(\{z_{k,N}(t)\}\) be defined by (2.12) and (2.13), respectively. Take \(z_{k,N}(0) = 0\) for all \(k\) and \(N\). Suppose that the diffusive spectrum \(\{\lambda_{k,N}\}\) converges to a shape function \(\varphi\) in the sense of Assumption 1. Furthermore, suppose the coefficients \(\{c_{k,N}\}\) satisfy Assumption 3 with limiting weight measure \(\mu\).

Then the family \(\{x_N(t)\}\) converges in distribution as \(N \to \infty\) to a mean zero Gaussian process \(x(t)\) defined by its auto-correlation function

\[
\mathbb{E}[x(t)x(s)] = \int_{0}^{1} \frac{e^{-\varphi(x)|t-s|}}{2\varphi(x)} \left(1 - e^{-2\varphi(x)(t\wedge s)}\right) \mu(dx). \tag{2.15}
\]

If the shape function \(\varphi\) furthermore satisfies Assumption 2 with spectral parameter \(\rho > 0\) and the limiting weight measure \(\mu\) is Lebesgue measure, then asymptotically, the limiting MSD function \(\sigma(t) := \mathbb{E}[x^2(t)]\) satisfies

\[
\sigma(t) \sim t, \quad t \text{ near zero.}
\]

and

\[
\sigma(t) \sim \begin{cases} 
  t^{1-\frac{1}{\rho}} & \rho > 1 \\
  \ln t & \rho = 1 \\
  1 & 0 < \rho \leq 1 
\end{cases} \tag{2.16}
\]

**Remark 2.1.** It is important to note that the limits with respect to \(N\) and \(t\) implicit in (2.16) are not interchangeable. For any finite \(N\), \(\mathbb{E}[x_N^2(t)] \sim t\) for large \(t\) because the Brownian term eventually dominates the dynamics. In the absence of the Brownian term \((c_{0,N} = 0)\), the process \(x_N(t)\) is positive recurrent.

**Proof.** Convergence in distribution follows from establishing two standard facts [20]: convergence of the finite-dimensional distributions, and tightness in the space \(C([0,T])\) of the family of processes \(\{x_N\}\) for any \(T > 0\). Since
each of the processes in this sequence is Gaussian, convergence of finite-dimensional distributions follows from pointwise convergence of the ACFs, 

\[ \sigma_N(t,s) := \mathbb{E}[x_N(t)x_N(s)]. \]

In order to establish tightness we will use the Kolmogorov criterion (2.18). Subsequently, the asymptotic analysis reduces to an application of Laplace’s method [19].

**Convergence of the finite-dimensional distributions:** We compute the ACF for \( x_N \). The explicit solution of the respective OU processes is given by

\[ z_k(t) = e^{-\alpha_k t}z_k(0) + \int_0^t e^{-\lambda_k (t-t')} dW_k(t') \]

where we have suppressed the dependence of the coefficients \( \{c_k\} \) and diffusive spectrum \( \{\lambda_k\} \) on \( N \). Since the modes are assumed to be independent with vanishing initial conditions, we see that for \( s, t > 0 \),

\[ \mathbb{E}[z_k(t)z_j(s)] = \delta_{kj} \frac{1}{2\lambda_k} e^{-\lambda_k |t-s|} \left( 1 - e^{-2\lambda_k (t\wedge s)} \right). \]

where \( \delta_{kj} \) is the Kronecker delta-function. Observing that cross-terms disappear and including the leading term \( \mathbb{E}[B_0(t)B_0(s)] = t \wedge s \), yields

\[ \sigma_N(t,s) = \epsilon_0^2 (t \wedge s) + \sum_{k=1}^{N-1} \frac{c_k^2}{2\lambda_k} e^{-\lambda_k |t-s|} \left( 1 - e^{-2\lambda_k (t\wedge s)} \right). \] (2.17)

In light of the assumption that \( \varphi(0) = 0 \), the above can be rewritten in terms of the coefficient measures defined in Assumption 3

\[ \sigma_N(t,s) = \int_0^1 \frac{e^{-\varphi(x)|t-s|}}{2\varphi(x)} \left( 1 - e^{-2\varphi(x)(t\wedge s)} \right) \mu_N(dx). \]

Note that the integrand is continuous for all \( x \in (0,1] \) and can be extended analytically to include \( x = 0 \) for each choice of \( t \) and \( s \). The integrand is bounded above by \( t \wedge s \) and therefore the weak convergence of the measures \( \mu_N \) implies the limiting expression (2.15).

**Tightness:** As mentioned, tightness of the family of processes \( \{x_N\} \) in \( C([0,T]) \) is implied by the Kolmogorov criterion: given \( T > 0 \), there exists an \( N_0 \in \mathbb{N} \) and strictly positive constants \( \alpha, \beta \) and \( C \) such that

\[ \sup_{N \geq N_0} \mathbb{E}[|x_N(t) - x_N(s)|^\alpha] \leq C |t - s|^{1+\beta} \] (2.18)

for all \( s, t \in [0,T] \).
From (2.17), we compute

$$E[(z_k(t) - z_k(s))(z_j(t) - z_j(s))] = \delta_{jk} \frac{1}{2\lambda_k}(2 - e^{-2\lambda_k(t\wedge s)})(1 - e^{-2\lambda_k|t-s|}),$$

while $E[(B_0(t) - B_0(s))^2] = |t-s|$. Cross-terms vanish and we find

$$E[(x_N(t) - x_N(s))^2] = c_0^2|t-s| + \sum_{k=1}^{N-1} \frac{c_k^2}{2\lambda_k}(2 - e^{-2\lambda_k(t\wedge s)})(1 - e^{-2\lambda_k|t-s|})$$

$$\leq c_0^2|t-s| + \sum_{k=1}^{N-1} \frac{c_k^2}{\lambda_k}(1 - e^{-2\lambda_k|t-s|})$$

$$\leq \left(2 \sum_{k=0}^{N-1} c_k^2\right)|t-s|$$

In the last line we applied the naive estimate $(1 - e^{\lambda t}) \leq \lambda t$ to each term of the sum. The sum appearing in the last line is exactly $\sum_{k=0}^{N-1} \delta(x - \frac{k}{N}) = \mu_N([0,1])$. By Assumption $\mu_N \to \mu$ weakly and by an equivalent statement we have

$$\limsup_{N \to \infty} \mu_N([0,1]) \leq \mu([0,1]).$$

As such, there exists an $N_0$ such that for all $N \geq N_0$, $\mu_N([0,1]) \leq 1 + \mu([0,1])$. Therefore, for all $N \geq N_0$,

$$E[(x_N(t) - x_N(s))^2] \leq (1 + \mu([0,1]))|t-s|.$$  

Finally, noting that $x_N(t) - x_N(s)$ is Gaussian, we see that

$$\sup_{N \geq N_0} E[(x_N(t) - x_N(s))^4] \leq 3(1 + \mu([0,1]))^2|t-s|^2,$$  

which confirms (2.18).

**Asymptotic analysis:** We now consider the large-$t$ asymptotic behavior of the limiting MSD function $\sigma(t) := E[x^2(t)]$ in the presence of Assumption $\mu_N$ with shape parameter $\rho$. First we observe that for a given constant $\lambda$

$$\lambda^{-1}(1 - e^{-\lambda t}) = \int_0^t e^{-\lambda s}ds.$$  

Applying this identity to the integrand in (2.17) and subsequently using Fubini’s Theorem to interchange the integrals yields

$$\sigma(t) = \int_0^t \int_0^1 e^{-2\rho(x)s} \mu(dx)ds.$$  

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Recalling our assumption that $\mu$ is simply Lebesgue measure, we write

$$\sigma(t) = \int_0^t \Phi(s) ds$$

where $\Phi(s)$ is the Laplace integral $\Phi(s) := \int_0^1 e^{-2\varphi(x)s} dx$.

Because $\varphi(x)$ is continuous (by Assumption 1) and therefore bounded, it follows that $\Phi(s)$ is also continuous. By the Fundamental Theorem of Calculus,

$$\lim_{t \to 0} \frac{1}{t} \int_0^t \Phi(s) ds = \Phi(0) = 1.$$  

This limit is finite and nonzero, which directly implies that near zero $\sigma(t) \sim t$.

In order to characterize large-$t$ behavior, we note that the minimum value of $\varphi(x)$ is assumed to be at $x = 0$ and therefore the only significant contribution to the large $s$ asymptotics will be in a small neighborhood near zero. Following [19], for example, we have

$$\int_0^1 e^{-\varphi(x)s} dx \sim \int_0^{\infty} e^{-x^\rho s} dx = s^{-\frac{1}{\rho}} \Gamma\left(\frac{1}{\rho}\right)$$

where in the last equality we applied the substitution $y = x^\rho s$ and $\Gamma$ is the Gamma function $\Gamma(z) := \int_0^{\infty} y^{z-1} e^{-y} dz$. Integrating this asymptotic expression while minding the various ranges of values of $\rho$ yields (2.16).

By generalizing (2.19) to higher and higher moments, one can show that the limiting process $x(t)$ is $\alpha$-Hölder continuous for any $\alpha \in (0, 1/2)$. This reinforces the notion that the limiting process is locally like Brownian motion, but asymptotically like fractional Brownian motion.

### 2.1.1 Robustness of the anomalous exponent with respect to perturbing the coefficients

As noted in [19], if one were interested in conducting statistical inference on a set of data, trying to fit to an ΣOU process, it would be a prohibitive task to fit the tens of thousands of coefficients. And Assumption 3 and the calculation for the ACF of distinguished particles processes (see proof of Theorem 3.1) can leave the false impression that the ability to calculate the anomalous exponent $\nu$ is restricted to special, delicately balanced coefficient families. In fact, the result is more robust than this. We demonstrate
this phenomenon with the following proposition which presumes random coefficients.

In what follows there are two senses of averaging. There is the probability space we use to select the coefficient family and for a fixed coefficient family, there is the probability space associated with the family of Brownian motions that drive the dynamics. We will use $E^c$ and $\text{Var}^c$ to denote the average and variance with respect to the coefficient probability space. and will continue to use $E$ and $\text{Var}$ to denote averages and variances with respect to instances of the Brownian motions.

**Proposition 2.2.** Suppose the triangular array of coefficients $\{c_{k,N}\}_{k \leq N}$ are independent random variables of the form $c_{k,N} = c/\sqrt{N}$ where $c$ is a random variable with a finite fourth moment. Then the associated coefficient measures $\{\mu_N\}_{N=1}^\infty$ converge weakly to $E[c^2]$ times Lebesgue measure almost surely.

Furthermore, the conclusions of Theorem 2.1 apply to the limiting process, $x(t)$.

**Proof.** The result follows from the Strong Law of Large Numbers.

Let $f : [0, 1] \to \mathbb{R}$ be a continuous function on $(0, 1)$ and denote $m_n := E^c[\epsilon^n]$, for $n = \{1, 2, 3, 4\}$. We also recall the definition of the coefficient measures $\mu_N$ from Assumption 3. Then the random variables

$$I_N := \int_0^1 f(x) \mu_N(dx) = \sum_{k=1}^{N-1} f\left(\frac{k}{N}\right) c_{k,N}^2$$

have mean $E^c[I_N] = m_2 \sum_{k=0}^{N-1} f\left(\frac{k}{N}\right) \frac{1}{N}$ and variance

$$\text{Var}^c(I_N) = E^c\left[\left(\sum_{k=1}^{N-1} f\left(\frac{k}{N}\right) (c_{k,N}^2 - \frac{m_2}{N})\right)^2\right]$$

$$= \sum_{k=1}^{N-1} f^2\left(\frac{k}{N}\right) E^c\left[(c_{k,N}^2 - \frac{m_2}{N})^2\right]$$

$$= \sum_{k=1}^{N-1} f^2\left(\frac{k}{N}\right) \left(m_4 - \frac{m_2^2}{N^2}\right) \frac{1}{N^2}$$

For the second equality, we note that cross-terms of the sum vanish due to independence of the coefficients. It remains to recognize the Riemann
approximation $\sum_{k=0}^{N-1} f^2(k/N)1/N = \int_0^1 f^2(x)dx + O(1/N)$, which implies that
\[
\text{Var}^c(I_N) = (m_4 - m_2^2) \frac{1}{N} \left( \int_0^1 f^2(x)dx + O(1/N) \right),
\]
which tends to 0 as $N \to \infty$. Therefore the sequence of random variables $I_N$ converges almost surely and we conclude that, in the language of Assumption 3, the coefficient measures $\mu_N$ converge to $m_2$ times Lebesgue measure almost surely.

\section{Anomalous diffusion of distinguished particles in bead-spring networks}

\subsection{General framework and main theorem}

When considering the large $N$ scaling limit of bead-spring systems, there are two distinct constructions. In the polymer physics community \cite{11,13}, it is typical to simply add a new bead to the bead-spring loop while keeping the spring constants the same. In mathematical developments, (see \cite{21} for example), it is typical to also increase the spring forces while rescaling magnitude of the noise in order to develop a continuum limit of the full bead-spring system. This is the so-called “random string” model.

While the distinguished particle limit exists in both cases, there is a marked qualitative difference in the behavior of the limiting process. In the physics development, the limiting process is of the type described in the preceding section: locally like a Brownian motion, but globally sub-diffusive. In contrast, the limiting distinguished particle process in the “random string” development is sub-diffusive on the shortest time scales and approaches a stationary distribution. As is further discussed in Section 3.6 the effect of “bringing the anomalous diffusion to the local scale” is that the resulting process is locally rougher than Brownian motion, having infinite quadratic variation, but finite quartic variation \cite{22}. Our focus is not on this development however, because we are interesting in processes which exhibit anomalous diffusion over arbitrarily large time scales. One may be concerned that the full chain does not have a limit in the polymer physics construction, but such a limit is not our goal. Rather, we proceed with the knowledge that there are a finite but large number of beads in the relevant physical systems and although there is no convergence of the full chain structure, there is \textit{convergence of the effect of the chain} on the distinguished particles.
Convergence of diffusive spectrum is sufficient for convergence in distribution of a family of ΣOU processes. We now argue the same principle holds for distinguished particle processes. The central insight is that the diffusive spectrum in this setting is given by the eigenvalues of the Laplacian matrix associated with the weighted connection graph $G$. A well-established characterization of stability of a family of graphs is convergence of the eigenvalues to some shape function, as seen for the Rouse chain model in Section 1.3.

The only technical detail is that the coefficient structure of the distinguished particle processes defined in Section 1.2 by Equations (1.9) and (1.10) may not precisely satisfy Assumption 3 on the coefficient family. However, after computing the ACF of the distinguished particle process, we see that it is equivalent in law to an effective ΣOU process to which Theorem 2.1 does apply.

**Theorem 3.1.** Let $\{G_N\}_{N \in \mathbb{N}}$ be a sequence of graphs, each having $N$ vertices respectively, with edge weight sets $\{E_N\}_{N \in \mathbb{N}}$ such that the triangular family $\{\lambda_{k,N}\}_{k \leq N}$ of eigenvalues of the associated Laplacian matrices $L_N$ satisfy Assumption 1. Furthermore, suppose that the graphs are constructed in such a way that the individual particle processes are exchangeable.

Then the conclusions of Theorem 2.1 hold for the family of processes $\{x_{i,N}(t)\}_{N \in \mathbb{N}}$ defined by (2.12) and (2.13).

**Proof.** Following the notation of Section 1.2 and suppressing dependence on $N$, the path of the $n$-th particle in the system is given by

$$x_n(t) = \frac{1}{\sqrt{N}}B_0(t) + \sum_{k=0}^{N-1} q_{n+1,k+1}z_k$$

where the family of OU-processes $\{z_{k,N}\}_{k=1}^{N-1}$ are defined by equation (2.13). The coefficients $\{q_{nk}\}_{k=1}^{N}$ are the $n$-th row of entries of the matrix $Q$, which we recall is the orthogonal matrix whose columns are the normalized eigenvectors of the Laplacian matrix $L_N$.

Because the particles are exchangeable,

$$\mathbb{E}[x_n(t)x_n(s)] = \frac{1}{N}\mathbb{E}[\mathbf{x}(t) \cdot \mathbf{x}(s)]$$

where $\mathbf{x}(t) = (x_1(t), \ldots, x_N(t))^\prime$ denotes the full vector of all $N$ particles in the system. Its dynamics are defined by the vector SDE (1.6) and the exact solution is given by Duhamel’s formula

$$\mathbf{x}(t) = \sigma e^{Lt}\mathbf{x}(0) + \sigma \int_0^t e^{L(t-s)}d\mathbf{W}(s)$$
Again, we recall the assumption that \( x(0) = 0 \).

In order to calculate the autocorrelation \( \mathbb{E}[x(t) \cdot x(s)] \), we observe:

\[
\mathbb{E} \left( \int_0^t e^{L(t-t')} d\mathbf{W}(t') \right) \cdot \left( \int_0^s e^{L(s-s')} d\mathbf{W}(s') \right)
\]

\[
= \mathbb{E} \sum_{k=1}^N \left( \int_0^t e^{L(t-t')} d\mathbf{W}(t') \right)_k \left( \int_0^s e^{L(s-s')} d\mathbf{W}(s') \right)_k
\]

\[
= \mathbb{E} \sum_{k=1}^N \left( \sum_{i=1}^N \int_0^t \left( e^{L(t-t')} \right)_{ki} dW_i(t') \right) \left( \sum_{j=0}^N \int_0^s \left( e^{L(s-s')} \right)_{kj} dW_j(s') \right)
\]

\[
= \sum_{k=1}^N \sum_{i=1}^N \sum_{j=1}^N \delta_{ij} \int_0^{t \wedge s} \left( e^{L(t-r)} \right)_{ki} \left( e^{L(s-r)} \right)_{kj} dr
\]

\[
= \int_0^{t \wedge s} \sum_{k=1}^N \sum_{j=1}^N \left( e^{L(t+s-2r)} \right)_{kj} dr
\]

\[
= \int_0^{t \wedge s} \| e^{L(t+s-2r)} \|_F^2 dr.
\]

In the last line we have used the Frobenius norm: \( \| A \|_F := \sum_{k=1}^N \sum_{j=1}^N a_{kj}^2 = \sum_k \lambda_k^2 \) where \( \{ \lambda_k \} \) is the set of eigenvalues of \( A \).

To complete the calculation above, we note that \( e^{Lt} \) is similar to \( e^{\Lambda t} \), where \( \Lambda \) is the diagonal matrix from (1.7) whose entries are the eigenvalues of \( L \). Therefore the eigenvalues of \( e^{Lt} \) are exactly the entries \( e^{\Lambda t} \), namely the set \( \{ e^{-\lambda_k t} \}_{k=0}^{N-1} \). Imposing the assumption that \( x(0) = 0 \), this implies

\[
\mathbb{E}[x(t) \cdot x(s)] = \sigma^2 \int_0^{t \wedge s} \sum_{k=0}^N e^{-\lambda_k (t+s-2r)} dr. \tag{3.21}
\]

Rearranging terms, we see that for each \( n \), the distinguished particle \( x_n \) is a mean-zero Gaussian process with ACF of the form found in Equation 2.17 with the coefficients identically set to \( c_{k,N} = \sigma / \sqrt{N} \). In this way, we see that the distinguished particle processes indexed by \( N \) are equivalent in law to a family effective ΣOU analogues \( \tilde{x}_N(t) \) defined by

\[
\tilde{x}_N(t) = \frac{\sigma}{\sqrt{N} + 1} \left( B_0(t) + \sum_{k=1}^N \tilde{z}_{k,N}(t) \right)
\]

where

\[
d\tilde{z}_{k,N}(t) = -\lambda_{k,N} \tilde{z}_{k,N}(t) dt + dB_{k,N}(t).
\]
The coefficient measures $\mu_N$, defined by (2.14), converge weakly to Lebesgue measure and the asymptotic conclusions of Theorem 2.1 apply to $\tilde{x}_N$ directly and therefore to the distinguished particle process by corollary.

3.1.1 Examples

We see from the argument above that, after collecting terms appropriately, the coefficient family $\{c_{k,N}\}$ of the effective distinguished particle process $\tilde{x}_N(t)$ is given by the respective multiplicities of the eigenvalue family $\{\lambda_{k,N}\}$. Whereas the coefficient measures in the Rouse model and its generalizations (Section 3.2) will all converge to Lebesgue measure, we take a moment discuss two examples where this is not the case.

Let $K_N$ denote a complete graph on $N$ vertices. Then there are only two eigenvalues: 0, which has multiplicity 1, and $N/(N-1)$ which has multiplicity $N-1$ [23]. The distinguished particle process associated to each $K_N$ is equivalent to an effective $\Sigma$OU process

$$\tilde{x}_N(t) = \frac{1}{\sqrt{N}} B_0(t) + \frac{\sqrt{N}}{N-1} \tilde{z}_N(t)$$

where

$$d\tilde{z}_N(t) = -\frac{N}{N-1} \tilde{z}_N(t) + dB_N(t).$$

The coefficient measures converge to the Dirac-$\delta$ distribution centered at $x = 1$. Recalling $x(0) = 0$, we see that the limiting MSD is given by $E[x^2(t)] = 1 - e^{-t}$, i.e. a one-dimensional OU process.

The same asymptotic behavior is observed from a system with a non-trivial coefficient family structure. An $N$-hypercube on $2^N$ vertices has eigenvalues of the form $\frac{2k}{N}$, with respective multiplicities $\left(\begin{array}{c} N \\ k \end{array}\right)$ [23]. By the de Moivre-Laplace Theorem we have the following large-$N$ characterization of the coefficients,

$$c_{k,N} = \left(\begin{array}{c} N \\ k \end{array}\right) \frac{1}{2^N} \approx \sqrt{\frac{2}{\pi N}} e^{-2N\left(\frac{k}{N} - \frac{1}{2}\right)^2}.$$

Rewriting the associated coefficients reveals a sequence of approximate Dirac-$\delta$ functions centered at $x = \frac{1}{2}$,

$$\mu_N(dx) \approx \sqrt{\frac{2}{\pi N}} \sum_{k=1}^{N} \delta^N(x) \frac{1}{N}$$

where $\delta^N(x) = \sqrt{N} e^{-2N\left(\frac{k}{N} - \frac{1}{2}\right)^2}$. 

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Since the eigenvalue shape function is $\varphi(x) = 2x$, the limiting MSD satisfies
\[ E[x^2(t)] = \int_0^t \int_0^1 e^{-2xs} \delta(x - \frac{1}{2}) dx ds = 1 - e^{-t}. \]

### 3.1.2 Higher-dimensional diffusions

The assumption that the particles are diffusing in one-dimensional space is not essential. Much like for standard Brownian motion, the dimension of the diffusion only has an effect on the ACF by a multiplicative constant. The exponent of the diffusion is unchanged and this principle holds for distinguished particle processes.

Consider the family $x(t) = \{x_1(t), x_2(t), \ldots, x_N(t)\}$, where for $i = 1, \ldots, N$, the particles have the form $x_i = (x_1^{i}, x_2^{i}, \ldots, x_d^{i})'$ where $d$ is the dimension of the space in which the particles are moving. The system-wide configuration potential is given by
\[ \Psi(x) = \frac{1}{2} \sum_{n \neq m} \kappa_{nm} |x_n - x_m|^2. \]

In this case the interactions decouple in the various components of the diffusion. The SDE for the $\alpha$-component of the $n$-th bead is given by
\[ dx_n^{\alpha} = \sum_{m \neq n} \sum_{\beta=1}^{d} \delta_{\alpha\beta} \kappa_{nm} (x_m^{\beta}(t) - x_n^{\alpha}(t)) dt + \sigma dW_n^{\alpha}(t) \]
where $\delta_{\alpha\beta}$ is the Kronecker $\delta$-function. We see that each component conducts its own diffusion independent of the other components and conclude that, assuming vanishing initial conditions as usual,
\[ E[x_n(t) \cdot x_n(s)] = \frac{\sigma^2 d}{N} \int_0^{t \wedge s} \sum_{k=1}^{N} e^{-2\lambda_k(t+s-2r)} dr \]
which is simply $d$ times the autocorrelation for one-dimensional distinguished particles, as in (3.21). In contrast to this observation, the dimension of the underlying connection graph does have significant effect, which we investigate in Section 3.3.

### 3.2 The Rouse polymer model

We return to the touchstone example from Section 1.3, the Rouse chain model. We recall that the connection graph $\mathcal{G}_R$ consists of edges $x_n \leftrightarrow x_{n+1}$
for all $n = \{0, \ldots N - 1\}$ as well as the edge $x_0 \leftrightarrow x_n$. This yields the system of SDEs

$$dx_n(t) = \kappa [x_{n-1}(t) - x_n(t)] + \kappa [x_{n+1}(t) - x_n(t)] + \sigma dW_n(t)$$

and the diffusive spectrum is given by $\lambda_{k,N} := 4 \sin^2\left(\frac{k\pi}{N}\right)$. In terms of Assumption \(\square\) the spectral shape function is

$$\varphi(x) = 4 \sin^2(\pi x)$$

with $x \in [0, 1)$. Using the Taylor expansion for $\sin(x)$, we see that this shape function essentially satisfies Assumption \(\square\) with shape parameter $\rho = 2$. (The only sense in which it does not satisfy the parameter assumption is that it is not strictly increasing on the full interval $[0, 1)$. However, this is easily overcome by restricting to the interval $[0, 1/2]$, and multiplying the MSD by two.)

By Theorem 3.1 the family of distinguished processes $x_{0,N}(t)$ are tight and the limiting process $x(t)$ has the MSD

$$E[x^2(t)] = 2\sigma^2 \int_0^t \int_0^t e^{-4\kappa \sin^2(\pi s)x} dx ds$$

(3.22)

It follows from the conclusions of Theorem 2.1 that the anomalous exponent is $\nu = 1/2$. For an explicit development of the above Laplace integral, including the order of the correction terms, Eq. 3.22 is happens to be a worked example in [19], Chapter 6.

### 3.3 Higher-dimensional Rouse analogues

While we showed in Section 3.1.2 that large-$t$ anomalous exponents do not depend on the dimension of the space in which the particles reside, we now observe that behavior does change if the bead-spring network has a higher dimensional connection graph. We employ a standard technique from graph theory of constructing complex graphs from simple ones [24].

The Cartesian product of two graphs $G_1$ and $G_2$, which have vertices $\{v_i\}_{i=1}^N$ and $\{w_j\}_{j=1}^M$, respectively, consists of vertices enumerated by the set of pairs $\{(v_i, w_j)\}$. There is an edge $(v_i, w_j) \leftrightarrow (v_k, w_\ell)$ if and only if either $v_i = v_k$ and $G_2$ contains the edge $w_j \leftrightarrow w_\ell$, or $w_j = w_\ell$ and $G_1$ contains the edge $v_i \leftrightarrow v_k$. When applied to a cycle graph such as the Rouse graph $G_R$ to itself, the Cartesian product yields the skeleton of a torus.

The adjacency matrix of a Cartesian product of two graphs is given by the Kronecker sum of their respective adjacency matrices $A_1 \oplus A_2$. If $G_1$
is a graph with $N$ vertices and $G_2$ has $M$ vertices, this sum is defined by $A_1 \oplus A_2 := A_1 \otimes I_M + I_N \otimes A_2$, where the Kronecker product $A \otimes B$ is a block matrix whose blocks are of the form $a_{ij}B$. The resulting Kronecker sum matrix has dimension $NM \times NM$. The only fact we will use here is that the set of eigenvalues of the Laplacian matrix associated to the Kronecker sum is given by the set \[ \alpha_{ij} = \{ \lambda_i + \mu_j : i \in 1 \ldots, N, j \in 1 \ldots, M \}. \]

where $\{\lambda_i\}$ and $\{\mu_j\}$ are the eigenvalues of the Laplace matrices for $G_1$ and $G_2$, respectively.

Denoting the $N$-bead Rouse eigenvalues by $\{\lambda_{j,N}\}$, the MSD of a distinguished particle in an $N \times N$ system is computed to be

$$E[x_N(t)^2] = \frac{1}{N^2} \int_0^t \sum_{i,j} e^{-\kappa(\lambda_{i,N} + \lambda_{j,N})s} ds$$

which converges as $N \to \infty$ to the integral

$$E[x(t)^2] = \int_0^t \int_0^1 \int_0^1 e^{-4\kappa(\sin^2(\pi x) + \sin^2(\pi y))s} dxdyds.$$ \hspace{1cm} (3.23)

The family of distinguished particles converges in distribution in the sense of Theorem 3.1 and it remains only to perform the Laplace integral asymptotic analysis on (3.23).

As before, we take the leading order behavior near the $(x, y)$-origin. For large $s$, we have

$$\Phi(s) := 4 \int_0^{\frac{1}{2}} \int_0^{\frac{1}{2}} e^{-4\kappa(\sin^2(\pi x) + \sin^2(\pi y))s} dxdy$$

$$\sim 4 \int_0^{\infty} \int_0^{\infty} e^{-4\kappa\pi^2(x^2+y^2)s} dxdy$$

which after a conversion to polar coordinates yields that for $s$ large, $\Phi(s) \sim s^{-1}$. Integrating this asymptotic relation implies that for large $t$,

$$E[x(t)^2] \sim \ln(t).$$

The Kronecker sum can be iterated arbitrarily many times for higher dimensional connectivity. Denoting the number of Kronecker sums by $D$, the following properties hold:

$$A_1 \oplus A_2 \oplus \cdots \oplus A_D$$
we see that the associated $\Phi(s)$ satisfies
\[
\Phi(s) \sim 2^D \int_{\mathbb{R}_+^D} \exp \left( -4\kappa \pi^2 s \sum_{i=1}^D x_i^2 \right) dx
= C \int_0^\infty e^{-4\kappa \pi^2 s r^2} r^{D-1} dr
= Cs^{\frac{D}{2}}
\]
where we have allowed the constant $C = C(D)$ to change from line to line. After integrating to get the MSD, we see that for $D \geq 3$, the Rouse model with $D$-dimensional connectivity has MSD that is bounded for all time.

### 3.4 Universality of the Rouse exponent

Returning our focus to the 1-D chain, we address an observation [11] that the long-term behavior is universal for a class of models. Such a class is never precisely described in the physics literature, but we provide in this section one characterization.

We construct a network by starting with a Rouse chain where nearest neighbor edges $x_n \leftrightarrow x_{n+1}$ are weighted by a single spring constant $\kappa_1 \geq 0$. We generalize the model by allowing edges of the form $x_n \leftrightarrow x_{n+j}$ which are respectively given uniform weights $\kappa_j \geq 0$. The weights are assigned uniformly in the spirit of preserving exchangeability of the beads. After the appropriate edges are added at the boundaries (e.g. the edge $x_0 \leftrightarrow x_{N-1}$ with weight $\kappa_2$) the resulting Laplace matrix is a circulant matrix. For example, under the assumption that $\kappa_j = 0$ for all $j \geq 3$, we have the Laplace matrix:

\[
L = \begin{pmatrix}
\kappa_0 & \kappa_1 & \kappa_2 & 0 & \cdots & 0 & \kappa_{-2} & \kappa_{-1} \\
\kappa_{-1} & \kappa_0 & \kappa_1 & \kappa_2 & \cdots & 0 & 0 & \kappa_{-2} \\
\kappa_{-2} & \kappa_{-1} & \kappa_0 & \kappa_1 & \cdots & 0 & 0 & 0 \\
0 & \kappa_{-2} & \kappa_{-1} & \kappa_0 & \cdots & 0 & 0 & 0 \\
0 & 0 & \kappa_{-2} & \kappa_{-1} & \cdots & 0 & 0 & 0 \\
\vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\
\kappa_{-2} & 0 & 0 & 0 & \cdots & \kappa_1 & \kappa_0 & \kappa_{-1} \\
\kappa_{-1} & \kappa_{-2} & 0 & 0 & \cdots & \kappa_2 & \kappa_1 & \kappa_0
\end{pmatrix}
\] (3.24)

where $\kappa_{-j} = \kappa_j$ and $\kappa_0 = -\sum_j \kappa_j$. By convention the set of indices for the weights $\{\kappa_j\}$ will be $j \in \{-\lfloor N/2 \rfloor, \ldots, \lceil N/2 \rceil\}$. 

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Theorem 3.2 (Universality of the Rouse exponent). Let \( \{G_N\} \) be a family of graphs whose associated Laplacian matrices are circulant with weights \( \{\kappa_j\}_{j \in \mathbb{Z}} \) which satisfy \( \kappa_{-j} = \kappa_j \) for all \( j \geq 1 \) and \( \kappa_0 = \sum_{j \in \mathbb{Z}} \kappa_j \). We assume that there exists an integer \( K > 0 \), such that \( \kappa_j = 0 \) for all \( j > K \).

Then the family of distinguished particle processes \( x_N \) converges in distribution to a mean zero Gaussian process \( x \) with ACF given by (2.15) where the shape function \( \varphi \) is defined by

\[
\varphi(x) := \sum_{j=-\infty}^{\infty} e^{2\pi i x j} \kappa_j
\]  

(3.25)

Furthermore MSD the limiting process \( x \) satisfies the asymptotic relationships

\[
\mathbb{E}[x^2(t)] \sim t, \quad t \text{ near zero};
\]

\[
\mathbb{E}[x^2(t)] \sim t^{\frac{3}{2}}, \quad t \text{ large}.
\]

Proof. The eigenvalues and eigenvectors of circulant matrices can be computed directly [25]. For any given set of weights \( \{\kappa_j\} \), the associated circulant matrix has a set of eigenvalue-eigenvector pairs \( \{(\lambda_k, \mathbf{v}_k)\}_{k=0}^{N} \) given by

\[
\lambda_k := \sum_{j=-[N/2]}^{[N/2]} e^{2\pi i k j / (N+1)} \kappa_j
\]

and

\[
\mathbf{v}_k := \frac{1}{\sqrt{N+1}} \left(1, e^{2k\pi i / (N+1)}, e^{2k\pi 2i / (N+1)}, \ldots, e^{2k\pi i N / (N+1)}\right)^t.
\]

Uniform convergence of the eigenvalues to the shape function (3.25) in the sense of Assumption 1 is clear. Tightness of the associated distinguished particles processes follow as in Theorem 3.1. The near zero asymptotic behavior of the MSD is as in Theorem 2.1. It remains only to demonstrate the large-\( t \) MSD behavior.

The restrictions that \( \kappa_{-j} = \kappa_j \) and \( \kappa_0 \) is the sum of all the other weights implies that

\[
\varphi(x) = \sum_{j=-K}^{K} e^{2\pi i x j} \kappa_j = \sum_{j=1}^{K} 2\kappa_j (1 - \cos(2\pi x j)) = 4 \sum_{j=1}^{K} \kappa_j \sin^2(\pi x j)
\]
We immediately see that the Rouse spectrum of Section 3.2 corresponds to the special case $K = 1, \kappa_1 = 1$. Since the sum is finite, applying the Taylor expansion term-by-term to the series yields

$$\varphi(x) \sim 4\pi^2 x^2 \sum_{j=1}^{K} j^2 \kappa_j$$

for $x < 1/K$. As such, the shape function satisfies Assumption 2 with shape parameter $\rho = 2$. The large-$t$ anomalous exponent $\nu = \frac{1}{2}$ follows immediately.

Readers familiar with the theory of Toeplitz matrices will recognize this type of weak convergence for eigenvalues from Szegő’s Theorem. In this more general light, we see that this notion of eigenvalue convergence is more robust than the case stated here, however if one wishes to carry out the program for non-exchangeable bead-spring systems, the convergence of the eigenvectors will have to be more carefully considered.

### 3.5 The inclusion of repulsive forces

Seeing this universal nature of the Rouse scaling discourages the notion that distinguished particle processes will be able to address the wide range of behaviors seen experimentally. It is interesting to note, at least from a mathematical point of view, that if we are allowed to include repulsive potentials between the beads, a larger class of exponents becomes available.

For example, suppose that for a generalized Rouse network with connectivity order 2, we have $\kappa_2 = -\kappa_1/4$. Then the leading order term of the expansion for the shape function $\varphi$ vanishes. One finds that in this case, the spectral parameter is $\rho = 4$, and the resulting large-$t$ MSD exponent is $\nu = 1 - \frac{1}{\rho} = \frac{3}{4}$.

In fact, one can create a process with large-$t$ MSD exponent $\nu = 1 - \frac{1}{2n}$ for any $n \in \mathbb{N}$, by Fourier inverting the shape function $\varphi(x) = \sin^{2n}(x)$. Such a shape function would satisfy Assumption 2 with parameter $\rho = 2n$.

To be specific about the coefficients, we let

$$\kappa_j := \int_0^1 e^{-2\pi ijx} (e^{\pi ix} - e^{-\pi ix})^2 n^2 dx.$$ 

for $j \in \{-2n, \ldots, 2n\}$. It follows that $\kappa_j = (-1)^{j+1} \binom{2n}{j}$. The choice to take only even powers of sine is made to ensure the symmetry $\kappa_j = \kappa_{-j}$.
3.6 Rescaled distinguished particle processes and linear SPDE

As a concluding note, we return to our discussion random string model which leads to another set of ΣOU processes which have qualitatively different behavior.

Consider again the Rouse chain model, but now we suppose that as the number of beads increases, we simultaneously increase the spring strength by a factor of $N^2$. Without also increasing the fluctuation strength by a factor of $\sqrt{N}$, the limiting structure would collapse to a single point. That is, we define $x_n$ to satisfy the SDE

$$dx_n(t) = \kappa N^2(x_{n+1} - 2x_n(t) + x_{n-1}(t)) + \sigma\sqrt{N}dW_n(t)$$

(3.26)

In [21] the author showed that there is a non-trivial limiting object under the above rescaling. We define a family of functions by

$$u_N(k/N, t) := x_{k,N}(t)$$

and take the linear interpolation for the value of $u_N(y, t)$, for all $y \in (k/N, (k+1)/N)$. Then $\{u_N(y, t)\}_{N=1}^{\infty}$ forms a tight family of functions and the limiting object $u(y, t)$ satisfies the stochastic heat equation

$$\partial_t u_N(y, t) = \Delta u_N(y, t) + W(dy, dt)$$

where $W(dx, dt)$ is a space-time white noise [26]. The second-derivative in space can be anticipated by seeing the double-difference spring operator in (3.26) as a discrete approximation to the Laplacian $\Delta$.

The limiting distinguished particle process is $u(y, \cdot)$. The exact solution can be expressed in the Fourier inversion

$$u(y, t) = \int_0^t \sum_{k=\infty}^{\infty} e^{2\pi iky/N}e^{-4\pi^2k^2(t-s)/N^2} \sigma dB_k(s)$$

where we recognize this is as limit of ΣOU processes given by (1.2) and (1.3) with coefficients and spectrum

$$\lambda_{k,N} = \left(\frac{2\pi k}{N}\right)^2, \quad c_{k,N} = \cos\left(\frac{2\pi k\ell}{N}\right)$$

One can show that these monomer paths exhibit anomalous diffusion, $\mathbb{E}[u(y, t)^2] \sim t^{1/2}$ for $t$ near zero rather than for large $t$. In fact, the process
approaches a stationary distribution for large times. As mentioned earlier in this section, this process $u(y, \cdot)$ has also received attention recently because its sample paths are locally rougher than Brownian motion, having finite quartic variation $[22]$.

Returning to the discussion in the previous subsection, setting $\kappa_2 = -\kappa_1/4$ results in the system of SDEs

$$dx_n(t) = \kappa(x_{n+1} - 2x_n(t) + x_{n-1}(t)) + \sigma dW_n(t)$$

Presumably by rescaling the spring constants by $N^4$ while strengthening the noise appropriately, one obtains the stochastic beam equation in the limit. One suspects that the local behavior will be rougher still and have anomalous exponent $\nu = 3/4$. Similar results should exist for any even number of spatial derivatives, but we do not pursue this line of thought here.

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\section*{References}

[1] Junghae Suh, Michelle Dawson, and Justin Hanes. Real-time multiple-particle tracking: applications to drug and gene delivery. \textit{Advanced Drug Delivery Reviews}, 57:63–78, 2005.

[2] Hirotoshi Matsui, Victoria E. Wagner, David B. Hill, Ute E. Schwab, Troy D. Rogers, Brian Button, Russell M. Taylor II, Richard Superfine, Michael Rubinstein, Barbara H. Iglewski, and Richard Boucher. A physical linkage between cystic fibrosis airway surface dehydration and pseudomonas aeruginosa biofilms. \textit{Proceedings of the National Academy of the Sciences}, 103(48):18131–18136, 2006.

[3] Jung Soo Suk, Junghae Suh, Samuel K. Lai, and Justin Hanes. Quantifying the intracellular transport of viral and nonviral gene vectors in primary neurons. \textit{Experimental Biology and Medicine}, 232:461–469, 2007.
[4] R. Morgado, F. A. Oliveira, G. G. Batrouni, and A. Hansen. Relation between anomalous diffusion and normal diffusion in systems with memory. *Physical Review Letters*, 89(10), 2002.

[5] Raz Kupferman. Fractional kinetics in kaczwanzig heat bath models. *Journal of Statistical Physics*, 114(1-2), 2004.

[6] Mendeli H. Vainstein, Luciano C. Lapas, and Fernando Oliviera. Anomalous diffusion. *Acta Physica Polonica B*, 39(5):1273, 2008.

[7] I. Santamaria-Holek. Anomalous diffusion in microrheology: A comparative study. 2008.

[8] S. C Kou. Stochastic modeling in nanoscale biophysics: Subdiffusion within proteins. *Annals of Applied Statistics*, 2(2):501–535, 2008.

[9] John Fricks, Lingxing Yao, Timothy C. Elston, and M. Gregory Forest. Time-domain methods for diffusive transport in soft matter. *SIAM Journal of Applied Mathematics*, 69(5):1277–1308, 2009.

[10] Scott A. McKinley, Lingxing Yao, and M. Gregory Forest. Transient anomalous diffusion of tracer particles in soft matter. *Journal of Rheology*, (6), 2009.

[11] M. Doi and S. F. Edwards. *The Theory of Polymer Physics*. Oxford University Press, 1986.

[12] Kurt Kremer and Gary S. Grest. Dynamics of entangled linear polymer melts: A molecular-dynamics simulation. *J. Chem. Phys.*, 92(8):5057–5086, 1990.

[13] Michael Rubinstein and Ralph H. Colby. *Polymer Physics*. Oxford University Press, 2003.

[14] R. Kupferman, A. M. Stuart, J. R. Terry, and P. F. Tupper. Long-term behaviour of large mechanical systems with random initial data. *Stochastics & Dynamics*, 2(4):533 –, 2002.

[15] R. Kupferman and A.M. Stuart. Fitting sde models to nonlinear kaczwanig heat bath models. *Physica D: Nonlinear Phenomena*, 199(3-4):279 – 316, 2004.

[16] R. Zwanzig. *Non-equilibrium Statistical Mechanics*. Oxford University Press, 2001.
[17] Bruno H. Zimm. Dynamics of polymer molecules in dilute solution: viscoelasticity, flow birefringence and dielectric loss. *The Journal of Chemical Physics*, 24(2):269–278, 1956.

[18] Hans Christian Öttinger and Yitzak Rabin. Diffusion equation versus coupled langevin equations approach to hydrodynamics of dilute polymer solutions. *Journal of Rheology*, 33:725–743, 1989.

[19] C. M. Bender and S. A. Orszag. *Advanced Mathematical Methods for Scientists and Engineers I: Asymptotic Methods and Perturbation Theory*. McGraw-Hill, 1978.

[20] Daniel Revuz and Marc Yor. *Continuous Martingales and Brownian Motion*. Springer-Verlag Berlin Heidlberg, 1991.

[21] Tadhisu Funaki. Random motions of strings and related stochastic evolution equations. *Nagoya Math Journal*, 89:129–183, 1983.

[22] Jason Swanson. Variations of the solution to a stochastic heat equation. *Annals of Probability*, 35(6):2122–2159, 2007.

[23] Fan Chung. *Spectral Graph Theory*. American Mathematical Society, 1997.

[24] Sridhar Mahadevan. *Representation Discovery using Harmonic Analysis*. Morgan and Claypool Publishers, 2008.

[25] Robert M. Gray. *Toeplitz and Circulant Matrices: A Review*. Foundations and Trends in Communications and Information. now Publishers Inc., 2006.

[26] John B. Walsh. An introduction to stochastic partial differential equations. In *École d’été de probabilités de Saint-Flour, XIV—1984*, volume 1180 of *Lecture Notes in Math.*, pages 265–439. Springer, Berlin, 1986.