

Chapter 2

Basics of Single-File Diffusion

The simple hard-core interaction does not affect collective properties of the system of point particles. These properties are described by quantities that are symmetric with respect to any permutation of the particles. However, in one dimension, the interaction has a prominent effect on the diffusion of a single marked particle—a tagged particle or a tracer. The present chapter studies basic dynamical features of the tracer dynamics under different conditions.

The chapter is organized as follows. Section 2.1 is introductory, it comprises definitions of basic concepts and the clarification of relation between the positions of interacting particles and order statistics of positions of noninteracting ones. The physical consequences of the interparticle interactions are reviewed in Sects. 2.2, 2.3, and 2.4. Namely, Sect. 2.2 is devoted to the subdiffusion of the tracer in an infinite homogeneous system. Section 2.3 contrasts the findings of Sect. 2.2 with the case of finite number of diffusing particles. The second topic treated in Sect. 2.3 concerns different dynamical regimes distinguished by different time-dependence of tracer's mean squared displacement. In Sect. 2.4 we recall asymptotic properties of the single-file diffusion front. The chapter is concluded by Sect. 2.5, where a few alternative approaches to SFD are pointed out.

2.1 Brownian Motion with Hard-Core Interaction

2.1.1 “Collisions” of Two Particles

From the point of view of the classical mechanics an elastic collision of two particles is an encounter at which the total energy of the particles as well as their total momentum are conserved. A result of such an impact in the case of two identical (same masses) particles moving in one dimension is that after the encounter the particles just *interchange their velocities* as compared to their states before the collision. Let us now discuss how one can define the elastic collision for identical particles

performing an overdamped Brownian motion, i.e., for the particles that possess *no well defined velocities*. We offer two (equivalent) solutions to this at a first glance ill-posed problem. The first one, and we can call it “the probabilistic approach” (sometimes referred to as “a heuristic approach” [1]), is due to Harris [2]. It is based on the equivalence of the positions of interacting particles and order statistics build on the positions of noninteracting ones. The second one, which we can call “the analytical approach”, stems from the definition of the reflecting boundary conditions for the diffusion equation. As we shall see throughout the thesis, the first approach provides us a quick and intuitive way to the most important quantities—exact probability density functions for individual particles, while the second yields a straightforward way to answer the frequently asked question: “Are you sure that your probabilistic reasoning is correct?”¹

Probabilistic Approach

Consider two identical (same mobilities) Brownian particles diffusing on a line. Their positions at time t are given by $\mathbf{X}_{1:2}(t)$ (the left one) and $\mathbf{X}_{2:2}(t)$ (the right one). We assume that except at the instants of their collisions the two particles are mutually independent. We suppose that due to the mutual interaction the particles cannot pass each other, thus the initial ordering, $\mathbf{X}_{1:2}(0) < \mathbf{X}_{2:2}(0)$, is preserved for all times. As long as the two particles are identical we can follow Harris [2] and relate the motion of interacting particles to order statistics of positions of independent noninteracting ones. To this end, let $\mathbf{X}_1(t)$ and $\mathbf{X}_2(t)$ be positions of the two identical noninteracting Brownian particles, then we can set

$$\begin{aligned}\mathbf{X}_{1:2}(t) &= \min \{ \mathbf{X}_1(t), \mathbf{X}_2(t) \}, \\ \mathbf{X}_{2:2}(t) &= \max \{ \mathbf{X}_1(t), \mathbf{X}_2(t) \}.\end{aligned}\tag{2.1}$$

The two equations embodies nothing but the very basic fact that, *except for the particle labeling, the space-time trajectories of two identical hard-core interacting particles are equivalent to the space-time trajectories of the noninteracting ones*, cf. Fig. 2.1. In other words, any collision event can be equivalently described as follows. We can imagine that instead of the mutual reflection the two approaching particles pass freely through each other and, just after they pass each other, we exchange their labels. Thus we can generate the dynamics of interacting particles simply by exchanging the labels of noninteracting ones. Notice that this picture is in agreement with the classical description of one-dimensional elastic collisions and, at the same time, it makes no reference to the particle velocities which presently do not exist.

¹ Actually, the original approach of the present author to the single-file diffusion was the analytical one, cf. Refs. [3, 4]. It was only after completing analytical derivations that the full power and beauty of the probabilistic interpretation has been recognized [5, 6]. In chapters of the present thesis devoted to SFD mainly the probabilistic reasoning is used. The alternative analytical route to the results is always outlined but not strictly followed.

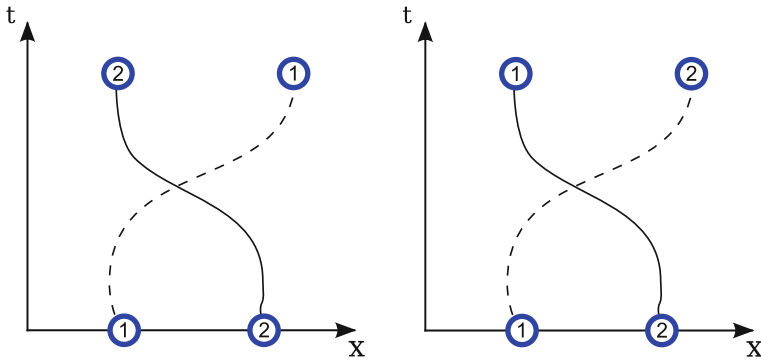


Fig. 2.1 Schematic illustration of space-time trajectories of two particles. *The left panel* Noninteracting particles pass freely through each other, their labels remain attached to individual trajectories. *The right panel* Interacting particles collide when they encounter hence the ordering of the labels is preserved. Except for the particle labeling, the two sets of trajectories are statistically equivalent

The correspondence between the interacting and the noninteracting pictures is behind the fact that the single-file model is exactly solvable and that many important quantities (PDFs of individual particles, their mean squared displacements, and others), could be derived by analytical methods.

Analytical Approach

Let us now formulate the SFD problem as the initial-boundary value problem for the two-particle Smoluchowski equation. For the two identical particles the equation reads [7]

$$\frac{\partial}{\partial t} p(x_1, x_2, t) = \sum_{i=1}^2 \left[D \frac{\partial^2}{\partial x_i^2} - \frac{\partial}{\partial x_i} \mathcal{F}(x_i, t) \right] p(x_1, x_2, t), \quad (2.2)$$

where D stands for the diffusion coefficient of each of the particles and $\mathcal{F}(x, t)$ is the external force acting on the particles. The above diffusion equation contains no evidence of interaction yet. In order to incorporate the hard-core interaction, it is convenient to map the two-particle diffusion in one dimension onto the diffusion of a single “representative particle” in two dimensions. In the latter picture, the coordinates of individual particles x_1, x_2 correspond to the vector components of the position of the representative particle. The hard-core interaction of two diffusing particles means that the representative particle is not allowed to cross the line $x_1 = x_2$ where the collisions occur. Thus the hard-core interaction can be incorporated as the reflecting boundary condition imposed along the line $x_1 = x_2$.

The perfectly reflecting boundary condition requires [7] that the component of the probability current which is perpendicular to the boundary vanishes at the boundary. In the present case, the components of the probability current parallel with the coordinate axes are given by

$$J_i(x_1, x_2, t) = \left[-D \frac{\partial}{\partial x_i} + \mathcal{F}(x_i, t) \right] p(x_1, x_2, t), \quad i = 1, 2. \quad (2.3)$$

Then the boundary condition that represents the hard-core interaction, *the non-crossing boundary condition*, reads

$$(J_1(x_1, x_2, t) - J_2(x_1, x_2, t))|_{x_1=x_2} = 0, \quad (2.4)$$

see Fig. 2.2 for more details. Explicitly, the above requirement reads

$$D \left(\frac{\partial}{\partial x_2} - \frac{\partial}{\partial x_1} \right) p(x_1, x_2, t) \Big|_{x_1=x_2} = 0. \quad (2.5)$$

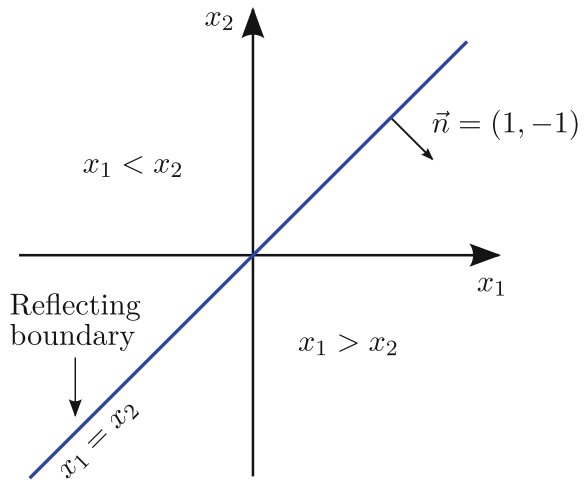
Thus the hard-core interaction splits the two-dimensional state space in two half-planes. Within which of the two half-planes ($x_1 < x_2$, or $x_1 > x_2$) the representative particle moves is dictated by the initial condition. For instance if we set

$$p(x_1, x_2, 0) = \delta(x_1 - y_1) \delta(x_2 - y_2), \quad y_1 < y_2, \quad (2.6)$$

then the particle ordering at any time t is in agreement with that in Eq. (2.1).

Notice that also this second approach to SFD maps the many particle problem with interaction onto the single-particle one. As we discuss below, for identical particles (same D and \mathcal{F} for all particles) the two approaches are equivalent. In contrast to the probabilistic approach, the analytical formulation can be easily extended to the case of *nonidentical* particles (unique D_i , and/or \mathcal{F}_i for each particle). However, this advantage is rather formal since for a general N , $N > 2$, little is known about the exact solution of the Smoluchowski equation when the interacting particles are

Fig. 2.2 The two-particle SFD is equivalent to the single-particle diffusion in 2d plane with the reflecting line $x_1 = x_2$. The (unnormalized) projection of the current vector $\vec{J} = (J_1, J_2)$ onto the direction perpendicular to the reflecting boundary, $\vec{J} \cdot \vec{n} = J_1 - J_2$, vanishes at the reflecting boundary which yields the non-crossing boundary condition (2.4)



different (see Sect. 2.5 for the review of the progress in this direction, and Refs. [8–11] for a discussion of some particular two-particle cases).

2.1.2 Propagator for General N

Having prepared the two approaches to the two-particle SFD, let us now formulate, solve and interpret the general N -particle problem. We assume that N interacting particles which are acted upon by the same external force \mathcal{F} are diffusing in one dimension, each with the diffusion coefficient D . The evolution of the joint PDF of particles positions is governed by the Smoluchowski equation

$$\frac{\partial}{\partial t} p(\vec{x}, t | \vec{y}, t_0) = \sum_{i=1}^N \left[D \frac{\partial^2}{\partial x_i^2} - \frac{\partial}{\partial x_i} \mathcal{F}(x_i, t) \right] p(\vec{x}, t | \vec{y}, t_0), \quad t > t_0. \quad (2.7)$$

Initially, at time t_0 , the particles are located at positions specified by the components of the vector \vec{y} , $\vec{y} = (y_1, y_2, \dots, y_N)$. Hence the initial condition to the above equation is given by

$$p(\vec{x}, t_0 | \vec{y}, t_0) = \delta(x_1 - y_1) \delta(x_2 - y_2) \dots \delta(x_N - y_N), \quad (2.8)$$

Due to the hard-core interaction, the initial ordering of the particles:

$$y_1 < y_2 < \dots < y_N, \quad (2.9)$$

is conserved for all times. This is ensured by $(N - 1)$ non-crossing boundary conditions (cf. Eq. (2.4))

$$D \left(\frac{\partial}{\partial x_{i+1}} - \frac{\partial}{\partial x_i} \right) p(\vec{x}, t | \vec{y}, t_0) \Big|_{x_i=x_{i+1}} = [\mathcal{F}(x_{i+1}, t) - \mathcal{F}(x_i, t)] p(\vec{x}, t | \vec{y}, t_0) \Big|_{x_i=x_{i+1}}, \quad (2.10)$$

$i = 1, 2, \dots, N - 1$.

Let us assume that $f(x, t | y, t_0)$ is the propagator (the Green function) for the corresponding problem with $N = 1$. That is, $f(x, t | y, t_0)$ satisfies the single-particle Smoluchowski equation

$$\frac{\partial}{\partial t} f(x, t | y, t_0) = \left[D \frac{\partial^2}{\partial x^2} - \frac{\partial}{\partial x} \mathcal{F}(x, t) \right] f(x, t | y, t_0), \quad (2.11)$$

subject to the initial condition

$$f(x, t_0|y, t_0) = \delta(x - y). \quad (2.12)$$

Then, as it has been demonstrated in Ref. [3], the propagator for the N -particle SFD problem, has a structure of the *permanent* [12] (which is similar to the determinant but not containing the minus signs). It reads

$$p(\vec{x}, t|\vec{y}, t_0) = \sum_{\sigma \in S_N} \prod_{j=1}^N f(x_{\sigma(j)}, t|y_j, t_0) \quad (2.13)$$

if components of the vector $\vec{x} = (x_1, x_2, \dots, x_N)$ satisfy

$$x_1 < x_2 < \dots < x_N, \quad (2.14)$$

and it vanishes, if at least one of the above inequalities is violated. In Eq. (2.13) the summation is taken over all $N!$ permutations σ of particle labels at time t (of course, equivalently, we can sum over all permutations of the initial positions). Notice that the normalization of the propagator $p(\vec{x}, t|\vec{y}, t_0)$ follows from the normalization of the PDF $f(x, t|y, t_0)$. Since $f(x, t|y, t_0)$ is normalized to one in the one-dimensional space, any summand in Eq. (2.13) is normalized to one in the *unrestricted* N -dimensional space. There are $N!$ such summands in Eq. (2.13), at the same time, the hard-core interaction, as expressed through the non-crossing boundary conditions, reduces the total volume of the N -particle state-space by the factor $1/N!$, which implies the required normalization of $p(\vec{x}, t|\vec{y}, t_0)$ and causes that $p(\vec{x}, t|\vec{y}, t_0)$ is different from zero only when \vec{x} lies in the N -dimensional wedge determined by inequalities (2.14) (the so called Weyl chamber of the symmetric group S_N [13, 14]).

Formula (2.13) expresses the exact solution of the many-particle problem with the hard-core interaction through a simpler object, which is the single-particle probability density. The special case of the above propagator for the unbiased ($\mathcal{F} = 0$) SFD model has been found by Rödénbeck et al. [15] employing the reflection principle, and by Lizana and Ambjörnsson [16, 17] using the Bethe Ansatz.

The permanent-like expression (2.13) possesses an interpretation in terms of non-interacting particles which is perfectly consistent with the probabilistic picture behind Eq. (2.1). Let $\mathbf{X}_i(t)$ be the position of the i th noninteracting particle distributed with the PDF $f(x_i, t|y_i, t_0)$, $i = 1, 2$. Hence $\mathbf{X}_i(t_0) = y_i$, $y_1 < y_2$, and for a moment we consider again that $N = 2$. Then the propagator

$$p(x_1, x_2, t|y_1, y_2, t_0) = f(x_1, t|y_1, t_0)f(x_2, t|y_2, t_0) + f(x_2, t|y_1, t_0)f(x_1, t|y_2, t_0), \quad (2.15)$$

which is different from zero only for $x_1 < x_2$, is nothing but the simultaneous PDF of random positions $\mathbf{X}_{1:2}(t)$, $\mathbf{X}_{2:2}(t)$ of two interacting particles (as defined by Eq. (2.1)) conditioned on the initial state: $\mathbf{X}_{1:2}(t_0) = y_1$, $\mathbf{X}_{2:2}(t_0) = y_2$. In other words, the propagator $p(x_1, x_2, t|y_1, y_2, t_0)$ accounts for all $2!$ possibilities, how the two

noninteracting particles can be ordered: either $\{\mathbf{X}_{1:2}(t), \mathbf{X}_{2:2}(t)\} = \{\mathbf{X}_1(t), \mathbf{X}_2(t)\}$ if $\mathbf{X}_1(t) < \mathbf{X}_2(t)$ (the first term on the right-hand side), or $\{\mathbf{X}_{1:2}(t), \mathbf{X}_{2:2}(t)\} = \{\mathbf{X}_2(t), \mathbf{X}_1(t)\}$ when $\mathbf{X}_1(t) > \mathbf{X}_2(t)$ (the second term with permuted x_1, x_2), cf. Fig. 2.1.

The correspondence between the interacting particles and the noninteracting ones based on definitions (2.1), can be extended to a general N [2]. To this end, at specified time t , we identify the position of the n th interacting particle, say $\mathbf{X}_{n:N}(t)$, with the position of the n th leftmost particle among the noninteracting ones. In statistics, the thus defined random variable $\mathbf{X}_{n:N}(t)$ is known as the n th order statistic [18] (it is the n th smallest one of independent random variables $\mathbf{X}_1(t), \dots, \mathbf{X}_N(t)$). Thus e.g. the first order statistic $\mathbf{X}_{1:N}(t)$ is the position of the leftmost interacting particle and it is identified with the position of the leftmost noninteracting one:

$$\mathbf{X}_{1:N}(t) = \min\{\mathbf{X}_1(t), \dots, \mathbf{X}_N(t)\}, \quad (2.16)$$

and similarly for any n . Then, similarly as in $N = 2$ case, the simultaneous PDF of positions of all N interacting particles (the simultaneous PDF of values of all N order statistics) conditioned on the initial positions is given exactly by the N -particle propagator (2.13).

2.1.3 PDF of a Tagged Particle

The noninteracting particles which has been used to construct the positions of the interacting ones are assumed to be identical as for their physical properties (same D and \mathcal{F}). This assumption is necessary for the permanent (2.13) to be the exact propagator for the interacting particles. A rather complicated structure of the propagator (sum of products) can be reduced to a simple product-like expression if we add a further assumption regarding the initial conditions.

Let us assume that the initial position of any noninteracting particle, $\mathbf{X}_i(t_0)$, $i = 1, \dots, N$, is drawn from the PDF $f(y, t_0)$. This choice of the initial condition implies that all noninteracting particles are identical as for all their statistical properties. That is, not only each particle diffuses with the same D and it is acted upon by the same force \mathcal{F} , but also the initial condition is, in a statistical sense, the same for all particles (in contrast to the previous case described by PDFs $f(x, t|y_i, t_0)$ which differ by initial deterministic positions). A remarkable simplification follows from this assumption in the corresponding interacting case. We get the result in two steps. First, the PDF for the position of any noninteracting particle at time t is the same and it is given by $f(x, t)$, which follows from $f(x, t_0)$ via the integration:

$$f(x, t) = \int dy f(x, t|y, t_0) f(y, t_0). \quad (2.17)$$

Second, the PDFs $f(x_i, t)$ replace the conditioned PDFs $f(x_i, t|y_j, t_0)$ in Eq. (2.13). Consequently, the sum on the right-hand side of Eq. (2.13) contains $N!$ *identical summands* and the simultaneous PDF for positions $\mathbf{X}_{1:N}(t), \dots, \mathbf{X}_{N:N}(t)$, of interacting particles reads

$$p(\vec{x}, t) = N! \prod_{j=1}^N f(x_j, t), \quad (2.18)$$

when the vector \vec{x} lies in the wedge (2.14) and it vanishes otherwise. In particular, for $t = t_0$ we obtain the initial simultaneous PDF in the factorized form

$$p(\vec{x}, t_0) = N! \prod_{j=1}^N f(x_j, t_0). \quad (2.19)$$

Such initial condition can be thought to describe e.g. the Gibbs equilibrium state as it will be discussed in Chap. 3, cf. Eq. (3.36). In particular, the factorized form of Eq. (2.18) may evoke an impression that the positions of interacting particles are not correlated. This is not the case, the interparticle correlations appear due to the fact that \vec{x} is restricted to the wedge (2.14).

Of course, one can follow a different line of reasoning, assuming first that the initial condition is given by Eq. (2.19), and, second, evolving the initial condition by the propagator (2.13). The result will be again given by Eq. (2.18). That is, for this specific initial condition the simultaneous PDF factorizes for all times $t, t \geq t_0$ [4].

The basic advantage of the factorized simultaneous PDF is that it yields an analytically tractable expression for the marginal PDF $p_{n:N}(x, t)$ for the position $\mathbf{X}_{n:N}(t)$ of the n th interacting particle:

$$p_{n:N}(x, t) = \frac{N!}{(n-1)!(N-n)!} f(x, t) \left[\int_{-\infty}^x dx' f(x', t) \right]^{n-1} \left[1 - \int_{-\infty}^x dx' f(x', t) \right]^{N-n}. \quad (2.20)$$

The interpretation of the right-hand side in terms of N statistically identical noninteracting particles, whose positions are distributed with the PDF $f(x, t)$, is rather straightforward. The expression $p_{n:N}(x, t)dx$ equals the probability that there is a single particle in $(x, x+dx)$ ($f(x, t)dx$) and, simultaneously, there are $(n-1)$ noninteracting particles to the left of x (with the probability $[\int_{-\infty}^x dx' f(x', t)]^{n-1}$), and the remaining $(N-n)$ particles are to the right of x (with the probability $[1 - \int_{-\infty}^x dx' f(x', t)]^{N-n}$). The combinatorial prefactor accounts for all possible permutations of labels.

In Chaps. 3 and 4 we will derive the generalization of the above marginal PDF for the SFD model with one (Eq. 3.39) and two (Eq. 4.13) absorbing boundaries.

2.2 SFD in Homogeneous System with Constant Density

Let us now turn to the key feature of the single-file dynamics—the subdiffusive behavior of the tagged particle. Consider an infinite line occupied by particles with constant density ρ . Particles are distributed randomly. This means that empty intervals between adjacent particles are exponentially distributed random variables with mean value $1/\rho$. At the initial time we choose a single particle (a tracer) and we follow its motion (alternatively, we can insert a single particle into the system). Clearly, the space available for the tracer diffusion is effectively reduced by the presence of other particles. This hindrance results in a slowdown of diffusive spreading of tracer PDF, as compared to the free diffusion. In the long-time limit, we observe a subdiffusive motion. Despite this anomalous behavior, the tracer PDF is still given by a Gaussian density but now the mean squared displacement (MSD) grows as $t^{1/2}$:

$$p_T(x, t) \sim \frac{1}{\sqrt{2\pi\langle \mathbf{X}_T^2(t) \rangle}} e^{-x^2/2\langle \mathbf{X}_T^2(t) \rangle}, \quad \langle \mathbf{X}_T^2(t) \rangle = \frac{2}{\rho} \sqrt{\frac{Dt}{\pi}}, \quad \text{as } t \rightarrow \infty. \quad (2.21)$$

This is one of the most highlighting results of the theory of the single-file diffusion which has already been confirmed in various experiments, e.g. in NMR studies of diffusion in zeolites [19–23], and in experiments on colloids confined in narrow channels [24–30].

From a general perspective, the SFD model belongs to the class of interacting models like phantom polymer chains [31, 32] or certain fluctuating interfaces [33]. The characteristic feature of all these models is that a tagged particle (or a tagged segment) undergoes a non-Markovian diffusion described by Gaussian PDF with associated mean squared displacement proportional to $t^{1/2}$. Such stochastic process is usually said to be of a fractional Brownian motion type [17, 34–36] rather than that of a continuous-time random walk type. Since for the latter the corresponding PDF is not Gaussian but it typically exhibits a sharp cusp around the initial position, see Ref. [37] for a numerical comparison. An approximative mapping (so called harmonization) between the long-time dynamics of SFD system and that of the Rouse polymer chain can be found in Refs. [38–40]. Further, in Ref. [35] a general phenomenological description for all these processes has been developed leading to a fractional Langevin equation. Let us now build some intuition with the way how the subdiffusion arises in the SFD system.

2.2.1 Heuristic Arguments

The time-dependence of the tracer displacement can be intuitively understood as follows [41, 42]. Consider a one-dimensional *lattice*. Each lattice site is either occupied by a particle or vacant, multiple occupation of sites is forbidden. On a nearly

full lattice, any particle is almost always surrounded by occupied sites and therefore it rarely moves. On the other hand, the concentration of *vacancies* on such a lattice is vanishingly small. Hence the vacancies rarely meet and we can approximate their dynamics by *independent* random walks. The crucial observation is that we can draw a certain conclusions about the tracer dynamics by considering the dynamics of almost freely diffusing vacancies. Indeed, a tracer will hop to the neighboring site only if that site contains a vacancy. Hence the displacement of the tracer is given by

$$\mathbf{X}_T(t) = \mathbf{N}_{R \rightarrow L}(t) - \mathbf{N}_{L \rightarrow R}(t), \quad (2.22)$$

where $\mathbf{N}_{R \rightarrow L}(t)$ is the number of vacancies that were initially to the right of the tracer and are now on the left, and vice versa for $\mathbf{N}_{L \rightarrow R}(t)$. Since the densities of the vacancies to the right and to the left of the tracer are equal, we expect that $\langle \mathbf{N}_{R \rightarrow L}(t) \rangle = \langle \mathbf{N}_{L \rightarrow R}(t) \rangle$. Thus the average tracer displacement, $\langle \mathbf{X}_T(t) \rangle$, is zero. From the diffusive motion of the vacancies it follows that $\langle \mathbf{N}_{R \rightarrow L}(t) \rangle = \langle \mathbf{N}_{L \rightarrow R}(t) \rangle \sim t^{1/2}$. Hence the difference on the right-hand side of Eq. (2.22) scales as $\sqrt{t^{1/2}}$ and the mean squared displacement of the tracer position grows as $t^{1/2}$. We recall that for the classical symmetric random walk both the number of left steps, $\mathbf{N}_L(t)$, and the number of right steps, $\mathbf{N}_R(t)$, behave as $\langle \mathbf{N}_L(t) \rangle = \langle \mathbf{N}_R(t) \rangle \sim t$. Then the particle position determined by the difference $\mathbf{X}(t) = \mathbf{N}_R(t) - \mathbf{N}_L(t)$ scales as $t^{1/2}$ and hence the mean squared displacement of the particle increases as t .

2.2.2 Derivation of Tracer PDF

The most elegant derivation of the basic result (2.21) is due to Levitt [43, 44] (but see also Refs. [45–47]). The main ideas behind Levitt's construction of the tracer PDF $p_T(x, t)$ are (A) the trajectories of interacting particles are statistically equivalent to the trajectories of noninteracting ones; (B) the PDF $p_T(x, t)$ is proportional to the probability $A_0(x, t)$ that, for the reference system of noninteracting particles, the number of particles to the left of the tracer (and hence to the right of it) has not changed as compared to the initial configuration.

Let us assume that initially the tracer is located at the origin of coordinates $x = 0$. We follow its dynamics up to time t and we ask for the probability that at this time the tracer is located in $(x, x + dx)$. An important quantity that will be used in construction of the tracer PDF is the mean number of noninteracting particles that initially were to the left of the tracer (i.e., to the left of $x = 0$) and, at time t are located to the right of x . It is given by the double integral

$$\nu_{L \rightarrow R}(x, t) = \rho \int_x^\infty dx' \int_{-\infty}^0 dy \frac{1}{\sqrt{4\pi Dt}} e^{-(x'-y)^2/4Dt}. \quad (2.23)$$

And vice versa, the mean number of particles that initially were to the right of the tracer and, at time t are to the left of x reads

$$\nu_{R \rightarrow L}(x, t) = \rho \int_{-\infty}^x dx' \int_0^{\infty} dy \frac{1}{\sqrt{4\pi Dt}} e^{-(x'-y)^2/4Dt}. \quad (2.24)$$

The above two quantities are merely mean values. A more complete description is provided by the corresponding probabilities. Since the reference particles are independent, the probability distribution for the overall number of crossings from left to right is the Poisson distribution with the mean value $\nu_{L \rightarrow R}(x, t)$ (and similarly for $\nu_{R \rightarrow L}(x, t)$). From the two Poisson distributions we can infer the probability that there were equal number of crossings from left to right as from right to left. The latter probability is given by the sum over all possible events which are compatible with the required condition:

$$A_0(x, t) = \sum_{k=0}^{\infty} \frac{[\nu_{L \rightarrow R} \nu_{R \rightarrow L}]^k}{k! k!} e^{-(\nu_{L \rightarrow R} + \nu_{R \rightarrow L})}, \quad (2.25)$$

or, expressed using the modified Bessel function:

$$A_0(x, t) = I_0(2\sqrt{\nu_{L \rightarrow R} \nu_{R \rightarrow L}}) e^{-(\nu_{L \rightarrow R} + \nu_{R \rightarrow L})}. \quad (2.26)$$

In the long-time limit, the tracer PDF $p_T(x, t)$ can be recovered from the non-interacting picture as follows. The probability that, at time t , the tracer is located in infinitesimal interval $(x, x + dx)$ is given by the product of the probability that there is a noninteracting particle in $(x, x + dx)$ which is (ρdx) , and the probability $A_0(x, t)$ that there were equal number of trajectory crossings. Therefore, we have [43]

$$p_T(x, t) \sim \rho A_0(x, t). \quad (2.27)$$

Let us now turn to the long-time behavior of the right-hand side of Eq. (2.27). All integrals in Eqs. (2.23), (2.24), can be evaluated analytically. This yields

$$\nu_{L \rightarrow R}(x, t) = \rho \left[\sqrt{\frac{Dt}{\pi}} e^{-x^2/4Dt} - \frac{x}{2} \left(1 - \operatorname{erf}\left(\frac{x}{\sqrt{4Dt}}\right) \right) \right], \quad (2.28)$$

$$\nu_{R \rightarrow L}(x, t) = \rho \left[\sqrt{\frac{Dt}{\pi}} e^{-x^2/4Dt} + \frac{x}{2} \left(1 + \operatorname{erf}\left(\frac{x}{\sqrt{4Dt}}\right) \right) \right]. \quad (2.29)$$

The both above expression increase with time. Therefore, in the long-time limit, $x \ll \sqrt{4Dt}$, we can use the asymptotic representation of the Bessel function, $I_0(2z) \sim e^{2z}/\sqrt{4\pi z}$, for $z \rightarrow \infty$, to get

$$p_T(x, t) \sim \rho (4\pi)^{-1/2} (\nu_{L \rightarrow R} \nu_{R \rightarrow L})^{-1/4} e^{-(\sqrt{\nu_{L \rightarrow R}} - \sqrt{\nu_{R \rightarrow L}})^2}, \quad t \rightarrow \infty. \quad (2.30)$$

Further, we approximate the error functions in Eqs. (2.28), (2.29) by their small-argument asymptotic behavior $\operatorname{erf}(z) \sim 2z/\sqrt{\pi}$ and, after some algebra, we obtain

$$(\sqrt{\nu_{L \rightarrow R}} - \sqrt{\nu_{R \rightarrow L}})^2 \sim x^2 \frac{\rho}{4} \sqrt{\frac{\pi}{Dt}}, \quad (2.31)$$

$$(\nu_{L \rightarrow R} \nu_{R \rightarrow L})^{-1/2} \sim \frac{1}{\rho} \sqrt{\frac{\pi}{Dt}}. \quad (2.32)$$

Returning to Eq. (2.27), the asymptotic tracer PDF is Gaussian:

$$p_T(x, t) \sim \frac{1}{\sqrt{4\pi \mathcal{D}_{1/2} \sqrt{t}}} e^{-x^2/4\mathcal{D}_{1/2}\sqrt{t}}, \quad t \rightarrow \infty, \quad (2.33)$$

where we have defined the generalized diffusion coefficient

$$\mathcal{D}_{1/2} = \frac{1}{\rho} \sqrt{\frac{D}{\pi}}, \quad (2.34)$$

which enters the subdiffusive law for the mean squared displacement

$$\langle \mathbf{X}_T^2(t) \rangle \sim 2\mathcal{D}_{1/2}\sqrt{t}. \quad (2.35)$$

Notice that the main ideas behind the above derivation of the Gaussian PDF (2.33), are essentially the same as those behind heuristic arguments based on Eq. (2.22). The only difference is that in the heuristic approach the freely diffusing entities are vacancies, whereas now the freely diffusing entities are noninteracting particles.

2.3 Comparison with SFD of N Particles

Harris's classical result concerning $t^{1/2}$ MSD growth and the Gaussian PDF (2.21) are derived under following conditions: the system is homogeneous with a constant density of particles, and, increasing time, the subdiffusive regime is the last one which occurs in the overall dynamical description. We now wish to comment on further details of the SFD model including finite-time behavior and the dynamics of the system with finite number of particles.

2.3.1 Entropic Repulsive Forces

First, let us consider the long-time dynamics of the system with zero density, namely, an infinite line containing N interacting particles. The dynamics of such a system has been studied in a great detail by Aslangul [8, 48].

In Ref. [8] the two-particle problem on a lattice has been solved exactly. In the continuum limit, the two particles undergo a Brownian motion with a hard-core interaction and the problem can be solved by a transition to the center of mass coordinate system. Then the difference coordinate behaves like a Brownian particle and the original hard-core interaction manifests itself as a perfectly reflecting wall for this particle at the origin. Under these conditions, the Brownian particle exhibits an anomalous drift away from the boundary, its average position increases as $t^{1/2}$, whereas the second moment has a normal diffusive spreading. Thus for two interacting particles the following overall picture emerges. The interaction induces a repulsive drift of entropic origin. The drift is anomalous with a vanishing velocity, the average distance between the particles grows at large times as $t^{1/2}$, whereas the second moment of the position of each particle grows linearly with time. Let $\mathbf{X}_{1:2}(t)$, $\mathbf{X}_{2:2}(t)$ be respectively the position of the left and of the right particle, then we have [8]

$$-\langle \mathbf{X}_{1:2}(t) \rangle = \langle \mathbf{X}_{2:2}(t) \rangle \sim \sqrt{\frac{2Dt}{\pi}}, \quad \langle \mathbf{X}_{1:2}^2(t) \rangle = \langle \mathbf{X}_{2:2}^2(t) \rangle \sim 2Dt. \quad (2.36)$$

In Ref. [48] similar issues have been clarified for N interacting particles. Aslangul has assumed that, at the initial time the particles form a compact point-like cluster located at the origin. In $t \rightarrow \infty$ limit, the mean position of the n th particle ($n = 1, \dots, N$), and its second moment evolve with time according to

$$\langle \mathbf{X}_{n:N}(t) \rangle \sim V_{n:N} \sqrt{t}, \quad \langle \mathbf{X}_{n:N}^2(t) \rangle \sim 2D_{n:N}t. \quad (2.37)$$

Hence the dynamical exponents are exactly the same as for two particles (2.36). Both the particle order and the total number of particles enters the result through the order-dependent transport coefficients $V_{n:N}$, $D_{n:N}$. The task of deriving exact expressions for $V_{n:N}$, $D_{n:N}$ is elusive [48], yet, for two special cases the asymptotic behavior can be given. For the particles located at the edges of the dispersing cluster the asymptotic behavior of the transport coefficients is given by $-V_{1:N} = V_{N:N} \propto [\log(N)]^{1/2}$, $D_{1:N} = D_{N:N} \propto [\log(N)]^{-1/2}$. For the central particle, we have $D_{c:N} \propto 1/N$, $c = (N+1)/2$.

Thus, when the total number of particles is finite, the mutual interactions induce an anomalous entropic drift but the diffusion is not anomalous in the long-time limit. On the other hand, notice that in the limit of $N \rightarrow \infty$, both $D_{N:N}$ and $D_{c:N}$ vanishes. This indicates a possible lowering of the dynamical exponent and the onset of a subdiffusive regime observed in the finite density situation. The middle particle is surrounded by infinitely many others and its diffusion constant vanishes as $1/N$. For the two edge particles, the logarithmic decrease of $D_{N:N}$ comes from the fact that these particles still face a free semi-infinite space to wander in (see Ref. [48] for a further discussion).

2.3.2 Three Dynamical Regimes

Let us consider a finite interval of the length L with N diffusing particles, and we put $\rho = N/L$. A thorough analysis of tracer dynamics in a finite interval with reflecting boundary conditions has been given by Lizana and Ambjörnsson in Refs. [16, 17]. Authors used Bethe Ansatz to derive the exact tracer PDF. In the present section we will paraphrase their results concerning different dynamical regimes for the dynamics of the middle particle. Recently, the results have been reproduced by the scaling method in Ref. [49].

The precise setting is the following. At the initial time $t = 0$ there are N interacting particles of the diameter Δ randomly distributed in the interval of the length L . We will follow the diffusion of the central particle located initially approximately near the center of the interval (the tracer). The dynamics of the tracer is rather complex. The exact analysis based on Bethe Ansatz has revealed three dynamical regimes: (A) short times, (B) intermediate times, and (C) long times.

(A) *Short times.* For time t much smaller than the collision time t_{coll} ,

$$t_{\text{coll}} = \frac{1}{\rho^2 D}, \quad (2.38)$$

the tracer “does not feel” other particles and, consequently, it undergoes a free diffusion. In this regime, the tracer PDF is Gaussian with the MSD given by

$$\langle [\mathbf{X}_T(t) - \mathbf{X}_T(0)]^2 \rangle = 2Dt, \quad t \ll t_{\text{coll}}. \quad (2.39)$$

(B) *Intermediate times.* For times t much larger than the collision time t_{coll} but still smaller than the equilibrium time t_{eq} ,

$$t_{\text{eq}} = \frac{L^2}{D}, \quad (2.40)$$

the tracer diffusion is anomalous, the tracer PDF is given by a Gaussian function with the mean squared displacement

$$\langle [\mathbf{X}_T(t) - \mathbf{X}_T(0)]^2 \rangle = \frac{1 - \rho\Delta}{\rho} \sqrt{\frac{4Dt}{\pi}}, \quad t_{\text{coll}} \ll t \ll t_{\text{eq}}. \quad (2.41)$$

The generalized diffusion coefficient predicted by Eq. (2.41) is in conformity with that obtained for infinite systems with point particles ($\Delta = 0$, cf. Eqs. (2.33–2.35)) and also with that for the SFD on a lattice [50, 51]. The latter correspondence is obtained when both the particle diameter Δ and the lattice spacing equals to one.

(C) *Long times.* In the long-time limit, $t \gg t_{\text{eq}}$, the tracer PDF approaches an equilibrium probability density function and its MSD saturates on a constant value. We have

$$\langle [\mathbf{X}_T(t) - \mathbf{X}_T(0)]^2 \rangle \propto \frac{L^2}{N}, \quad t \gg t_{\text{eq}}. \quad (2.42)$$

Only regimes (A) and (B) are found in the infinite system with constant particle density (discussed in Sect. 2.2), where t_{eq} diverges. Notably, in the setting discussed by Aslangul (cf. Sect. 2.3) the regime (C) is replaced by the normal diffusion and the regime (A) should be absent since the particles initially form a compact point-like cluster. In a finite interval with periodic boundary conditions the regime (C) is also different. For a periodic system at long times, all particles become highly correlated – they behave as a single effective particle and undergo a normal diffusion with the renormalized diffusion coefficient D/N [52]. A different (even superdiffusive) MSD behavior in regime (B) is reported in Ref. [53] where effects induced by the choice of initial conditions are discussed by means of Monte Carlo simulations.

2.4 Single-File Diffusion Front

In the finite- N case studied by Aslangul the particle near the boundary of the cluster is repelled by a finite number of its neighbors. This repulsion induces an anomalous drift proportional to $t^{1/2}$. An important question is in order. What if the edge particle has *infinite* number of others to its left (say)? How strong is the entropic repulsion in this case? To obtain the answer let us turn to the study of statistical properties of the single-file diffusion front. Namely, in the present section we consider SFD on an infinite line. Initially the negative half-line is occupied by (infinitely many) particles distributed with the mean density ρ . There are no particles on the positive half-line. We are interested in the motion of the right-most particle.

The evolution of the density of particles $\rho(x, t)$ is governed by the diffusion equation with the step initial condition: $\rho(x, 0) = \rho$ for $x < 0$ and $\rho(x, 0) = 0$ otherwise. The density profile at time t is given by the complementary error function:

$$\rho(x, t) = \frac{\rho}{2} \operatorname{erfc}\left(\frac{x}{\sqrt{4Dt}}\right), \quad (2.43)$$

from which we obtain the mean number of particles located to the right of x :

$$\nu(x, t) = \int_x^\infty dx' \rho(x', t). \quad (2.44)$$

Let us number the particles from right to left. Hence the rightmost particle is labeled by $n = 1$. How can we construct the PDF $p_n(x, t)$ of the n th interacting particle? Again we provide an answer by a proper construction based on the reference noninteracting picture. The sought probability that the n th interacting particle is in $(x, x + dx)$ equals to the probability that there is a noninteracting particle in $(x, x + dx)$, i.e., $\rho(x, t)dx$, times the probability that there are $(n - 1)$ particles to the

right of x . Since the reference noninteracting particles are statistically independent, the latter probability is given by the Poisson distribution with the mean value $\nu(x, t)$. Altogether, we get

$$p_n(x, t) = \rho(x, t) \frac{[\nu(x, t)]^{n-1}}{(n-1)!} e^{-\nu(x, t)}. \quad (2.45)$$

Let us now focus on statistical properties of the right-most particle (sometimes called as the single-file diffusion front, or just a diffusion front). Its cumulative distribution function, $F_1(x, t) = \int_{-\infty}^x dx' p_1(x', t)$, equals

$$F_1(x, t) = \exp[-\nu(x, t)]. \quad (2.46)$$

In the long-time limit $F_1(x, t)$ converges to Gumbel distribution:

$$F_1(x, t) \sim \exp\left[-\exp\left(-\frac{x}{b(t)} + a(t)\right)\right], \quad t \rightarrow \infty, \quad (2.47)$$

with parameters

$$b(t) = \sqrt{\frac{2Dt}{\log(2Dt)}}, \quad a(t) = \log\left(\frac{2\rho Dt}{\sqrt{2\pi} \log(2Dt)}\right). \quad (2.48)$$

For the proof of the convergence we refer to the proof of Theorem 3 in Ref. [54] (Arratia in Ref. [54] has used λ instead of our ρ and has worked with a standard Brownian motion for which $D = 1/2$).

Gumbel distribution (2.47) gives us asymptotic behavior of all moments of the front position. The asymptotic mean position assumes the form

$$\langle \mathbf{X}_1(t) \rangle \sim \sqrt{\frac{2Dt}{\log(2Dt)}} \left[\gamma + \log\left(\frac{2\rho Dt}{\sqrt{2\pi} \log(2Dt)}\right) \right], \quad t \rightarrow \infty. \quad (2.49)$$

where γ stands for Euler's constant, $\gamma \approx 0.5772156649$. For the variance we obtain

$$\langle [\mathbf{X}_1(t) - \langle \mathbf{X}_1(t) \rangle]^2 \rangle \sim \frac{\pi^2}{6} \frac{2Dt}{\log(2Dt)}, \quad t \rightarrow \infty. \quad (2.50)$$

Thus an anomalous entropic drift produced by infinite number of particles scales with time faster than $t^{1/2}$ -law observed in Aslangul's finite- N setting. Interestingly enough, an effective one-sided restriction of particle's motion results in a slowdown of its diffusion. The asymptotic variance (2.50) grows with time slower than that in the case of the normal diffusion (i.e., slower than t) but still faster than in the case of $t^{1/2}$ subdiffusion.

Finally, a few remarks are in order. First, Gumbel distribution $\exp(-\exp(-x))$ is one of the three possible limiting distributions for extreme order statistics. The three distributions with brief comments on the related theory are presented in App. A. Second, there exists a recent work [55] concerning diffusion front.² Third, in Refs. [56, 57] fluctuations of the current through the origin has been studied for the simple symmetric exclusion process with a similar initial condition as that of the present section. For the asymmetric simple exclusion process the similar initial conditions have been discussed in Refs. [58–66], in particular in connection to random matrix theory.

2.5 Further Reading

Let us now mention a few selected directions of research which has not been covered in the preceding text.

(1) Recently SFD of *nonidentical* particles (different diffusion constants) has attracted a considerable attention. In this case the correspondence between the interacting particles and the noninteracting ones breaks down and the model is no-longer integrable. Various approximative [67] and numerical methods have been developed including scaling arguments [68] and the harmonization technique [10, 39] which approximates the SFD system by the particles interconnected by harmonic springs (the Rouse model). With the aid of this mapping, in Ref. [40] a force-response relation for tracer has been studied. Rigorously, a convergence to a fractional Brownian motion, a law of large numbers and a central limit theorem has been proven in Ref. [69].

(2) Several studies are devoted to SFD in one dimension with *more general interparticle interactions than just the hard-core one* [70–76]. For instance, typical $t^{1/2}$ subdiffusive behavior is reported also for inelastically colliding particles [77, 78]. What if the interaction is long-ranged? This important generalization has been studied in seminal work [70] with the following conclusion: provided that the correlation length between the particles is finite the tracer MSD grows asymptotically as $t^{1/2}$ and the generalized diffusion coefficient is related to the compressibility of the system. These predictions were tested experimentally for colloidal particles [25, 26] and for charged millimetric steel balls [73, 74]. Hydrodynamic interactions, yet another effect, are screened significantly in one dimension; cf. Ref. [27] for both experimental and theoretical study, and Ref. [76] for extensive numerical analysis.

Above examples may evoke an impression that $t^{1/2}$ scaling of the MSD must be observed in any one-dimensional diffusive system regardless the form of interparticle interaction. Of course this is not the case. A notable counterexample where long-

²Notice that Sabhapandit's expression for the cumulative distribution function of the front position (Eq. (7) in Ref. [55]) differs from $F_1(x, t)$ in Eq. (2.46) by a nontrivial multiplicative factor. Probabilistic interpretation of Eq. (7) in Ref. [55] remains unclear to the present author (actually, $F_1(x, t)$ corresponds to the right-hand side of Eq. (5) in Ref. [55]).

ranged interactions modify the subdiffusive regime is provided by Brownian particles interacting by the logarithmic potential (Dyson's Brownian motion). In this case the tracer MSD grows as $\log(t)$ [79]. Other cases are listed in next paragraphs. There, deviations from typical $t^{1/2}$ subdiffusion are caused by interaction with external fields and/or with confining channel, and even by a certain type of initial conditions.

(3) Single-file dynamics *in spaces with dimension greater than one* is of considerable interest in recent years. In particular, a reduction of the confined two-dimensional single-file dynamics of discs to the one-dimensional longitudinal motion of rods has been carried out in Refs. [80–83]. When the diameter of the tube is slightly greater than the doubled diameter of the disc a crossover from the subdiffusion to a normal diffusion occurs. An accurate description of this phenomenon is still under active debate [84–86]. For particles interacting by Yukawa potential, numerical analysis of Ref. [87] reveals rather different diffusive regimes and transitions depending on the shape of the channel. The screened Coulomb potential (described through a modified Bessel function of the second kind K_0 , as inspired by experiments [73, 74]) leads to nontrivial properties of fluctuations in the vicinity of transitions between different equilibrium conformations of the system [88–90].

(4) Effects induced by *external fields* acting on particles have become the subject of several studies [3, 38, 40, 91–101]. Strictly speaking, the previous point (3) also belongs to this category. A particularly hard and still unsolved problem is when the external field acts on the tagged particle only. Theoretical advances in this direction can be found in Refs. [38, 40, 98, 99]. The external field acting on all particles can model, for example, entropic forces stemming from inhomogeneities of real channels [102]. SFD in random potentials have been studied both theoretically [100, 103] and experimentally [101]. Channels with random walls have been considered in Ref. [104]. Diffusion of magnetic dipoles in modulated channels is discussed in Refs. [91–93].

(5) *Initial conditions* may imply two unexpected effects on the dynamics of the tracer. First, the power law initial distribution results in t^α subdiffusion, where α is neither 1 nor $1/2$ [49, 95, 105]. Second, the initial condition determines the value of the generalized diffusion coefficient [106], which is a long-memory effect unobserved in the normal diffusion (where the diffusion coefficient is determined by Einstein's relation).

(6) In some studies the *dynamics of individual particles is not normal Brownian motion*. Instead, the particles may follow e.g. the deterministic dynamics [107–110] or some kind of an anomalous kinetics [105, 111–113]. An outstanding result valid for all these systems is the so called Percus diffusion formula [95, 107]. The formula relates MSD of the tracer in a system with interaction with motion of a single particle in the absence of interaction: $\langle [\mathbf{X}_T(t) - \mathbf{X}_T(0)]^2 \rangle \sim \langle |\mathbf{X}(t) - \mathbf{X}(0)| \rangle / \rho$. It is valid for an infinite homogeneous system with constant density of particles and in Ref. [95] it has been derived for a rather broad class of anomalous processes including e.g. the continuous-time random walk and the fractional Brownian motion. Thus for instance if for a free diffusion $\langle |\mathbf{X}(t) - \mathbf{X}(0)|^2 \rangle \propto t^\alpha$ then for the tracer motion $\langle [\mathbf{X}_T(t) - \mathbf{X}_T(0)]^2 \rangle \propto t^{\alpha/2}$.

(7) The *first-passage* time density for a tracer in a homogeneous system has been discussed in Ref. [36]. An open single-file system (the interval with at least one absorbing boundary) has been studied numerically for a biased SFD [114], for an unbiased SFD [15] (briefly discussed as a particular example), and analytically for an unbiased diffusion in Refs. [4–6]. The latter works form a basis of the following Chaps. 3 and 4. A closely related problem of orders statistics of first-passage times for independent random walkers [115–125] will be discussed in a more detail in Chap. 3.

Last but not least, in the above brief review we have restricted ourselves mainly to the physically-oriented literature. Rigorous (mathematical) results concerning the dynamics of the tracer can be found in the following references. Besides the seminal works of Harris [2] and Spitzer [126], central limit theorems for a tagged particle are discussed in Refs. [54, 69, 127], and reviewed in Ref. [128].

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