Anomalous and nonanomalous behaviors of single-file dynamics

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ABSTRACT

We study the dynamics of a tagged particle that undergoes single-file diffusion in an environment of point Brownian particles. Specifically, we examine the effect of the particle density on the well-known anomalous sub-diffusion behavior of the tagged particle. We compare two single-file systems; the first maintains a fixed average particle density and the second experiences a dilution with time. Both our analytical predictions and computational results, that study the time evolution of the mean square displacement per particle for both systems, show that the behavior of the tagged particle transforms from anomalous sub-diffusive (if the average particle density is kept fixed) to normal if a reduction in the average particle density takes place during the diffusion. Our computational results are based on a discrete Monte-Carlo technique that captures perfectly the dynamics of the continuum formulation of single-file systems.

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1. Introduction

Particle systems governed by stochastic dynamics and exclusion processes have been a research focus [1,2]. An infinite system of interacting Brownian particles hopping on a one-dimensional lattice is referred to as single-file dynamics, and it was first solved by Harris [3]. In nature, many physical systems are found to obey single-file dynamics; such as ion transport through channels in biological membranes [4], zeolites in one-dimensional channel systems [5–7], and super-ionic or organic conductors [8].

Both the ordinary and single-file diffusion properties of the individual tagged Brownian particles (sometimes referred to as the tracer particles) have been a research focus [9–13]. Harris found that if the average particle density is kept fixed, the single-file diffusion of the tracer particles is anomalous sub-diffusive [3], in contradiction to ordinary diffusion, with the tracer particle's mean square displacement growing as time to the one half, $\Delta x^2 \propto t^{1/2}$, and not t, as in ordinary diffusion. Moreover, for a tracer particle in a finite system, Δx^2 reaches equilibrium at very large times; $\lim_{t\to\infty} \Delta x^2 = \text{constant}$ [14,15], and the probability-density function (PDF) is a Gaussian in position with variance Δx^2 [3,12,13].

For the vast majority of cases, single-file diffusion has been treated in the context of homogeneous initial states, in which the particles are mostly equally spaced, with a constant average particle density [16–27]. The main research focus in this paper is to investigate the effect of the particle density on the anomalous sub-diffusion behavior and $t^{1/2}$ dependence of the tracer particles. We compare two single-file systems; the first has a homogeneous initial state and maintains a fixed average particle density with time (see Sec. 3), and the second has an inhomogeneous (Gaussian) initial state (see Sec. 4), where the particle density is maximum near the center of the lattice (through which the particles diffuse) and minimum near the tails, and experiences a progressive drop in the average particle density with time, where the single-file restriction directs the diffusion of the individual tagged particles away from the crowded center and toward the empty tails.

For both single-file systems considered here we study, both analytically and computationally, the time evolution of the mean square displacement per particle. Our computational results utilize a Monte-Carlo technique that simulates the continuum formulation of single-file dynamics (Sec. 2). This technique provides a discrete stepwise approach to how single-file systems evolve with time, and we will show that it captures perfectly the dynamics of the continuum limit.

The role of anomalous diffusion has received attention in literature to describe many physical processes, most prominently within crowded systems; such as ultra-cold atoms in one-dimensional polarization optical lattice [28], crowded fluids such as the cytoplasm of living cells (where the cytoplasm and nucleoplasm of living cells are crowded with a plethora of macromolecules, often rendering the diffusion in these intracellular fluids anomalous) [29–32], two-dimensional Yukawa liquids [33], protein hydration water [34], single-particle movement in cytoplasm [35], worm-like micellar solutions [36], and heart-beat intervals and DNA sequences [37]. In

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Sec. 3 we discuss the anomalous sub-diffusion behavior of single-file dynamics with a fixed average particle density. Our computational results confirm once again that the diffusion constant of the tracer particles D_T is very sensitive to the way the initial state is prepared (such as the spacing between neighboring particles), as predicted in literature [16–19,27]. We also study the effect of the average particle density on the time evolution of Δx^2. Finally, single-file dynamics with a time-variant average particle density is studied in detail in Sec. 4. Note that for the system with the Gaussian density distribution, the dynamical behavior of the central particle was studied before [38,39], wherein it is analytically shown that its Δx^2 grows as t at late times. Here we consider all the particles (both core and tail particles) in the Gaussian distribution when solving for Δx^2. Are the anomalous sub-diffusion behavior and $t^{1/2}$ dependence of single-file dynamics still preserved if a reduction in the average particle density takes place during the diffusion? This is a very crucial question. Further, if not, how does the mean square displacement scale with time in such a case?

2. The Monte-Carlo technique

The Monte-Carlo technique we present here is a discrete stepwise approach that simulates how particle systems evolve with time with the single-file restriction. We will show in next sections that this quantized approach captures perfectly the dynamics of the continuum limit. We start with a finite number of particles N that undergo single-file diffusion in a one-dimensional lattice with a fixed number of cells N_{cells} (in our model $N_{cells} = 10001$). The single-file restriction implies that each cell can be occupied by one particle at most at any moment in time. The x coordinates of the leftmost, central, and rightmost cells in the lattice are -5000, 0, and 5000, respectively. We take the particle distribution through a finite number of Monte-Carlo (time) steps. In each time step, every particle in the distribution attempts a hop once to either the right or left direction, with a probability of $1/2$ for each. The order at which the particles attempt to hop in each time step is random. For simplicity, for a given particle, let's assume that the chosen hopping direction is to the right, the transition probability to the right cell is expressed as

$$T_i^+ = (1 - u_{i+1}), \tag{1}$$

where T_i^+ is the transition probability of a particle located in the ith cell to the $(i+1)$th cell and u_j represents the occupancy states of the cells (1 if occupied and 0 if empty). Similarly, the transition probability to the left cell is expressed as

$$T_i^- = (1 - u_{i-1}). \tag{2}$$

At each Monte-Carlo step, the mean square displacement per particle is calculated according to

$$\Delta x^2 = \frac{1}{N} \sum_{i=1}^{N} (x_i(t) - x_i(0))^2, \tag{3}$$

where $x_i(t)$ and $x_i(0)$ are the positions of the particles at times t and 0 (initial state), respectively.

We consider two different single-file systems in our simulations. The first is a homogeneous system that maintains a fixed average particle density during the diffusion. Its initial state is constructed by distributing a fixed number of particles almost homogeneously over the lattice cells. To maintain a fixed average particle density, we prevent the particles from escaping off by utilizing periodic boundary conditions (similar to diffusion in a circle); that is, if the leftmost cell in the lattice is empty and a particle located in the rightmost cell attempts a hop to the right, it relocates to

the leftmost cell (and vice versa). For such a system, the average particle density ϕ is expressed as

$$\phi = N/N_{cells}, \tag{4}$$

and we will show that it preserves the anomalous sub-diffusion behavior with time.

The second is an inhomogeneous (Gaussian) system that experiences a reduction in the average particle density during the diffusion. Its initial state is constructed as follows; at $t = 0$ we distribute the particles among the cells according to the function

$$P(x, t = 0) = e^{-x^2/\sigma^2}, \tag{5}$$

where $P(x, 0)$ is the cellular occupancy probability at $t = 0$ and σ is a parameter that characterizes the width of the Gaussian function. For the central cell in the lattice (the cell with $x = 0$), $P(0, 0) = 1$; that is, it is guaranteed to be occupied by a particle at $t = 0$, and as the x coordinates of the cells increase in both directions, $P(x, 0)$ decreases exponentially; as a consequence, tail cells are almost guaranteed to be initially unoccupied; that is, the localized particle density is maximum near the center and minimum near the tails of the lattice at $t = 0$. We can calculate a numerical estimate of the average number of particles in the system N_{ave} as

$$N_{ave} = \sum_{x_{\min}}^{x_{\max}} e^{-x^2/\sigma^2}, \tag{6}$$

where $x \in \{x_{\min}, x_{\max}\}$. It is clear that N_{ave} increases as σ increases. If $1 \ll \sigma \ll x_{\max}$, we have

$$N_{ave} \approx \int_{-\infty}^{\infty} e^{-x^2/\sigma^2} dx = \sigma \sqrt{\pi}. \tag{7}$$

3. Anomalous behavior of single-file dynamics

We discuss here the anomalous sub-diffusion behavior of single-file dynamics for a system that maintains a fixed average particle density during the diffusion; see Fig. 1. Consider a uniform, initial distribution $x_{0,j} = j\Delta$, where $x_{0,j}$ denotes the positions of the particles at $t = 0$ and Δ is the spacing between neighboring particles ($\Delta = 1/\phi$), the probability distribution of a tagged particle with coordinate x can be expressed as [40]

$$P(x, t|x_0) \propto e^{-(x-x_0)^2/\sqrt{\Delta^2 Dt}}, \tag{8}$$

where x_0 is the initial position of the tagged particle and D is the diffusion constant of the entire particle system. Equation (8) implies

$$\Delta x^2 = \langle (x - x_0)^2 \rangle = \frac{1}{2}\sqrt{\Delta^2 Dt} = 2D_T t^{1/2}, \tag{9}$$

corresponding to anomalous sub-diffusion and establishing the famous statistical property in [3], where D_T is the diffusion coefficient of the individual tagged particles (also referred to as the tracer diffusion coefficient). For a distribution in which the particles are not perfectly equally spaced (the initial positions of the particles are chosen randomly, which is similar to the case we consider in our simulation), Eq. (9) can be written as [41]

$$\Delta x^2 = 2\left(\frac{1-\phi}{\phi}\right)\left(\frac{Dt}{\pi}\right)^{1/2}. \tag{10}$$

Fig. 2 depicts the anomalous sub-diffusion behavior and $t^{1/2}$ dependence for single-file diffusion with a fixed average particle density. In Fig. 2(a) we show the time evolution of Δx^2, calculated according to Eq. (3), for sixty different simulations with $\phi = 0.5$,