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# Diffusion of tagged particle in an exclusion process

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We study the diffusion of tagged hard-core interacting Brownian point particles under the influence of an external force field in one dimension. Using the Jepsen line we map this many-particle problem onto a single particle one. We obtain general equations for the distribution and the mean-square displacement $\langle (x_T)^2\rangle$ of the tagged center particle valid for rather general external force fields and initial conditions. The case of symmetric distribution of initial conditions around the initial position of the tagged particle on $x=0$ and symmetric potential fields $V(x)=V(-x)$ yields zero drift $\langle x_T\rangle=0$ and is investigated in detail. We find $\langle (x_T)^2\rangle=\mathcal{R}(1-\mathcal{R})/2Nr^2$ where $2N$ is the (large) number of particles in the system. $\mathcal{R}$ is a single particle reflection coefficient, i.e., the probability that a particle *free of collisions* starts on $x_0>0$ and remains in $x>0$ while $r$ is the probability density of noninteracting particles on the origin. We show that this equation is related to the mathematical theory of order statistics and it can be used to find $\langle (x_T)^2\rangle$ even when the motion between collision events is not Brownian (e.g., it might be ballistic or anomalous diffusion). As an example we derive the Percus relation for non-Gaussian diffusion. A wide range of physical behaviors emerge which are very different than the classical single file subdiffusion $\langle (x_T)^2\rangle \sim t^{1/2}$ found for uniformly distributed particles in an infinite space and in the absence of force fields.

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## I. INTRODUCTION

Systems of particles governed by stochastic dynamics and exclusion interactions have been studied for a long time [1–3]. One aspect of this problem is the motion of a tagged particle sometimes called the tracer particle [4–7]. The diffusion of a tagged particle, in a one-dimensional system of Brownian particles, interacting via hard-core interaction is a model for the motion of a single molecule in a crowded one-dimensional environment such as a biological pore or channel [8–11], and in experimentally studied physical systems such as zeolites [12], confined colloid particles [13–15], and charged spheres in circular channels [16]. Since particles do not pass each other such diffusion processes are called single file diffusion.

Confinement of a tagged Brownian particle, due to its interaction with other Brownian particles, leads to a slowdown of the diffusion of the tagged particle $\langle (x_T)^2\rangle \propto t^{1/2}$ instead of normal diffusion $\langle (x_T)^2\rangle \propto t$ when the particles in the system are uniformly distributed [4,6]. Such many-body problems can be treated using methods which exploit the relation between the dynamics of the interacting tagged particle and the motion of a particle free of interactions [5,6,17–20]. In recent years at least seven new directions of research emerged. (i) The effect of an external field acting on all the particles [21] or on the tagged particle only [22,23] has attracted attention since pores induce entropic barriers [10] and are generally inhomogeneous. In this category the examples of single file motion in a periodic potential [24] or in a box [25] were considered in detail. (ii) Initial conditions may have a profound impact on diffusion of the tagged particle. For example, if particles start as a narrow Gaussian packet the diffusion of the tagged center particle increases linearly in time $\langle (x_T)^2\rangle \propto t$ [26] (see details below). Power-law initial conditions induce $\langle (x_T)^2\rangle \propto t^{\xi}$ and $\xi$ is neither 1 nor 1/2 [27] (see further details in text). When an external field is acting on the system, it is important to consider nonuniform initial conditions where the density of particles is determined naturally from Boltzmann's distribution. In addition the method of averaging plays a crucial role [28,29]. For example, if we start from a fixed configuration of initial conditions (drawn from the stationary distribution) and average only over stochastic trajectories the behavior of tagged particle fluctuations is qualitatively different compared with the usual procedure of averaging, which involves an average both over initial conditions (drawn from the stationary distribution) and over the noise generating the stochastic trajectories. (iii) In some investigations the underlying motion is not normal diffusion, instead the particles may be non-Brownian, and following anomalous kinetics [27,30]. (iv) Usually hard-core interactions are considered, although the hard problem of more general interactions has been recently treated in [23,31,32]. Screened hydrodynamic interactions which seem important at short times were investigated in [33] both theoretically and experimentally. Granular single file diffusion with inelastic collisions shows the typical $t^{1/2}$ subdiffusion [34,35]. (v) In the presence of a constant drift force several interesting effects are found [36]. Among the more recent findings are oscillations in the mean-square displacement [29] which are due to finite-size effects. (vi) Interacting particles in systems with quenched disorder is yet another challenge. The motion of a tagged particle was recently treated in the context of single file diffusion in the Sinai model [37]. (vii) Finally, if the motion of the tagged particle is not normal Brownian motion, what stochastic theory replaces the usual Brownian-Langevin framework? In this direction interesting connections to fractional calculus emerged [23,38,39]. Roughly speaking and under certain conditions half order time derivatives ($d^{1/2}/dt^{1/2}$) enter in the Langevin equation [23] and fractional Brownian noise replaces white noise.

Here we provide a general theory of single file diffusion of the center tagged particle, valid in the presence or the absence of an external potential field $V(x)$, as well as for thermal and nonthermal initial conditions. Our main results reproduce previously obtained formulas and many new ones by mapping the many-particle problem onto a single particle model. Our method, explained in Sec. II, exploits the theoretical concept of the Jepsen line [5], is limited to hard-core point particles, but, as we show in Sec. V, is not limited to Brownian particles. After providing general results in Sec. III we limit our attention to symmetric initial conditions and potentials where the tagged particle has no average drift. A general relation between the mean-square displacement of the tagged particle and reflection probability of the noninteracting particle is given in Eq. (41). Detailed calculations of the mean-square displacement of the tagged particle then follow, for special choices of force fields and initial conditions, in Sec. IV. As we discuss in Sec. III D, in certain limits our problem is related to order statistics [40], a fact worth mentioning since it allows us to solve our problem and related ones using known methods. In Sec. V, we discuss non-Brownian kinds of motion and the Percus relation. A brief report of part of our results was recently published [21].

## II. MODEL AND METHODS

In our model, $2N+1$ identical point particles with hard-core particle-particle interactions are undergoing Brownian motion in one dimension, so particles cannot pass each other. The diffusion constant of particles free of interaction is $D$. As mentioned, toward the end of the paper we discuss the more general case where the dynamics between collision events is not necessarily Brownian. An external potential $V(x)$ acts on the particles. The system stretches from $-\bar{L}$ to $\bar{L}$; however, unless stated otherwise we will let $\bar{L}\to\infty$ and obtain a thermodynamic limit where $N/\bar{L}$ is fixed. We tag the center particle, which clearly has $N$ particles to its left and $N$ to it right. Initially the tagged particle is at the origin $x=0$. The motion of a single particle in the absence of interactions with other particles is described by a single particle Green function $g(x,x_0,t)$, with the initial conditions $g(x,x_0,0)=\delta(x-x_0)$. In the case of over damped Brownian motion the Green function is the solution of the Fokker-Planck equation [41].

$$\frac{\partial g(x,x_0,t)}{\partial t} = D\left[\frac{\partial^2}{\partial x^2} - \frac{1}{k_b T}\frac{\partial}{\partial x}F(x)\right]g(x,x_0,t), \qquad (1)$$

where $F(x)=-V'(x)$ is the force field, $T$ is the temperature, and $k_b$ is Boltzmann's constant. The initial conditions of $N$ particles residing initially to the right (left) of the test particle are drawn from the probability density function (PDF) $f_R(x_0)$ ($f_L(x_0)$), respectively. We consider an ensemble of trajectories and average over trajectories and initial conditions (see details below). Our goal is to obtain the PDF $P(x_T)$ where $P(x_T)dx_T$ is the probability of finding the tagged particle in a small interval $(x_T,x_T+dx)$.

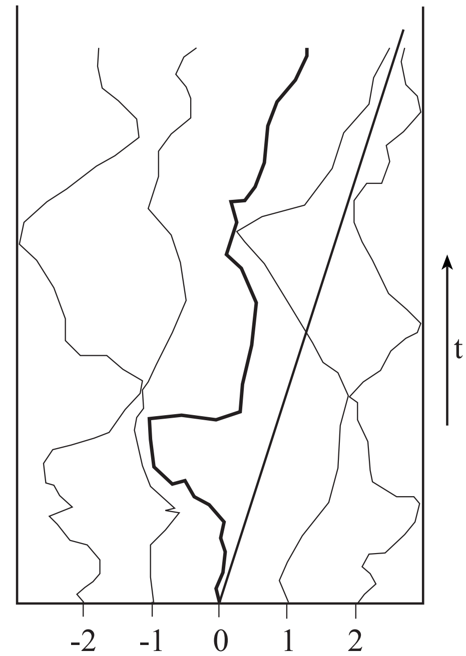


FIG. 1. Schematic motion of Brownian particles in a box, where particles cannot penetrate through each other. The center tagged particle label is 0, its trajectory is restricted by collisions with neighboring particles. The straight line is the Jepsen line, it follows $vt$ as explained in the text. In an equivalent noninteracting picture, we allow particles to pass through each other, and at time $t$ we search for the position of the particle which has $N$ particles to its right and $N$ to its left (i.e., the center particle).

### Jepsen line

A schematic diagram of the problem is presented in Fig. 1 for particles in a box. Initial positions of particles are given by $x_0^j$ where $j=-N,\ldots,0,\ldots N$ where $j$ is the label of the interacting particles (see Fig. 1). The tagged particle whose coordinate is denoted with $x_T(t)$, is the center particle $j=0$ (bold line in Fig. 1). Initially the tagged particle is at the origin $x_T(0)=0$. Since particles do not pass each other, their order is clearly maintained, and the number of particles to the left and right of the tagged particle $N$ is fixed.

In Fig. 1 the straight line which starts at $x=0$ is called the Jepsen line and follows $x(t)=vt$, where $v$ is a test velocity [5,6]. We label the interacting particles according to their initial position, increasing to the right (see Fig. 1). The tagged particle starts just to the right of the Jepsen line so at $t=0$ the label of the particle to the right of the Jepsen line is zero. In this system we have $2N+1$ particles. Hence initially we have $N$ particles to the left of the Jepsen line and including the tagged particle $N+1$ particles to the right.

Let $\tilde{\alpha}(t)$ be the label number of the first particle situated to the right of the Jepsen line. According to our rules, at $t=0$ we have $\tilde{\alpha}=0$, and then the random variable $\tilde{\alpha}$ will increase or decrease in steps of $+1$ or $-1$ according to:

(i) if a particle crosses the Jepsen line from left to right $\tilde{\alpha}\to\tilde{\alpha}-1$;

(ii) if a particle crosses the Jepsen line from right to left $\tilde{\alpha}\to\tilde{\alpha}+1$. Thus the counter $\tilde{\alpha}$ is performing a random walk decreasing or increasing its value $+1$ or $-1$ at random times.

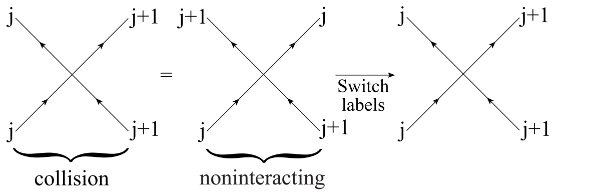


FIG. 2. In one dimension, the paths of a pair of particles in a hard-core collision event can be represented by two noninteracting particles which pass through each other, and then their label numbers are switched.

A collision between two hard-core particles is represented schematically in Fig. 2. In one dimension a hard-core collision event is equivalent to two particles that pass through each other, i.e., noninteracting particles, and then after the particles cross each other, the labels of the pair of particles are switched (see Fig. 2). Instead of relabeling particles after each collision, we let particles pass through each other, and then at time $t$ we label our particles (or if we are interested only in tagged particle, locate the central particle). Operationally this means that in the time interval $(0,t)$ we view the particles as noninteracting, and then find the particle with $N$ particles to its right and $N$ to its left, which is equivalent to the tagged particle in the interacting system. Hence the problem is related to the mathematical topic of order statistics [40] as we will discuss briefly later.

Following Jepsen [5] and Levitt [6] we introduce the stochastic process for the noninteracting particles $\alpha(t)$ where:

(i) if a particle crosses the Jepsen line from left to right $\alpha \to \alpha - 1$;

(ii) if a particle crosses the Jepsen line from right to left $\alpha \to \alpha + 1$. The process $\alpha(t)$ is the same as the process $\tilde{\alpha}(t)$, in statistical sense.

As mentioned our goal is to find the PDF $P(x_T)$ which is related to the probability that $x_t < vt$ in the usual way

$$\Pr(x_T < vt) = \int_{-\infty}^{vt} P(x_T) dx_T. \tag{2}$$

Let $P_N(\alpha)$ be the probability of the random variable $\alpha$. The event $x_T < vt$ is statistically equivalent to finding $\alpha = 1$ or $\alpha = 2$ etc since if $\alpha \geq 1$ we have particle label $\alpha \geq 1$ to the right of the Jepsen line (hence the tagged particle is to the left of the line $x_T < vt$). Hence

$$\Pr(x_T < vt) = \sum_{\alpha=1}^{N} P_N(\alpha). \tag{3}$$

So our plan is to find $P_N(\alpha)$ and then using Eqs. (2) and (3) we will get $P(x_T)$. Note that from Eqs. (2) and (3) it becomes clear that the straight Jepsen line following $vt$ is merely a tool which could be replaced by any deterministic trajectory.

The random variable $\alpha$ is a sum of many random variables

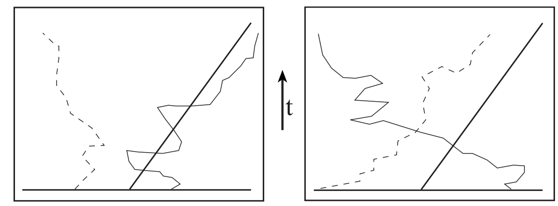


FIG. 3. Trajectories crossing the Jepsen line. In the left panel one particle started on $L$ and ended on $L$ the other on $R$ and ended on $R$. These two paths are assigned the probability $P_{LL}(x_0^{-1})P_{RR}(x_0^{1})$ and yield in Eq. (6) $\alpha = 0$. Similarly the trajectories on the right panel correspond to $P_{LL}(x_0^{-1})P_{RL}(x_0^{1})$ and they contribute $\alpha = 1$.

$$\alpha = \sum_{j=-N}^{N} \delta\alpha_j \tag{4}$$

where $\delta\alpha_j$ is the number of times particle $j$ crossed the Jepsen line from right to left minus the number of times it crossed the line from left to right. Clearly $\delta\alpha_j$ may attain the values $-1$ or 0 if the particle started on the left, or 1 or 0 if it started on the right. Since we are interested in the large $N$ limit we may neglect the contribution of $\delta\alpha_0$, which is indicated by the prime in the sum [42].

We calculate the probability $P_N(\alpha)$ of the random variable $\alpha$. For that we designate $P_{LL}(x_0^{-j})$, the probability that particle $-j$, starting to the left of the Jepsen line at $t=0$ at $x_0^{-j} < 0$, is found at time $t$ to the left of the Jepsen line. Clearly for the corresponding trajectory $\delta\alpha_{-j} = 0$ since the particle crossed the Jepsen line an even number of times or did not cross it at all. Similarly, $P_{LR}(x_0^{-j})$ is the probability to start to the left of the line and end to its right, and $P_{RR}(x_0^{j})$, $P_{RL}(x_0^{j})$ are defined similarly for particles starting on $x_0^{j} > 0$ to the right of the line.

In our noninteracting picture, the motion of particles is independent, hence we can use random-walk theory [43] and Fourier series to find $P_N(\alpha)$. It is convenient to rewrite Eq. (4)

$$\alpha = \sum_{j=1}^{N} \Delta\alpha_j \tag{5}$$

where $\Delta\alpha_j = \delta\alpha_j + \delta\alpha_{-j}$ may attain the values 1, 0, and $-1$. Each summand $\Delta\alpha_j$ takes into account one particle starting to the left of the Jepsen line and one to the right.

First consider $N=1$, that is one particle that starts on the left of the Jepsen line and one to its right. Then $\alpha = \Delta\alpha_1 = \delta\alpha_1 + \delta\alpha_{-1}$ and as mentioned $\alpha = 1$ or 0 or $-1$. Examples for possible trajectories are shown in Fig. 3. It is easy to see that

$$P_{N=1}(\alpha) = \begin{cases} \alpha = 1 & P_{RL}(x_0^{1})P_{LL}(x_0^{-1}) \\ \alpha = 0 & P_{LL}(x_0^{-1})P_{RR}(x_0^{1}) + P_{LR}(x_0^{-1})P_{RL}(x_0^{1}) \\ \alpha = -1 & P_{RR}(x_0^{1})P_{LR}(x_0^{-1}). \end{cases} \tag{6}$$

We define the structure function

$$\lambda(\phi,x_0^{-j},x_0^j) = e^{i\phi}P_{LL}(x_0^{-j})P_{RL}(x_0^j) + [P_{LL}(x_0^{-j})P_{RR}(x_0^j) + P_{LR}(x_0^{-j})P_{RL}(x_0^j)] + e^{-i\phi}P_{LR}(x_0^{-j})P_{RR}(x_0^j). \quad (7)$$

The structure function describes a single step in random-walk Eq. (5) in the following usual way: the coefficient of $\exp(i\phi)$ is the probability that $\Delta\alpha_j$ is equal one (i.e., $P_{LL}P_{RL}$), the coefficient of $\exp(i\phi)=1$ (i.e., $\phi=0$) yields the probability $\Delta\alpha_j=0$, and similarly for $\exp(-i\phi)$. Since the summands in Eq. (5) are independent, Fourier analysis gives

$$P_N(\alpha) = \frac{1}{2\pi}\int_{-\pi}^{\pi} d\phi \Pi_{j=1}^{N}\lambda(\phi,x_0^{-j},x_0^j)e^{-i\alpha\phi}. \quad (8)$$

We average Eq. (8) with respect to the initial conditions $x_0$ which are assumed independent identically distributed random variable and we find

$$\langle P_N(\alpha)\rangle = \frac{1}{2\pi}\int_{-\pi}^{\pi} d\phi\langle\lambda(\phi)\rangle^N e^{-i\alpha\phi} \quad (9)$$

where from Eq. (7)

$$\langle\lambda(\phi)\rangle = e^{i\phi}\langle P_{LL}\rangle\langle P_{RL}\rangle + \langle P_{LL}\rangle\langle P_{RR}\rangle + \langle P_{LR}\rangle\langle P_{RL}\rangle + e^{-i\phi}\langle P_{LR}\rangle\langle P_{RR}\rangle. \quad (10)$$

Here $\langle P_{ij}\rangle$ is the probability of starting in $i=L,R$ (relative to the Jepsen line) and ending in $j=L,R$ and $\langle\cdots\rangle$ denotes an average over initial condition. The probability $\langle P_{LR}\rangle$ is given in terms of the Green's function of the noninteracting particle $g(x,x_0,t)$ and the initial density of particles situated initially to the left of the Jepsen line $f_L(x_0)$

$$\langle P_{LR}(vt)\rangle = \int_{-\bar{L}}^{0} f_L(x_0)\int_{vt}^{\bar{L}} g(x,x_0,t)dxdx_0. \quad (11)$$

We see that for $\langle P_{LR}\rangle$ we average over initial conditions in the domain $(-\bar{L},0)$ weighted by $f_L(x_0)$ (since the starting point is to the left of the Jepsen line) and also integrate over $x$ in the domain $(vt,\bar{L})$ with the weight $g(x,x_0,t)$ (since the end point is to the right of the line). Similarly

$$\langle P_{RR}(vt)\rangle = \int_{0}^{\bar{L}} f_R(x_0)\int_{vt}^{\bar{L}} g(x,x_0,t)dxdx_0. \quad (12)$$

As mentioned $f_L(x_0)$ $[f_R(x_0)]$ is the PDF of initial positions of particles that initially are at $x_0<0$ $(x_0>0)$, respectively; hence, $f_L(x_0)=0$ when $x_0>0$ and $\int_{-\bar{L}}^{0} f_L(x_0)dx_0=1$, while $f_R(x_0)$ is normalized and nonzero only in $(0,\bar{L})$. $\langle P_{LL}\rangle$ and $\langle P_{RR}\rangle$ are defined similarly, and they satisfy $\langle P_{LL}\rangle=1-\langle P_{LR}\rangle$, and $\langle P_{RL}\rangle=1-\langle P_{RR}\rangle$.

## III. DYNAMICS OF THE TAGGED PARTICLE

We now apply the central limit theorem to analyze sum Eq. (5) using Eq. (9) when $N\to\infty$. The small $\phi$ expansion of structure function Eq. (10) is

$$\langle\lambda(\phi)\rangle = 1 + i\langle\Delta\alpha\rangle\phi - \frac{1}{2}\langle(\Delta\alpha)^2\rangle\phi^2 + O(\phi^3) \quad (13)$$

where

$$\langle\Delta\alpha\rangle = \langle P_{RL}\rangle - \langle P_{LR}\rangle \quad (14)$$

as expected, and the variance $\sigma_{\Delta\alpha}^2=\langle(\Delta\alpha)^2\rangle-\langle\Delta\alpha\rangle^2$ is

$$\sigma_{\Delta\alpha}^2 = \langle P_{RL}\rangle\langle P_{RR}\rangle + \langle P_{LR}\rangle\langle P_{LL}\rangle. \quad (15)$$

According to the central limit theorem in the large $N$ limit

$$P_N(\alpha) \sim \frac{1}{\sqrt{2\pi N}\sigma_{\Delta\alpha}}\exp\left[-\frac{(\alpha-N\langle\Delta\alpha\rangle)^2}{2N\sigma_{\Delta\alpha}^2}\right]. \quad (16)$$

This simple result, valid for a large class of Green's functions and initial conditions, is suited for the investigation of a large number of single file problems.

To find the distribution of $x_T$ we use Eqs. (3) and (16) replacing a sum with an integral

$$\Pr(x_T < vt) \sim \frac{1}{\sqrt{2\pi N}\sigma_{\Delta\alpha}}\int_0^{\infty}\exp\left(-\frac{(\alpha-N\langle\Delta\alpha\rangle)^2}{2N\sigma_{\Delta\alpha}^2}\right)d\alpha. \quad (17)$$

Changing variables according to $\eta=(\alpha-N\langle\Delta\alpha\rangle)/\sqrt{N}\sigma_{\Delta\alpha}$ we have

$$\Pr(x_T < vt) \sim \frac{1}{\sqrt{2\pi}}\int_{-\langle\Delta\alpha\rangle\sqrt{N}/\sigma_{\Delta\alpha}}^{\infty}\exp\left(-\frac{\eta^2}{2}\right)d\eta \quad (18)$$

which is the main result so far. Taking the derivative of Eq. (18) with respect to $vt$, following Eq. (2) switching $vt\to x_T$, and using Eqs. (14) and (15) we find the PDF of the tagged particle position

$$P(x_T) \sim C\exp\left\{-\frac{N[\langle P_{LR}(x_T)\rangle - \langle P_{RL}(x_T)\rangle]^2}{2[\langle P_{LL}(x_T)\rangle\langle P_{LR}(x_T)\rangle + \langle P_{RR}(x_T)\rangle\langle P_{RL}(x_T)\rangle]}\right\}. \quad (19)$$

In this large $N$ limit we neglected small corrections depending on $x_T$ in the prefactor of the exp, namely $C$ is a normalization constant independent of $x_T$. Equation (19) is a starting point for further approximation: below we expand the expression in the exponent around its extremum exploiting the fact that $N$ is large [see Eqs. (25), (30), and (40)]. In Eq. (19) and what follows $\langle P_{ij}(x_T)\rangle$ is given by Eqs. (11) and (12) with $vt\to x_T$. Equation (19) yields the PDF of the center particle $P(x_T)$ in terms of $\langle P_{ij}(x_T)\rangle$ which according to Eq. (12) depends on the free particle Green's function and the initial conditions. Thus the information contained in the noninteracting Green function is sufficient for the determination of the single file diffusion of the tagged particle [44].

### A. Thermal equilibrium

In the long time limit, and in the presence of a binding potential field, e.g., harmonic field or particles in a box, an equilibrium is reached. Then initial conditions do not play a role. For example, $\langle P_{LR}(x_T)\rangle = P_R^{\text{eq}}(x_T)$ with

$$P_R^{\text{eq}}(x_T) = \frac{1}{Z}\int_{x_T}^{\bar{L}} \exp\left(-\frac{V(x)}{k_b T}\right)dx \tag{20}$$

where $Z$ is the normalizing partition function

$$Z = \int_{-\bar{L}}^{\bar{L}} \exp\left[-\frac{V(x)}{k_b T}\right]dx. \tag{21}$$

Similarly

$$P_L^{\text{eq}}(x_T) = \frac{1}{Z}\int_{-\bar{L}}^{x_T} \exp\left(-\frac{V(x)}{k_b T}\right)dx. \tag{22}$$

In Eqs. (20) and (22) we used the steady-state solution, $\lim_{t\to\infty} g(x,x_0,t) = \exp[-V(x)/k_b T]/Z$, which is Boltzmann's distribution suited for a system in thermal equilibrium. Using Eq. (19) the position PDF of the tagged particle is $\lim_{t\to\infty} P(x_T) = P^{\text{eq}}(x_T)$

$$P^{\text{eq}}(x_T) \sim C\exp\left\{-\frac{N[\langle P_R^{\text{eq}}(x_T)\rangle - \langle P_L^{\text{eq}}(x_T)\rangle]^2}{4\langle P_L^{\text{eq}}(x_T)\rangle\langle P_R^{\text{eq}}(x_T)\rangle}\right\}. \tag{23}$$

If the potential is symmetric $V(x)=V(-x)$, e.g., particles in a box or harmonic field, we have for not too large $x_T$, $P_L^{\text{eq}}(x_T)\simeq 1/2$, $P_R^{\text{eq}}(x_T)\simeq 1/2$; hence, from Eq. (19)

$$P^{\text{eq}}(x_T) \sim C\exp\{-N[\langle P_R^{eq}(x_T)\rangle - \langle P_L(x_T)\rangle]^2\}. \tag{24}$$

Expanding the expression in the exponent in $x_T$ (since $N$ is large) we find using Eqs. (20), (22), and (23)

$$P^{\text{eq}}(x_T) \sim \frac{2\sqrt{N}}{\sqrt{\pi}Z}\exp\left[-\frac{4N}{Z^2}(x_T)^2\right] \tag{25}$$

where with out loss of generality we assigned $V(x=0)=0$. Hence the standard deviation is

$$\langle (x_T)^2\rangle \sim \frac{Z^2}{8N}. \tag{26}$$

The same expression is found in the Appendix using the many-body Boltzmann distribution, and integrating over all the particles except the tagged particle.

### B. Simple illustration

We now consider the situation of particles free of a force $F(x)=0$ with open boundary conditions $\bar{L}\to\infty$ where initially all the particles are on the vicinity of the origin. More precisely, the tagged particle is initially situated at $x_T=0$, $N$ particles to its right on $\epsilon\to 0^+$ and $N$ particles on $-\epsilon$. This problem was solved already by Aslangul [26], and here we recover the known result using our formulas. The Green's function $g(x,x_0,t)$ of a free particle is

$$g(x,x_0,t) = \frac{\exp\left[-\frac{(x-x_0)^2}{4Dt}\right]}{\sqrt{4\pi Dt}} \tag{27}$$

where as mentioned $D$ is the diffusion coefficient of the free particle. With the specified initial conditions we have

$$\langle P_{RL}(x_T)\rangle = \lim_{\epsilon\to 0}\int_0^\infty \delta(x_0-\epsilon)\int_{-\infty}^{x_T}\frac{\exp\left[-\frac{(x-x_0)^2}{4Dt}\right]}{\sqrt{4\pi Dt}}dxdx_0$$
$$= \frac{1}{2} + \int_0^{x_T}\frac{e^{-x^2/4Dt}}{\sqrt{4\pi Dt}}dx. \tag{28}$$

Similarly

$$\langle P_{LR}(x_t)\rangle = \frac{1}{2} - \int_0^{x_T}\frac{e^{-x^2/4Dt}}{\sqrt{4\pi Dt}}dx. \tag{29}$$

When $x_T \ll \sqrt{2Dt}$ we Taylor expand in $x_T$ to find $(\langle P_{LR}\rangle - \langle P_{RL}\rangle)^2 \sim (x_T)^2/\pi Dt$, using Eq. (19) we recover the result in [26]

$$P(x_T) \sim \frac{1}{\pi}\sqrt{\frac{N}{Dt}}\exp\left[-\frac{N(x_T)^2}{\pi Dt}\right], \tag{30}$$

hence

$$\langle (x_T)^2\rangle \sim \frac{\pi Dt}{2N}. \tag{31}$$

The diffusion is normal in the sense that the mean-square displacement increases linearly in time. However the diffusion of the tagged particle is slowed down compared with a free particle by a factor of $1/N$ which is due to the collisions with all other Brownian particles in the system. Clearly the approximation breaks down if one is interested in the tails of $P(x_T)$ since we used $x_T \ll \sqrt{2Dt}$. Though clearly when $N$ is large, the probability of finding such a particle is extremely small [i.e., use Eq. (30) $P(x_T=\sqrt{2Dt}) \sim \exp(-N2/\pi)$].

### C. Formula for $\langle (x_T)^2\rangle$

We now consider symmetric potential fields $V(x)=V(-x)$ and symmetric initial conditions. The latter means that the density of particles at time $t=0$ to the left of the tagged particle, i.e., those residing in $x_0<0$, is the same as for those residing to the right, $f_R(x_0)=f_L(-x_0)$ (e.g., uniform initial conditions). In this case the subscript $R$ and $L$ is redundant and we use $f(x_0)=f_R(x_0)=f_L(-x_0)$, where $f(x_0)=0$ if $x_0<0$, $f(x_0)\geq 0$, and $\int_0^\infty f(x_0)dx_0=1$. From symmetry it is clear that the tagged particle is unbiased, namely, $\langle x_T\rangle=0$. Further, since $N$ is large we may expand the expressions in the exponent in Eq. (19) in $x_T$ to obtain the leading term

$$\langle P_{RL}\rangle - \langle P_{LR}\rangle = \frac{\partial}{\partial x_T}[\langle P_{RL}(x_T)\rangle - \langle P_{LR}(x_T)\rangle]\Big|_{x_T=0} x_T + O[(x_T)^2]. \tag{32}$$

Similarly for small $x_T$

$$\langle P_{LL}\rangle\langle P_{LR}\rangle + \langle P_{RR}\rangle\langle P_{RL}\rangle = 2\langle P_{RR}(x_T)\rangle[1 - \langle P_{RR}(x_T)\rangle]|_{x_T=0} + O(x_T). \tag{33}$$

To derive Eq. (32) we used the symmetry of the problem, which means that the probability of crossing the point $x_T=0$ from left to right is the same as the probability to cross from right to left $\langle P_{LR}\rangle_{x_T=0}=\langle P_{RL}\rangle_{x_T=0}$ and similarly $\langle P_{LL}\rangle_{x_T=0}=\langle P_{RR}\rangle_{x_T=0}$ by symmetry. We designate the reflection coefficient,

$$\mathcal{R} = \langle P_{RR}\rangle_{x_T=0} \tag{34}$$

[or $\mathcal{R}=\langle P_{LL}\rangle_{x_T=0}$] since it is the probability that a particle starting at $x_0>0$ is found in $x>0$ at time $t$ when an average over initial conditions is made

$$\mathcal{R} = \int_0^{\bar{L}} f(x_0)\int_0^{\bar{L}} g(x,x_0,t)dxdx_0. \tag{35}$$

A transmission coefficient is defined through $\mathcal{T}=\langle P_{RL}\rangle_{x_T=0}=\langle P_{LR}\rangle_{x_T=0}$ which is related to the reflection coefficient in the usual way $\mathcal{T}=1-\mathcal{R}$.

Turning our attention to Eq. (32), from left-right symmetry we have

$$\frac{\partial}{\partial x_T}\langle P_{RL}(x_T)\rangle\Big|_{x_T=0} = -\frac{\partial}{\partial x_T}\langle P_{LR}(x_T)\rangle\Big|_{x_T=0}. \tag{36}$$

Hence we define

$$r = \frac{\partial}{\partial x_T}\langle P_{RL}(x_T)\rangle\Big|_{x_T=0} \tag{37}$$

where from Eq. (12)

$$r = \int_0^{\bar{L}} f(x_0)g(0,x_0,t)dx_0. \tag{38}$$

So $r$ is the density of noninteracting particles at $x=0$ for an initial density $f(x_0)$. Note that since $\langle P_{RL}(x_T)\rangle+\langle P_{RR}(x_T)\rangle=1$ we have

$$r = -\frac{\partial}{\partial x_T}\langle P_{RR}(x_T)\rangle\Big|_{x_T=0}. \tag{39}$$

Inserting Eq. (37) in Eq. (32) using Eq. (36) we have $\langle P_{RL}\rangle-\langle P_{LR}\rangle=2rx_T+\cdots$. Inserting Eq. (34) in Eq. (33) we find our main result: the probability density function of the position of the tagged central particle

$$P(x_T) \sim \frac{1}{\sqrt{2\pi\langle(x_T)^2\rangle}}\exp\left[-\frac{(x_T)^2}{2\langle(x_T)^2\rangle}\right], \tag{40}$$

where

$$\langle(x_T)^2\rangle = \frac{\mathcal{R}(1-\mathcal{R})}{2Nr^2} \tag{41}$$

is the mean-square displacement of the tagged particle. The single particle probability $\langle P_{RR}(x_T)\rangle$ gives $\mathcal{R}$ Eq. (34) and $r$ Eq. (39) which in turn yield the mean-square displacement of tagged particle Eq. (41). We will soon use this equation to demonstrate a variety of physical behaviors. However first we establish a connection between our work and the theory of order statistics.

### D. Order statistics

We generate $n$ independent identically distributed random variables drawn from a PDF $\hat{r}(x)$ and arrange them in increasing order. Order statistics deals with the $m$th observable $m=1,\ldots,n$ among $n$ observations taken in the increasing order, which is denoted $x_m$. The PDF of $x_m$, $\phi(x_m)$ depends on the PDF $\hat{r}(x)$, the sample size $n$, and the order $m$. Let $\hat{R}(x)$ be the cumulative distribution of $x$; e.g., if the domain of $x$ is $-\infty<x<\infty$, $\hat{R}(x)=\int_{-\infty}^{x}\hat{r}(x)dx$ as usual. Following well-known result [40], define $\hat{x}$ with

$$\hat{R}(\hat{x}) = \frac{m}{n+1} \tag{42}$$

then when $n$ is large and $m/n$ is of the order 1/2,

$$\phi(x_m) = \text{const}\exp\left\{-\frac{n(x-\hat{x})^2\hat{r}^2(\hat{x})}{2\hat{R}(\hat{x})[1-\hat{R}(\hat{x})]}\right\}. \tag{43}$$

Hence the variance of $x_m$,

$$(\sigma_m)^2 = \frac{\hat{R}(\hat{x})[1-\hat{R}(\hat{x})]}{n\hat{r}^2(\hat{x})} \tag{44}$$

which has some resemblance to Eq. (41).

The problem of the motion of a tagged particle is mathematically identical to the problem of order statistics in two cases: (i) in the presence of a binding potential and in the long time limit and (ii) when all the particles start on the same point. In both cases the single particle PDF $g(x,x_0,t)$ of all the particles are identical since it is either independent of $x_0$ [case (i)] or we have a unique initial condition (case treated in Sec. III B). For example, in the presence of a binding field $\lim_{t\to\infty} g(x,x_0,t)=\exp[-V(x)/k_bT]/Z$ which is independent of the initial position of the particle. Hence in equilibrium, to find the center particle we may draw $(2N+1)$ random variables from Boltzmann's distribution and search for the center particle (which will give the position of the interacting tagged particle) or, using the language of order statistics, we have $\hat{r}(x)=\exp[-V(x)/k_bT]/Z$. Using a symmetric potential $V(x)=V(-x)$ and Eq. (42) we insert $n=2N+1$, and $m=N+1$; hence, when $N$ is large we have

$$\hat{R}(\hat{x}) = \int_{-\infty}^{\hat{x}} \frac{\exp\left[-\frac{V(\hat{x})}{k_bT}\right]}{Z}dx = \frac{1}{2}. \tag{45}$$

Thus, $\hat{x}=0$. Then using Eq. (44) we find

$$\langle (x_T)^2 \rangle = \frac{Z^2}{8N} \tag{46}$$

which is the same as Eq. (26) [recall $V(0)=0$].

While Eq. (44) has superficially a structure similar to Eq. (41) they are different. Our $\mathcal{R}$ Eq. (34) is generally not equal half but neither must it be close to that value [so Eq. (42) is not generally related to our problem]. In fact when $t \to 0$ we must have $\langle (x_T)^2 \rangle \to 0$ which is found when $\lim_{t\to 0} \mathcal{R}=1$ (see examples below). In the problem of motion of a tagged particle, the number of particles which can interact with the center particle is usually increasing with time (hence $n$ is not fixed). For example, consider the classical case of uniformly distributed particles in infinite space and in the absence of forces. Roughly speaking particles at distances of the order of $l_{\text{eff}}=\sqrt{Dt}$ or shorter can influence the tagged particle motion via collisions. So in this case roughly $N_{\text{eff}}=\rho\sqrt{Dt}$ particles participate in the process. In contrast, if all particles are initially at the vicinity of the origin $N$ particles participate, i.e., influence the motion of the tagged particle. Interestingly this gives an argument for the well-known behavior of the mean-square displacement of the tagged particle, with uniform density of particles, namely, use Eq. (31) $\langle (x_T)^2 \rangle \sim \pi D t/2N$ and replace $N$ with $N_{\text{eff}}=\rho\sqrt{Dt}$ to find $\langle (x_T)^2 \rangle \simeq \sqrt{Dt}/\rho$ which of course misses the correct numerical prefactor (see Eq. (54) below).

## IV. PHYSICAL ILLUSTRATIONS

### A. Particles in a box

Consider particles in a finite box extending from $-\bar{L}$ to $\bar{L}$ which was recently treated with the Bethe ansatz and numerical simulations by Lizana and Ambjörnson [25]. The tagged particle initially at $x_T=0$ has $N$ particles to its right and $N$ to its left. These particles are assumed uniformly distributed; hence,

$$f(x_0) = \begin{cases} \dfrac{1}{\bar{L}} & 0 < x_0 < \bar{L} \\ 0 & \text{otherwise} \end{cases}. \tag{47}$$

In the limit $\bar{L}\to\infty$ and $N\to\infty$ in such a way that the density $\rho=N/\bar{L}$ is fixed, we obtain single file diffusion in an infinite system, a case well studied long ago [4,6].

The single particle Green's function of a particle in a box, with reflecting boundary conditions $\partial g(x,x_0,t)/\partial x|_{x=\pm\bar{L}}=0$ is solved using an eigenfunction expansion [41]

$$g(x,x_0,t) = \frac{1}{2\bar{L}} + \frac{1}{\bar{L}}\sum_{n=1}^{\infty} \cos\left[\frac{n\pi}{2\bar{L}}(x+\bar{L})\right]\cos\left[\frac{n\pi}{2\bar{L}}(x_0 + \bar{L})\right]\exp\left(-D\frac{n^2\pi^2}{4\bar{L}^2}t\right). \tag{48}$$

With Eqs. (35), (47), and (48) we find

$$\mathcal{R}(t) = \frac{1}{2} + \frac{4}{\pi^2}\sum_{n=1,\text{Odd}}^{\infty} \frac{\exp\left(-D\frac{n^2\pi^2}{4\bar{L}^2}t\right)}{n^2} \tag{49}$$

where the summation is over odd $n$. At $t=0$, $\mathcal{R}=1$ since all particles initially in $(0,\bar{L})$ did not have time to move to the other side of the box, and $\lim_{t\to\infty}\mathcal{R}=1/2$ since in the long time limit there is equal probability for a noninteracting particle to occupy each half of the box. Using Eqs. (38), (47), and (48) we find

$$r = \frac{1}{2\bar{L}} \tag{50}$$

hence Eq. (41) gives the mean-square displacement of the tagged particle

$$\langle (x_T)^2 \rangle \sim 2\frac{\mathcal{R}(t)[1-\mathcal{R}(t)]\bar{L}^2}{N}. \tag{51}$$

The eigenvalues of the noninteracting particle determine the multi exponential type of decay of $\mathcal{R}(t)$ with time, which in turn determines the dynamics of the interacting tagged particle [46].

Let $\delta^2=D\pi^2 t/4\bar{L}^2$; hence, the limit $\delta \ll 1$ gives the short time dynamics before the particles interact with the walls, or equivalently the limit of an infinite system. The reflection coefficient is rewritten

$$\mathcal{R} = \frac{1}{2} + \frac{4}{\pi^2}\left(\delta\sum_{n=1,\text{Odd}}^{\infty}\frac{e^{-\delta^2 n^2}-1}{\delta^2 n^2}\delta + \sum_{n=1,\text{Odd}}^{\infty}\frac{1}{n^2}\right). \tag{52}$$

When $\delta \ll 1$ we may replace the first summation with integration

$$\sum_{n=1,\text{Odd}}^{\infty}\frac{e^{-\delta^2 n^2}-1}{\delta^2 n^2}\delta \simeq \frac{1}{2}\int_0^{\infty}\frac{e^{-y^2}-1}{y^2}dy = \frac{-\sqrt{\pi}}{2} \tag{53}$$

where the factor 1/2 on the RHS comes from the summation over only odd $n$ on the LHS. Using $\sum_{n=1,\text{Odd}}^{\infty}1/n^2=\pi^2/8$ we have $\mathcal{R}=1-\frac{\sqrt{Dt}}{\bar{L}\sqrt{\pi}}+\cdots$, and hence

$$\langle (x_T)^2 \rangle \sim \frac{2}{\sqrt{\pi}}\frac{\sqrt{Dt}}{\rho}. \tag{54}$$

This result was obtained in [4,6], and it describes the dynamics of the tagged particle in a box, before particles have time to interact with the walls, namely, when $\delta$ is small.

In the opposite limit of long times and finite systems we attain equilibrium, then $\lim_{t\to\infty}\mathcal{R}=1/2$ and

$$P(x_T) \sim \frac{\sqrt{N}}{\sqrt{\pi}\bar{L}}e^{-N(x_T)^2/\bar{L}^2}, \tag{55}$$

hence

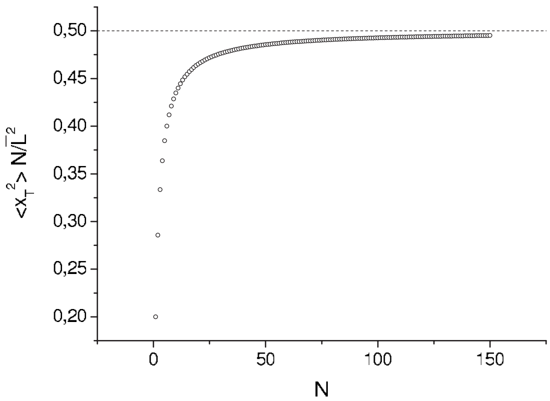


FIG. 4. For particles in a box we show $\langle (x_T)^2\rangle N/\bar{L}^2$ of the tagged particle, in equilibrium versus $N$. Exact expression obtained in [25] valid for all $N$ (dots) converges in the limit of $N\to\infty$ to the behavior predicted by our theory (dashed line) Eq. (56). For $N=70$ clear deviations between our asymptotic theory and the exact result in [25] are found.

$$\lim_{t\to\infty}\langle (x_T)^2\rangle = \bar{L}^2/2N. \tag{56}$$

Equation (55) is a special case of the more general equation [Eq. (25)] since the single particle normalizing partition function for our example is $Z=2\bar{L}$.

As mentioned, in [25] the Bethe ansatz was used to solve the problem of tagged particle motion in a box. Among other things an exact expression for the long time limit of $\langle (x_T)^2\rangle$, valid for all $N$ was found [25]

$$\lim_{t\to\infty}\langle (x_T)^2\rangle = \bar{L}^2\left(\frac{1}{4}\right)^{N+1}\frac{\Gamma\left(\frac{1}{2}\right)\Gamma[2(N+1)]}{\Gamma(N+1)\Gamma\left(N+\frac{5}{2}\right)}. \tag{57}$$

Since our formalism is valid only in the large $N$ limit, comparison of our solution to an exact result like Eq. (57) provides insight to the question of convergence. In Fig. 4 we plot $\lim_{t\to\infty}\langle (x_T)^2\rangle N/\bar{L}^2$ versus $N$ using Eq. (57) comparing it to our Eq. (56) which gives $\lim_{t\to\infty}\langle (x_T)^2\rangle N/\bar{L}^2=1/2$. Not surprisingly we see that the two results yield asymptotically the same result. The figure illustrates that even for $N=100$ deviations between exact results and the present theory are observable.

In [25] numerical simulation of systems with $N=1$, 10, and 70 (maximum of 141 particles) were performed, and favorably compared with the Bethe ansatz solution. These simulations were made for finite-size hard-core particles whose diameter is $\Delta$. To make comparison between our theory and simulation we scale the size of the box according to $2\bar{L}\to 2\bar{L}-(2N)\Delta$. In Fig. 5 the scaled mean-square displacement versus $t/\tau_{\text{eq}}$ is shown, where $\tau_{\text{eq}}=4\bar{L}^2/D$. Some general features of our theory can now be discussed. First, at short times simulations show normal behavior $\langle (x_T)^2\rangle=2Dt$, which is a trivial effect: particles did not have time to collide and hence the tagged particle diffuses normally as if it is free. After particles start to collide, deviations from normal diffusion are observed (for $N=70$ but as expected not for $N=1$). These are mainly due to collisions with other particles. Finally saturation due to the finite size of the system is found. While our theory shows the general trend of simulations (say for $N=70$ and for not too short times) it is clearly not in perfect agreement. We argue that this is due to the small number of particles $N=70$ since as we showed in Fig. 4, at least for large times and large $N$ our theory gives the exact result. It would be nice to have simulations with point particles, with larger $N$ and since there are three phases of the motion: normal diffusion, single file diffusion without the influence of the walls and finally saturation to equilibrium. Separation of time scales is needed to demonstrate these behaviors clearly.

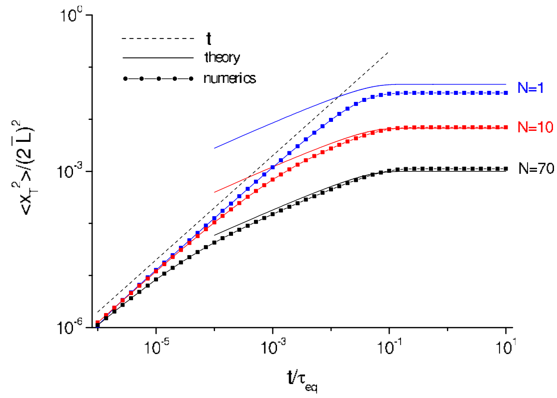


FIG. 5. (Color online) Motion of tagged particle in a box is shown for $N=1$, 10, and 70. Simulation results (squares) are taken from [25] (see text). At short time simulations exhibit normal diffusion $\langle (x_T)^2\rangle=2Dt$ as illustrated by the straight dashed line which is a guide to the eyes. Our theory is expected to work well in the large $N$ limit and when many collision events between tagged particle and surrounding Brownian particles took place. Hence agreement between theory (solid line) and simulation is reasonable at most only for $N=70$ and not for too short times.

### B. Gaussian packet

Consider particles without external forces $V(x)=0$ in an infinite system. Initially particles are spread with a Gaussian packet with width $\xi$,

$$f(x_0) = \frac{\sqrt{2}}{\sqrt{\pi}\xi}\exp\left[-\frac{(x_0)^2}{2\xi^2}\right] \tag{58}$$

for $x_0>0$. As before we consider the tagged particle motion, which is initially at $x_T=0$, with $N$ particles to its left and $N$ to its right. With the free particle Green's function $g(x,x_0,t)$ [Eq. (27)] we proceed to find $\langle (x_T)^2\rangle$.

Reflection probability Eq. (35) is

$$\mathcal{R} = \int_0^\infty dx_0\sqrt{\frac{2}{\xi^2\pi}}e^{-(x_0)^2/2\xi^2}\int_0^\infty \frac{dx}{\sqrt{4\pi Dt}}e^{-(x-x_0)^2/4Dt}. \tag{59}$$

Changing variables according to $y^2/2=(x-x_0)^2/4Dt$ and using dimensionless parameter $\tilde{\xi}=\xi/\sqrt{2Dt}$, we find

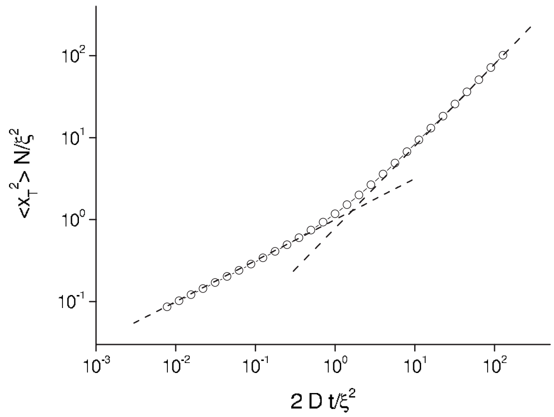


FIG. 6. Scaled mean-square displacement of the tagged particle with Gaussian initial conditions of the packet of particles exhibits a transition between short time $\langle(x_T)^2\rangle \propto t^{1/2}$ law to $\langle(x_T)^2\rangle \propto t$ behavior. Dashed lines are short and long time asymptotic behavior [Eq. (64)], circles represent Eq. (63).

$$\mathcal{R} = \frac{1}{2} + \frac{1}{\tilde{\xi}}\sqrt{\frac{2}{\pi}}\int_0^{\infty} d\tilde{x}_0 e^{-(\tilde{x}_0)^2/2\tilde{\xi}^2}\frac{\mathrm{Erf}(\tilde{x}_0/\sqrt{2})}{2} \tag{60}$$

where $\mathrm{Erf}(\tilde{x}_0/\sqrt{2})/2=\int_0^{\tilde{x}_0}e^{-y^2/2}dy/\sqrt{2\pi}$ is the error function [45]. MATHEMATICA solves the integral in Eq. (60) and we find

$$\mathcal{R} = \frac{1}{2} + \frac{1}{\pi}\mathrm{arccot}\left(\frac{\sqrt{2Dt}}{\xi}\right). \tag{61}$$

For short times $\sqrt{Dt} \ll \xi$ we have $\mathcal{R} \sim 1-\frac{\sqrt{2Dt}}{\pi\xi}$, namely most particles did not have time to cross the origin, while in the opposite limit $\lim_{t\to\infty}\mathcal{R}=1/2$ due to the symmetry of initial conditions. The calculation of $r$ Eq. (38) using Eqs. (27) and (58) is straightforward

$$r = \frac{1}{2\sqrt{\pi Dt}\sqrt{1+\xi^2/2Dt}}, \tag{62}$$

Inserting Eqs. (61) and (62) in Eq. (41) we find

$$\langle(x_T)^2\rangle \sim \xi^2\frac{\pi}{N}\left(1+\frac{2Dt}{\xi^2}\right)\left[\frac{1}{4}-\frac{1}{\pi^2}\mathrm{arccot}^2\left(\sqrt{\frac{2Dt}{\xi^2}}\right)\right]. \tag{63}$$

This solution is shown in Fig. 6 with its two limiting behaviors

$$\langle(x_T)^2\rangle \sim \begin{cases} \xi\dfrac{\sqrt{2Dt}}{N} & \text{short times } 2Dt \ll \xi^2 \\ \dfrac{\pi D}{2N}t & \text{long times } 2Dt \gg \xi^2. \end{cases} \tag{64}$$

For short times the particles do not have time to disperse; hence, the motion of the tagged particle is slower than normal, increasing as $t^{1/2}$ which is similar to the single file diffusion with a uniform density [Eq. (54)]. Roughly speaking, for short times the tagged particle sees a uniform density of particles with $\rho=N/\xi$. For long times we recover the behavior in Eq. (31) since the scale of diffusion is much larger than $\xi$. Hence if we start with a Gaussian or delta function packet we get in the long time limit similar behavior, as we showed.

### C. Particles in harmonic oscillator

Consider particles in a harmonic potential $V(x)=m\omega^2x^2/2$ where $\omega>0$ is the harmonic frequency. The single particle undergoes an Ornstein Uhlenbeck process [41] and the corresponding single particle Green's function is

$$g(x,x_0,t) = \frac{1}{\sqrt{2\pi D\tau(1-e^{-2t/\tau})}}\exp\left[-\frac{(x-x_0e^{-t/\tau})^2}{2D\tau(1-e^{-2t/\tau})}\right], \tag{65}$$

where $(\tau)^{-1}=Dm\omega^2/k_bT$ is the inverse relaxation time.

We assume thermal initial conditions

$$f(x_0) = \frac{2\sqrt{m\omega^2}}{\sqrt{2\pi k_bT}}\exp\left(-\frac{m\omega^2x^2}{2k_bT}\right), \quad x_0>0. \tag{66}$$

Using Eq. (38) it is easy to show that

$$r = \frac{1}{\sqrt{2\pi}\xi_{\mathrm{th}}}, \tag{67}$$

where the thermal length is $\xi_{\mathrm{th}}=\sqrt{D\tau}=\sqrt{m\omega^2/k_bT}$. Note that one can write $r=1/Z$ which as we will soon prove is a general result valid for all potential fields satisfying $V(x)=V(-x)$, provided that the initial condition $f(x_0)$ is the thermal equilibrium. The reflection coefficient [Eq. (35)] is

$$\mathcal{R} = \frac{1}{2} + \sqrt{\frac{1}{2\pi}}\eta\int_0^{\infty} e^{-\eta^2y^2/2}\,\mathrm{Erf}\left(\frac{y}{\sqrt{2}}\right)dy, \tag{68}$$

where $\eta=e^{t/\tau}\sqrt{1-e^{-2t/\tau}}$. Using MATHEMATICA

$$\mathcal{R} = \frac{1}{2} + \frac{1}{\pi}\mathrm{arccot}(\sqrt{e^{2t/\tau}-1}). \tag{69}$$

For short times $t/\tau \ll 1$, $\mathcal{R}\sim 1-\sqrt{2t}/(\pi\sqrt{\tau})$, and for long time $\mathcal{R}\sim 1/2+e^{-t/\tau}/\pi$.

Using Eqs. (41), (67), and (69) the mean-square displacement of the tagged particle is

$$\langle(x_T)^2\rangle = \frac{\pi}{N}\xi_{\mathrm{th}}^2\left[\frac{1}{4}-\frac{1}{\pi^2}\mathrm{arccot}^2(\sqrt{e^{2t/\tau}-1})\right]. \tag{70}$$

For short times $t \ll \tau$

$$\langle(x_T)^2\rangle \sim \frac{\xi_{\mathrm{th}}}{N}\sqrt{2Dt}. \tag{71}$$

Such a behavior is expected, as well known for short times the diffusion process of the Ornstein Uhlenbeck process $x\sim t^{1/2}$ is faster than the drift $x\sim t$ and dominates the process; i.e., take $t\ll\tau$ in Eq. (65) and get the Green's function of the force free particle Eq. (27). Hence for short times we can neglect the external field, but use of course Gaussian initial condition Eq. (66). Then the problem reduces to the short time behavior of the Gaussian packet, free of external forces (compare short time behavior in Eq. (64) with Eq. (71) when $\xi\to\xi_{\mathrm{th}}$). The long time limit of Eq. (70) gives $\langle(x_T)^2\rangle \sim \pi\xi_{\mathrm{th}}^2/4N$ which is the thermal equilibrium behavior predicted more generally in Eq. (25). Behavior of the scaled mean-square displacement and its asymptotic behaviors is presented in Fig. 7.

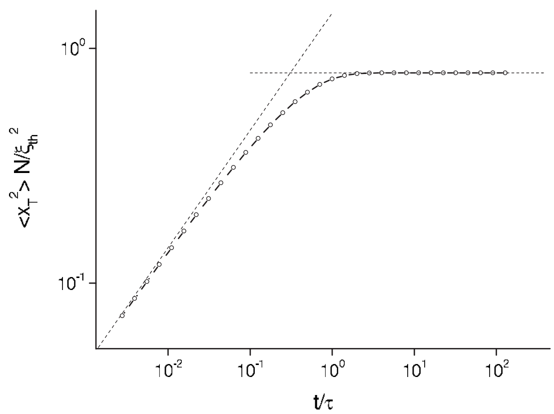


FIG. 7. Scaled mean-square displacement of tagged particle in harmonic field Eq. (70) exhibits a transition between a short time $\langle (x_T)^2\rangle \propto t^{1/2}$ law to saturation due to the binding field. The horizontal dashed line is the long time $\langle (x_T)^2\rangle = \pi\xi_{\rm th}^2/4N$ behavior, the dashed line is short time limit Eq. (71), and the dotted dashed line is Eq. (70).

### D. Thermal initial conditions

If we assume that initially the particles are in thermal equilibrium, our simple formulas simplify even more. If $f(x_0)=2\exp[-V(x_0)/k_bT]/Z$ then $r=1/Z$. To see this notice that for symmetric potentials $V(x)=V(-x)$ we have $g(0,-x_0,t)=g(0,x_0,t)$ and

$$r=\frac{2}{Z}\int_0^\infty \exp\left[-\frac{V(x_0)}{k_bT}\right]g(0,x_0,t)dx_0 \tag{72}$$

yields

$$r=\int_{-\infty}^{\infty}\frac{\exp\left[-\frac{V(x_0)}{k_bT}\right]}{Z}g(0,x_0,t)dx_0, \tag{73}$$

where we assumed that the potential is binding so a stationary solution of the Fokker-Planck equation is reached; i.e., the free particle is excluded. Therefore $r$ [Eq. (73)] is the probability of finding a noninteracting particle at the origin, with thermal initial conditions. Since the thermal equilibrium density is the stationary solution of the Fokker-Planck operator, $r$ is time independent and equal to $r=\exp[-V(0)/k_bT]/Z$. We can always take $V(0)=0$ and then $r=1/Z$. Examples for this behavior are the already analyzed cases of particles in a box with uniform initial density [Eq. (50)] (since $Z=2\bar{L}$ for that case) and similarly for particles in a harmonic potential with initial thermal density [Eqs. (66) and (67)]. Hence using Eq. (41)

$$\langle (x_T)^2\rangle = \frac{\mathcal{R}(1-\mathcal{R})Z^2}{2N}. \tag{74}$$

For the symmetric and binding potentials under consideration, we have $\lim_{t\to\infty}\mathcal{R}=1/2$ and hence Eq. (74) in the long time limit yields equilibrium behavior Eq. (26).

### E. Power-law type of initial conditions

Flomenbom and Taloni [27] considered particles free of external forces; hence, the free particle Green' function is

$$g(x,x_0,t)=\frac{1}{\sqrt{4\pi Dt}}\exp\left[-\frac{(x-x_0)^2}{4Dt}\right], \tag{75}$$

with initial conditions of power law type

$$f(x_0)=B|x_0|^{-\beta} \quad 0<x_0<L \tag{76}$$

for $0<\beta<1$. Here the system size $\bar{L}\to\infty$ and the reader should not confuse $\bar{L}$ with $L$. The normalization of the PDF of Eq. (76) yields $B=(1-\beta)L^{\beta-1}$. In the limit $\beta\to 0$ and $L\to\infty$ in such a way that $\rho=N/L$ remains fixed, we anticipate the classical case of single file diffusion in the presence of a uniform density of particles: $\langle x^2\rangle\propto t^{1/2}$ [Eq. (54)]. In the opposite limit of $\beta\to 1$ the particles are initially concentrated at the origin, and we expect the behavior $\langle x^2\rangle \propto t$ [Eq. (31)]. Thus $0<\beta<1$ bridges between these two known behaviors, indeed one finds $\langle (x_T)^2\rangle \propto t^{(\beta+1)/2}$ as shown in [27]. The latter is valid for times $\sqrt{4Dt}\ll L$ as discussed below. This indicates that specially chosen initial condition may control the qualitative behavior of the diffusion of the tagged particle. Here we analyze this case using our formalism finding analytical expressions for the mean-square displacement.

To obtain $\langle (x_T)^2\rangle$ all we need to do is to find $r$ and $\mathcal{R}$. Using Eqs. (38), (75), and (76),

$$r=\frac{(1-\beta)}{\sqrt{\pi}}\frac{L^{\beta-1}}{(\sqrt{4Dt})^\beta}\int_0^{L/\sqrt{4Dt}} y^{-\beta}e^{-y^2}dy, \tag{77}$$

solving the integral

$$r=\frac{(1-\beta)}{\sqrt{\pi}}\frac{L^{\beta-1}}{(\sqrt{4Dt})^\beta}\frac{1}{2}\left[\Gamma\left(\frac{1-\beta}{2}\right)-\Gamma\left(\frac{1-\beta}{2},\frac{L^2}{4Dt}\right)\right], \tag{78}$$

where $\Gamma(a,z)$ is the incomplete Gamma function [45]. The following behaviors are found for short and long times:

$$r=\begin{cases} c_r\dfrac{L^{\beta-1}}{(\sqrt{4Dt})^\beta} & \sqrt{4Dt}\ll L \\ \dfrac{1}{\sqrt{4\pi Dt}} & \sqrt{4Dt}\gg L. \end{cases} \tag{79}$$

In the short time limit we took the upper bound in integration in Eq. (77) to $\infty$ so

$$c_r=\frac{(1-\beta)}{\sqrt{\pi}}\int_0^\infty y^{-\beta}e^{-y^2}dy=\frac{1-\beta}{\sqrt{\pi}}\frac{\Gamma(1-\beta/2)}{2}. \tag{80}$$

Inserting Eqs. (75) and (76) in Eq. (35) we find the reflection coefficient

$$\mathcal{R}=\frac{1}{2}+\frac{1}{2}(1-\beta)\left(\frac{L}{\sqrt{4Dt}}\right)^{\beta-1}\int_0^{L/\sqrt{4Dt}} dy\, y^{-\beta}\,\mathrm{Erf}(y). \tag{81}$$

In the limit of long times we get the expected behavior $\lim_{t\to\infty}\mathcal{R}=1/2$ since then half of the particles are to the left of the origin and half to the right (in statistical sense). MATHEMATICA solves the integral in the last equation in terms of tabulated functions

$$\int_0^x y^{-\beta}\,\mathrm{Erf}(y)dy = \frac{x^{-\beta}}{(1-\beta)\sqrt{\pi}}\left\{x[\sqrt{\pi}\,\mathrm{Erf}(x) + xE_{\beta/2}(x^2)] - x^{\beta}\Gamma\left(1-\frac{\beta}{2}\right)\right\}, \tag{82}$$

where $E_n(z)=\int_1^\infty dt\,\exp(-zt)/t^n$ is the exponential integral function.

To analyze the short time behavior we use integration by parts in Eq. (81) and find

$$\mathcal{R} = \frac{1}{2} + \frac{1}{2}\left(\frac{L}{\sqrt{4Dt}}\right)^{\beta-1}\left[\left(\frac{L}{\sqrt{4Dt}}\right)^{1-\beta}\mathrm{Erf}\left(\frac{L}{\sqrt{4Dt}}\right) - \frac{2}{\sqrt{\pi}}\int_0^{L/\sqrt{4Dt}} y^{1-\beta}e^{-y^2}dy\right]. \tag{83}$$

Using asymptotic properties of the Erf function [45], neglecting terms of the order of $\exp(-L^2/4Dt)$, Eq. (83) for $\sqrt{4Dt} \ll L$ gives

$$\mathcal{R} \sim 1 - c_{\mathcal{R}}\left(\frac{\sqrt{4Dt}}{L}\right)^{1-\beta}, \tag{84}$$

with

$$c_{\mathcal{R}} = \frac{1}{\sqrt{\pi}}\int_0^\infty y^{1-\beta}e^{-y^2}dy = \frac{\Gamma\left(1-\frac{\beta}{2}\right)}{2\sqrt{\pi}}. \tag{85}$$

Equations (78), (81), and (82) yield the mean-square displacement Eq. (41). The short time behavior $\sqrt{4Dt} \ll L$,

$$\langle (x_T)^2\rangle \sim \frac{1}{2N}\frac{2\sqrt{\pi}}{(1-\beta)^2\Gamma(1-\beta/2)}L^{1-\beta}(\sqrt{4Dt})^{1+\beta}, \tag{86}$$

while for long times $\sqrt{4Dt} \gg L$,

$$\langle (x_T)^2\rangle \sim \frac{\pi Dt}{2N}. \tag{87}$$

Thus after a long time the diffusion is normal $\langle (x_T)^2\rangle \propto t$, exactly like the case where all particles started initially on the origin [Eq. (31)]. While for short times $\langle (x_T)^2\rangle \propto t^{(1+\beta)/2}$.

Taking the limit $\beta \to 0$ in Eq. (86), we get the well-known result of single file motion in uniform density of particles [4,6] Eq. (54), with the density $\rho = N/L$. In the opposite limit $\beta \to 1$ we have $\langle x^2\rangle = \frac{\pi Dt}{2N}$ for all times which is the same as in Eq. (31). Note that the limit $\beta \to 1$ must be treated with care, the short time limit and the $\beta \to 1$ limit do not commute due to the $1/(1-\beta)^2$ divergence in Eq. (86). When $\beta \to 1$ all particles are centered on the origin hence we get the same behavior as in Eq. (31).

## V. PERCUS RELATION: BEYOND BROWNIAN PARTICLES

So far we considered the case where particles are diffusing according to the laws of Brownian motion in between collision events. What happens for other types of motion? For example, what happens when the underlying motion itself is anomalous [27,30].

Percus [18] (see also [27,47]) investigated a general relation between the diffusion of the tagged particle and motion in the absence of interactions (free motion) $\langle (x_T)^2\rangle \sim \langle |x|\rangle_{\text{free}}/\rho$. Such a relation was suggested for normal diffusion where we have $\langle |x|\rangle_{\text{free}} \propto t^{1/2}$, so $\langle (x_T)^2\rangle \propto t^{1/2}$ and for a particle moving ballistically between collision events hence $\langle |x|\rangle_{\text{free}} \propto t$ and therefore when we turn on the interactions $\langle (x_T)\rangle^2 \propto t$. This simple relation between free particle motion and the mean-square displacement of the tagged interacting particle is expected to work for an infinite system, with a uniform density $\rho$ of particles, and when external forces are zero $[F(x)=0]$. Here we will derive the Percus relation from our formalism for more general dynamics.

Assume that the Green's function of the noninteracting particle can be written in the scaling form

$$g(x,x_0,t) = \frac{1}{\sqrt{K_\alpha t^{\gamma/2}}}G\left(\frac{x-x_0}{\sqrt{K_\gamma t^{\gamma/2}}}\right). \tag{88}$$

We assume $G(y)=G(-y)$ and from normalization $\int_{-\infty}^{\infty}G(y)dy=1$. Here the free particle motion is anomalous, so that $\langle |x|\rangle_{\text{free}} \propto t^{\gamma/2}$ for $0<\gamma$ and not equal unity. For example the underlying motion might be subdiffusive continuous time random walk (CTRW) [48–52] or fractional Brownian motion, where in the latter case $G(y)$ is Gaussian and in the former $G(y)$ is expressed in terms of Lévy distributions (see some details below). We assume that moments of the process are finite. The constant $K_\gamma$ has units of $\mathrm{m}^2/\mathrm{s}^\gamma$.

To obtain the mean-square displacement of the tagged interacting particle we calculate reflection coefficient Eq. (35)

$$\mathcal{R} = \frac{1}{\bar{L}}\int_0^{\bar{L}} dx_0\int_0^{\bar{L}} G\left(\frac{x-x_0}{\sqrt{K_\gamma t^{\gamma/2}}}\right)\frac{dx}{\sqrt{K_\gamma t^{\gamma/2}}}. \tag{89}$$

Here we used uniform density of particle $f(x_0)=1/\bar{L}$, and we will consider the limit $\bar{L}\to\infty$ with the density $\rho$ being kept fixed. Change in variables $y=(x-x_0)/\sqrt{K_\gamma t^{\gamma/2}}$ and using $\bar{L}/\sqrt{K_\gamma t^{\gamma/2}} \to \infty$ we have

$$\mathcal{R} \sim \frac{1}{\bar{L}}\int_0^{\bar{L}} dx_0\int_{-x_0/\sqrt{K_\gamma t^{\gamma/2}}}^{\infty} G(y)dy. \tag{90}$$

Integrating by parts, changing variables $y=x_0/\sqrt{K_\gamma t^{\gamma/2}}$, and using the normalization condition, we have

$$\mathcal{R} \sim 1 - \frac{\langle |x|\rangle_{\text{free}}}{2\bar{L}} \tag{91}$$

where the mean of the absolute value of the free particle motion is by its definition

$$\langle |x|\rangle_{\text{free}} = \int_{-\infty}^{\infty} |x| G\left(\frac{x}{\sqrt{K_\gamma t^{\gamma/2}}}\right)\frac{dx}{\sqrt{K_\gamma t^{\gamma/2}}}. \tag{92}$$

Here we used the assumed symmetry $G(y)=G(-y)$ which means that the underlying random walk is not biased, as a result $\langle |x|\rangle = \sqrt{K_\gamma t^{\gamma/2}}2\int_0^\infty yG(y)dy$. It is easy to see that $r$

$=1/2\bar{L}$. In the limit where $N\to\infty$ and $\bar{L}\to\infty$ we find using Eqs. (41) and (91) the Percus formula for a general class of stochastic dynamics

$$\langle (x_T)^2\rangle = \frac{\langle |x|\rangle_{\text{free}}}{\rho}. \tag{93}$$

Clearly this equation gives a useful relationship between motion of a free particle and the same particle moving in single file when it is surrounded by identical particles whose density is $\rho$,

As a simple example consider fractional Brownian motion where $g(x,x_0,t)=(\sqrt{4\pi K_\gamma t^\gamma})^{-1}\exp[-(x-x_0)^2/4K_\gamma t^\gamma]$, where $0<\gamma<2$. Then Eq. (93) gives

$$\langle (x_T)^2\rangle = \frac{2\sqrt{K_\gamma t^\gamma}}{\rho\sqrt{\pi}}. \tag{94}$$

Hence if the underlying motion is ballistic $\gamma\to 2$ the motion of the tagged particle undergoing single file dynamics is normal with respect to time $\langle (x_T)^2\rangle \propto t$. For a CTRW particle in the continuum approximation the noninteracting single particle green function is governed by the fractional diffusion equation [50–52]

$$\frac{\partial^\gamma}{\partial t^\gamma} g(x,x_0,t) = \bar{K}_\gamma \frac{\partial^2}{\partial x^2} g(x,x_0,t) \tag{95}$$

with $0<\gamma<1$. From this equation it is easy to find [53] $\langle |x|\rangle_{\text{free}}=\sqrt{\bar{K}_\gamma t^\gamma}/\Gamma(1+\gamma/2)$. Hence using Eq. (93)

$$\langle (x_T)^2\rangle = \frac{\sqrt{\bar{K}_\gamma} t^{\gamma/2}}{\rho\Gamma(1+\gamma/2)}. \tag{96}$$

We see that independent of the mechanism of the underlying anomalous diffusion (i.e., fractional Brownian motion, or CTRW) we get for the tagged particle $\langle (x_T)^2\rangle \sim t^{\gamma/2}$. Further our general results show that the Green's function of the tagged particle is Gaussian even though the Green's function of noninteracting CTRW particles is highly non-Gaussian.

Warning: one should be careful when applying our results to the CTRW model, namely Eq. (96) should not be abused. One mechanism of anomalous diffusion are the power-law waiting times of Scher and Montroll [48] which yield slow dynamics, as captured by the CTRW [49,50] and the fractional Eq. (95) [53]. Single file diffusion with such subdiffusive motion as the starting point was considered recently theoretically and with simulations in [27,30]. It should be noted that the meaning of collision in such a model should be taken with care. For a random walk on a lattice with waiting times on each lattice point, one can envision several collision rules. For example, one might allow two particles to occupy the same site at a given time, or one may consider a mechanism were a particle once hopping into a trap already occupied will eject the particle previously residing in the trap. Or a particle is allowed to jump only into an empty site, as is usually assumed. These types of collision rules might yield behaviors different than ours. For example, a particle stuck with a very large sojourn time, might be ejected by another particle; hence, one can imagine a situation where some form of interaction causes the particles to move faster. In our work the collision implies that we can let particles go past one another as if they were noninteracting (so on a lattice two particles may occupy the same point at the same time) and eventually we look for the center particle. Even more interesting will be to investigate interacting particles in systems with quenched disorder since the latter, when strong enough, is known to lead to non-Gaussian subdiffusion [48,49]. There simple formula Eq. (93) is generally not expected to hold. Indeed in [37] single file motion of a tagged particle in the Sinai model was considered, the results are much richer when compared with Eq. (93).

## VI. DISCUSSION

The one-dimensional problem of motion of a tagged particle interacting via hard-core interactions with other particles was solved using the Jepsen line. The formalism we developed treats both Brownian and non-Brownian motion in between collision events, is suited for rather general external fields acting on the particles, for open and closed system, and handles also different types of initial conditions. Following others we have mapped the problem onto a noninteracting problem using the Jepsen line. The motion of the tagged particle belongs to the general problem of order statistics. The problem reduces to considering a list of $2N+1$ random variables and finding the distribution of the variable which has $N$ variables smaller than it and $N$ larger corresponding to center particle (note that the right most particle we will have an extreme value problem). Classical theory of order statistics deals however with the case where all the random variables have identical distributions. In contrast in the exclusion process under consideration, particles have nonidentical distribution. Thus except for two cases: (i) all the particles initially on the same position and (ii) equilibrium state, the problem deals with nonidentically distributed random variables (since the initial condition are nonidentical). While we treated the problem of symmetric potential and symmetric initial condition for the center particle in detail, it is left for future work to consider nonsymmetric potential fields, nonsymmetric initial conditions, and the dynamics of the particle in the tails of the packet. We believe that the methods developed here with some modifications can treat these cases too.

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## APPENDIX

In this appendix we use Boltzmann's distribution for the interacting system to find the PDF of the tagged center particle in equilibrium. The multidimensional PDF for $2N+1$ interacting particles, in the presence of an external binding field $V(x)$, with $V(x)=V(-x)$, acting on all of them is

$$P(x_{-N},\ldots,x_{-1},x_0,x_1,\ldots,x_N)=\frac{1}{Z_{2N+1}}\exp\left[-\sum_{j=-N}^{N}\frac{V(x_j)}{k_bT}\right]\theta(x_{-N+1}-x_{-N})\theta(x_{-N+2}-x_{-N+1})\cdots\theta(x_N-x_{N-1}) \tag{A1}$$

where $Z_{2N+1}$ is a normalizing factor, and $\theta(x)$ is a step function: $\theta(x)=0$ if $x<0$, $\theta(x)=1$ for $x\geq 0$. The center tagged particle is $x_0=x_T$. To find the PDF of $x_T$ in equilibrium, which we call $P^{\text{eq}}(x_T)$, we must integrate Eq. (A1) over all coordinates besides $x_0\to x_T$

$$P^{\text{eq}}(x_T)=\frac{\exp\left[-\frac{V(x_T)}{k_bT}\right]}{Z_{2N+1}}\int_{-\infty}^{x_T}dx_{-N}\int_{x_{-N}}^{x_T}dx_{-N+1}\cdots\int_{x_{-2}}^{x_T}dx_{-1}\exp\left[-\frac{\sum_{j=-N}^{-1}V(x_j)}{k_bT}\right]\int_{x_T}^{\infty}dx_1\int_{x_1}^{\infty}dx_2\cdots\int_{x_{N-1}}^{\infty}dx_N\exp\left[-\frac{\sum_{j=1}^{N}V(x_j)}{k_bT}\right]. \tag{A2}$$

We rearrange the integration limits, as explained in Fig. 8

$$\int_{-\infty}^{x_T}dx_{-N}\int_{x_{-N}}^{x_T}dx_{-N+1}\cdots=\int_{-\infty}^{x_T}dx_{-N}\int_{-\infty}^{x_{-N}}dx_{-N+1}\cdots. \tag{A3}$$

Hence we can use

$$\int_{-\infty}^{x_T}dx_{-N}\int_{x_{-N}}^{x_T}dx_{-N+1}\cdots=\frac{1}{2}\left[\int_{-\infty}^{x_T}dx_{-N}\int_{x_{-N}}^{x_T}dx_{-N+1}\cdots+\int_{-\infty}^{x_T}dx_{-N}\int_{-\infty}^{x_{-N}}dx_{-N+1}\cdots\right]=\frac{1}{2}\int_{-\infty}^{x_T}dx_N\int_{-\infty}^{x_T}dx_{-N+1}\cdots. \tag{A4}$$

Repeating this procedure we rewrite Eq. (A4) as

$$P^{\text{eq}}(x_T)=\text{Nor}\left\{\int_{-\infty}^{x_T}dx\frac{\exp\left[-\frac{V(x)}{k_BT}\right]}{Z}\right\}^N\left\{\int_{x_T}^{\infty}dx\frac{\exp\left[-\frac{V(x)}{k_BT}\right]}{Z}\right\}^N\frac{\exp\left[-\frac{V(x_T)}{k_BT}\right]}{Z}. \tag{A5}$$

where Nor is a normalization constant and $Z$ is defined in Eq. (21).

Thus Eq. (A5) describes a problem of order statistics which is extensively investigated by mathematicians, as mentioned in Sec. III D. $P^{\text{eq}}(x_T)$ Eq. (A5) is the PDF of the random variable which has exactly $N$ random variable larger than it and $N$ smaller. In this sense we have transformed the problem to a noninteracting system, similar to the noninteracting picture in the main text. The information contained in the single noninteracting particle; i.e., the single particle Boltzmann distribution $\exp[-V(x)/k_bT]/Z$ is all what is needed for the calculation of the position of the tagged particle.

Using the symmetry $V(x)=V(-x)$ we have

$$\int_{-\infty}^{x_T}\frac{e^{-V(x)/k_BT}}{Z}dx=\frac{1}{2}+\int_0^{x_T}\frac{e^{-V(x)/k_BT}}{Z}dx, \tag{A6}$$

and

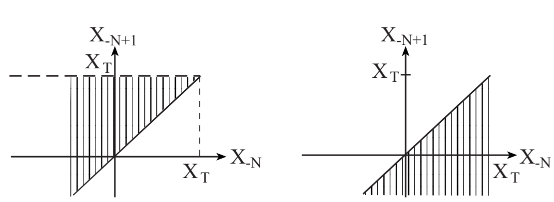


FIG. 8. Left panel integration in the domain $-\infty<x_{-N}<x_T$, $x_{-N}<x_{-N+1}<x_T$ is equivalent to integration $-\infty<x_{-N}<x_T$, $-\infty<x_{-N+1}<x_{-N}$ (right panel).

$$\int_{x_T}^{\infty}\frac{e^{-V(x)/k_BT}}{Z}dx=\frac{1}{2}-\int_0^{x_T}\frac{e^{-V(x)/k_BT}}{Z}dx. \tag{A7}$$

Using Eqs. (A6) and (A7), we rewrite Eq. (A5) as

$$P^{\text{eq}}(x_T)=\text{Nor}\frac{e^{-V(x_T)/k_bT}}{Z}e^{N\ln 1/4}\times\exp\left\{N\ln\left[1-4\left(\frac{\int_0^{x_T}e^{-V(x)/k_bT}dx}{Z}dx\right)^2\right]\right\}. \tag{A8}$$

In the limit $N\to\infty$ only $x_T$ with $\int_0^{x_T}\exp[-V(x)/k_bT]dx/Z\ll 1$ will have a measurable contribution to $P^{\text{eq}}(x_T)$ since if this condition is not satisfied, the value of $P^{\text{eq}}(x_T)$ is exponentially small in $N$. Expanding ln in Eq. (A8) we have

$$P^{\text{eq}}(x_T)\propto\exp\left[-\frac{V(x_T)}{k_bT}\right]\exp\left[-4N\left(\frac{\int_0^{x_T}dxe^{-V(x)/k_bT}}{Z}\right)^2\right]. \tag{A9}$$

Since $N\gg 1$ we expand $\int_0^{x_T}\exp(-V(x)/k_bT)dx=x_T$ where we used $V(0)=0$. We use $V(x_T)/k_bT \ll N(x_T)^2/Z^2$ which holds in the center part of the PDF of the tagged particle [since $N \gg 1$, $V(0)=0$, and $V(x)$ is analytic] $P^{\text{eq}}(x_T) \sim C \exp[-4N(x_T)^2/Z^2]$ where $C$ is a normalization constant. This final approximate result is the same as Eq. (25), justifying the tricks used to derive our main results.


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