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Single-file diffusion with non-thermal initial conditions

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ABSTRACT

Single-file diffusion is a theoretically challenging many-body problem where the calculation of even the simplest observables, e.g. mean square displacement, for a tracer particle requires an elaborate mathematical machinery. There is therefore a need for simple approaches which provide intuitive understandings and predict qualitatively correct behaviours. Here we put forward a scaling-type method which we use to investigate the influence of non-thermal initial conditions on the dynamics of a tracer particle. With our new approach we reproduce, up to scaling, several known long and short time asymptotic results for the tracer particle mean square displacement.

1. Introduction

Q2

The dynamics of diffusing particles in one dimension which are unable to pass each other, often referred to as single-file diffusion, has attracted great theoretical interest for at least 50 years, see Refs. [1–14]. More recent progress in the field addresses single-file diffusion in a potential [15] and that of particles with different diffusion constants [16]. One of the main theoretical predictions is that a tagged (or a tracer) particle, explores the system subdiffusively even though the collective behaviour is identical to that of non-interacting particles [16,17].

Nowadays single-file diffusion also finds experimental realisations. A few examples are diffusion in colloidal systems [18,19], transport in microporous materials [20,21], and permeability of potassium ions in nerve fibres [22]. Also, exclusion effects have been proposed to be of importance for transcription factor (DNA binding proteins) dynamics [23].

In order to calculate dynamical properties of a tagged particle in a single-file system one needs to deal with a theoretically challenging many-body problem. This typically requires rather elaborate mathematics (e.g. Refs. [1,2,12,13,15,24]) which may cloud fundamental understanding. There is therefore a need for simplified methods that captures correct qualitative behaviour and at the same time provide new insights to the problem. A few such papers already exist [9,14] for thermal initial conditions and identical particles. To the best of our knowledge there has not been a similar progress on simple approaches for non-thermal initial conditions. Some aspects have, however, been addressed [25–28] using rather lengthy calculations. The main goal of this paper is to put forward a new but simple method to calculate tagged particle properties, in particular the particle's mean square displacement $\mathcal{S}(t)$, under non-thermal conditions. Our approach relies on two main assumptions: (i) we know the functional form of $\mathcal{S}(t)$ at equilibrium, and (ii) particle concentration gradients decay rapidly compared to the motion of the tagged particle. Based on this, which we denote a quasi-equilibrium approach, we are able to reproduce known scaling behaviours pertaining to different types of initial conditions.

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Table 1
Summary of results ($\tau = \Delta^2/D$).

$\rho_0(x_0)$	$\mathcal{S}(t) \propto$	
	$t/\tau \ll 1$	$t/\tau \gg 1$
$\frac{N}{2\Delta}\, e^{-\lvert x_0\rvert/\Delta}$	$\sqrt{t}$	t
$\frac{N}{\sqrt{2\pi\Delta^2}}\, e^{-x_0^2/(2\Delta^2)}$	$\sqrt{t}$	t
$\sum_{n=-\infty}^{\infty} \delta(x_0 - n\Delta)$	t	$\sqrt{t}$
$\frac{1}{\Delta}\left(\frac{\lvert x_0\rvert}{\Delta}\right)^{-\beta}$	$t^{(1+\beta)/2}$	

2. The quasi-equilibrium approach

Imagine a single-file system extending to infinity in both directions. The particles are identical, point-like and undergo Brownian motion in between hard-core repulsive interactions. Now we tag one particle, label it "0", and place it at time $t = 0$ in the origin, that is, $x_0(t = 0) = 0$. The remaining particles are initially distributed symmetrically around $x_0 = 0, \ldots x_{-2}, x_{-1}, x_0, x_1, x_2, \ldots$, according to some non-thermal distribution $\rho_0(x)$. We then ask: what is the mean square displacement, $\mathcal{S}(t)$, of particle 0?

Our result for $\mathcal{S}(t)$ is based on a quasi-equilibrium argument. For an equilibrated single-file it is well known that the MSD for a tagged particle in the long time limit is (see e.g. Ref. [1]) $\mathcal{S}(t) = (1/\varrho)\sqrt{4Dt/\pi}$ where ϱ is the constant average particle concentration (average inverse inter-particle distance), and D is the single-particle diffusion constant (assumed equal for all particles). Now we assume that this equation holds for all, even non-thermal, initial conditions if we replace ϱ with the time-dependent concentration $\rho(x, t)$ in the vicinity of the tagged particle: $\varrho \approx \rho(x = 0, t)$. This leads to our proposed form for the tracer particle MSD in a single-file system for arbitrary choice of symmetric initial particle densities:

$$\mathcal{S}(t) = \frac{1}{\rho(x = 0, t)}\sqrt{\frac{4Dt}{\pi}} \tag{1}$$

Eq. (1) is nothing but a quasi-equilibrium approach to the problem and is expected to hold whenever concentration relaxations are faster than the motion of the tracer particle.[1] Now, since the macroscopic particle concentration in a single-file system and in a system of non-interacting particles are indistinguishable [17] we can calculate $\rho(x = 0, t)$ by simply solving the diffusion equation in one dimension, and subsequently setting $x = 0$ in the associated solution. In effect this amounts to convoluting $\rho_0(x_0)$ with a Gaussian propagator[2]

$$\rho(x = 0, t) = \int_{-\infty}^{\infty} \frac{e^{-x_0^2/(4Dt)}}{\sqrt{4\pi Dt}}\, \rho_0(x_0)\, dx_0, \tag{2}$$

From here it is easy to see that Eqs. (1) and (2) become exact for a uniform distribution $\rho_0(x_0) = \varrho$, and leads to the classical result by Ref. [1]. Eqs. (1) and (2) constitute our main scaling result: in the subsequent sections we demonstrate that the scaling with time as determined by those two equations agree with all known results for non-thermal initial conditions available in the literature. In the Appendix we motivate our approach further based on the known expression for the velocity–velocity correlation function for a particle in a single-file diffusion system.

3. Special cases

In this section we will investigate four different types of $\rho_0(x_0)$ and show that our simple model gives correct results up to scaling in t. The results are summarised briefly in Table 1 and depicted in Fig. 1.

3.1. Exponential distribution

Here we consider the case where the initial particle density decays exponentially from the origin

$$\rho_0(x_0) = \frac{N}{2\Delta}\, e^{-\lvert x_0\rvert/\Delta}, \tag{3}$$

1 The average absolute distance covered by a tagged particle scales as $(Dt)^{1/4}$ whereas the particle density close to equilibrium is $\rho(x, t) \simeq \rho(x, t = \infty)[1 + \text{const.}/\sqrt{Dt}]$. Tracer particle dynamics is therefore much slower than concentration relaxations. See also Ref. [27] for more details.

2 Consider diffusion on an infinite line with the initial density $\rho_0(x)$. Here the solution to the diffusion equation, $\partial\rho(x, t)/\partial t = D\partial^2\rho(x, t)/\partial x^2$, gives a solution for density according to $\rho(x, t) = \int_{-\infty}^{\infty} \frac{e^{-(x-y)^2/(4Dt)}}{\sqrt{4\pi Dt}}\rho_0(y)\, dy$.