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On the role of adhesion in single-file dynamics

Ahmed M. Fouad *, John A. Noel

Department of Physics, Temple University, Philadelphia, PA 19122, USA

HIGHLIGHTS

- We introduce adhesion to single-file dynamics.
- Adhesion causes a noticeable convergence in the particle trajectories.
- The probability-density functions of single-file and ordinary diffusion are identical.
- The collective single-file diffusion is nonanomalous.
- The diffusion of the individual tagged articles is anomalous sub-diffusive.

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ABSTRACT

For a one-dimensional interacting system of Brownian particles with hard-core interactions (a single-file model), we study the effect of adhesion on both the collective diffusion (diffusion of the entire system with respect to its center of mass) and the tracer diffusion (diffusion of the individual tagged particles). For the case with no adhesion, all properties of these particle systems that are independent of particle labeling (symmetric in all particle coordinates and velocities) are identical to those of non-interacting particles (Lebowitz and Percus, 1967). We clarify this last fact twice. First, we derive our analytical predictions that show that the probability-density functions of single-file (ρ_{sf}) and ordinary (ρ_{ord}) diffusion are identical, $\rho_{sf} = \rho_{ord}$, predicting a nonanomalous (ordinary) behavior for the collective single-file diffusion, where the average second moment with respect to the center of mass, $\langle x(t)^2 \rangle$, is calculated from ρ for both diffusion processes. Second, for single-file diffusion, we show, both analytically and through large-scale simulations, that $\langle x(t)^2 \rangle$ grows linearly with time, confirming the nonanomalous behavior. This nonanomalous collective behavior comes in contrast to the well-known anomalous sub-diffusion behavior of the individual tagged particles (Harris, 1965). We introduce adhesion to single-file dynamics as a second inter-particle interaction rule and, interestingly, we show that adding adhesion does reduce the magnitudes of both $\langle x(t)^2 \rangle$ and the mean square displacement per particle Δx^2; but the diffusion behavior remains intact independent of adhesion in both cases. Moreover, we study the dependence of both the collective diffusion constant D and the tracer diffusion constant D_T on the adhesion coefficient α.

1. Introduction

Single-file dynamics refers to the one-dimensional diffusion of incompressible Brownian particles (so-called tracer or tagged particles) with hard-core interactions, and it has been widely used to model numerous systems such as the diffusion

* Corresponding author.
E-mail address: ahmed.fouad@temple.edu (A.M. Fouad).

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of a single molecule in a crowded one-dimensional environment such as nanochannels [1–4], experimentally studied physical systems such as zeolites [5], confined colloid particles [6–9], and charged spheres in circular channels [10], and particles with long-range interactions [11]. The particles' incompressibility implies that their mutual passage is excluded. Since the sequence of particles in such a situation remains unaffected over time, this leads to deviation from normal diffusion. For an infinite system and uniform initial particle density, Harris [12] and Levitt [13] first showed that the diffusion of a tagged particle is anomalous sub-diffusive (where the tracer particle's mean square displacement grows as the square root of time, $\Delta x^2 \sim t^{1/2}$), rather than normal (where $\Delta x^2 \sim t$); because the diffusion of a tagged particle is always hindered by collisions with all surrounding particles (the many-body confinement effect). This many-body problem has been treated using the methods of Percus [14,15], Lebowitz [16], and Jepsen [17].

All statistical properties of single-file systems that are insensitive to the labeling of the individual tagged particles are identical to those of non-interacting particles [16]. One such property is the probability-density function ρ from which the average second moment with respect to the center of mass $\langle x(t)^2\rangle$ can be obtained. The collective single-file diffusion, which is the diffusion of an entire particle system with respect to a reference point such as the center of mass, is characterized by monitoring the time evolution of $\langle x(t)^2\rangle$. Since $\langle x(t)^2\rangle$ is an insensitive quantity, the collective single-file diffusion is nonanomalous, exactly as the diffusion of non-interacting particles, where $\langle x(t)^2\rangle$ grows linearly with time.

The role of adhesion in the diffusion of many physical systems in nature (most prominently polymers) is an area of great interest [18–32]. In this paper, we introduce adhesion to single-file dynamics and examine its effect on both the nonanomalous behavior of the collective single-file diffusion and the anomalous sub-diffusion behavior of the individual tagged particles, where we conduct extensive computer simulations, which exploit Monte-Carlo techniques and high-performance computing resources, to study the time evolutions of both $\langle x(t)^2\rangle$ and Δx^2 for a range of values of the adhesion coefficient α. Moreover, we study the dependence of both the collective diffusion constant D and the tracer diffusion constant D_T on α.

In Section 2 we discuss the simulation method behind our numerical results. The nonanomalous behavior of the collective single-file diffusion with no adhesion is discussed in detail in Section 3, including our analytical predictions for the probability-density functions of both single-file (ρ_{sf}) and ordinary (ρ_{ord}) diffusion. In Section 4 we present our computational results for the time evolutions of both $\langle x(t)^2\rangle$ and Δx^2 at various α values and the dependence of both D and D_T on α. Moreover, we examine the particle trajectories both with and without adhesion.

2. Simulation method

We start with a one-dimensional lattice that consists of N_{sites} sites (in our model $N_{sites} = 10\,001$). The x coordinates of the leftmost, central, and rightmost sites are -5000, 0, and 5000, respectively. The single-file restriction implies that each site can be occupied by one particle at most at any moment in time. The initial state (at time $t = 0$) is configured as follows. We distribute particles only within the 1000 sites closest to the center of the lattice ($x = 0$); that is, for example, if the local particle density ϕ is 0.5, we distribute 500 particles among the 1000 central sites uniformly, with an occupied site followed by an empty site, and so forth. The number of particles has to be much smaller than the number of sites; because [as we will show in detail in the computational-results section, where we will let the particle system evolve for two million time steps (see Fig. 3)] this will help avoid the particles reaching the two ends of the lattice (before the simulation ends) then bouncing back in, causing a retarded diffusion. For such an initial configuration, the anomalous sub-diffusion behavior of the individual tagged particles is expected to be exhibited by core particles at early times (before a significant drop in the average particle density takes place), as will be discussed in Section 4.

The particle system evolves with time as follows. We take the system through a specific number of time (Monte-Carlo) steps. In each time step, every particle in the system is considered once in a random order, where a hopping direction is picked for every particle at random, either to the right or left, with a probability of ½ for each. For a given particle, let us assume that the chosen direction is to the right, the transition probability to the right site, T_i^+, is expressed as

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

where u_j is the occupancy states of the sites (1 if occupied and 0 if empty); see Fig. 1 for possible numerical values of T_i^+. Similarly, the transition probability to the left site is given by

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

As the system evolves with time, $\langle x(t)^2\rangle$ is calculated according to

$$\langle x(t)^2\rangle = \sum_{i=1}^{N} x_i(t)^2, \tag{3}$$

where N is the total number of particles in the simulation and $x_i(t)$ is the displacements of the particles with respect to the origin ($x = 0$).