Diffusion of finite-sized hard-core interacting particles in a one-dimensional box: Tagged particle dynamics

L. Lizana[*]

Niels Bohr Institute, Blegdamsvej 17, DK-2100 Copenhagen, Denmark

T. Ambjörnsson[†]

Department of Theoretical Physics, Lund University, Sölvegatan 14A, SE-223 62 Lund, Sweden
and Department of Chemistry, Massachusetts Institute of Technology, 77 Massachusetts Avenue, Cambridge, Massachusetts 02139, USA

We solve a nonequilibrium statistical-mechanics problem exactly, namely, the single-file dynamics of N hard-core interacting particles (the particles cannot pass each other) of size Δ diffusing in a one-dimensional system of finite length L with reflecting boundaries at the ends. We obtain an exact expression for the conditional probability density function $\rho_T(y_T, t | y_{T,0})$ that a tagged particle T $(T = 1, \ldots, N)$ is at position y_T at time t given that it at time $t=0$ was at position $y_{T,0}$. Using a Bethe ansatz we obtain the N-particle probability density function and, by integrating out the coordinates (and averaging over initial positions) of all particles but particle T, we arrive at an exact expression for $\rho_T(y_T, t | y_{T,0})$ in terms of Jacobi polynomials or hypergeometric functions. Going beyond previous studies, we consider the asymptotic limit of large N, maintaining L *finite*, using a nonstandard asymptotic technique. We derive an exact expression for $\rho_T(y_T, t | y_{T,0})$ for a tagged particle located roughly in the middle of the system, from which we find that there are three time regimes of interest for finite-sized systems: (A) for times much smaller than the collision time $t \ll \tau_{\text{coll}} = 1/(\varrho^2 D)$, where $\varrho = N/L$ is the particle concentration and D is the diffusion constant for each particle, the tagged particle undergoes a normal diffusion; (B) for times much larger than the collision time $t \gg \tau_{\text{coll}}$ but times smaller than the equilibrium time $t \ll \tau_{\text{eq}} = L^2/D$, we find a single-file regime where $\rho_T(y_T, t | y_{T,0})$ is a Gaussian with a mean-square displacement scaling as $t^{1/2}$; and (C) for times longer than the equilibrium time $t \gg \tau_{\text{eq}}$, $\rho_T(y_T, t | y_{T,0})$ approaches a polynomial-type equilibrium probability density function. Notably, only regimes (A) and (B) are found in the previously considered infinite systems.

PACS number(s): 05.40.Fb, 02.50.Ey, 05.10.Gg

I. INTRODUCTION

Recent development of single fluorophore tracking techniques allows experimental studies of the motion of particles in cellular environments with nanometer resolution [1]. The cell interior represents a crowded environment, in which the motion of an individual particle is strongly affected by the presence of other particles: crowding affects, for instance, the folding of proteins, diffusional motion [2,3], as well as rates of biochemical reactions [4,5]. Crowding is also important during ribosomal translation on mRNA [6] and binding protein diffusion along DNA [7,8], where bound proteins are hindered from passing each other. Furthermore, advances in nanofluidics allow studies of geometrically constrained nanosized particles [9,10]. The system considered in this paper, the diffusion of a tagged particle immersed in a one-dimensional bath of hard-core interacting particles—in the literature referred to as single-file diffusion (SFD)—represents one of the simplest systems governed by crowding effects, but with possible applications for obstructed one-dimensional protein diffusion along DNA molecules and transport in nanofluidic systems.

SFD phenomena emerge in quasi-one-dimensional geometries. The particle order is under these circumstances conserved over time t, which results in interesting dynamics for a tagged particle, quite different from what is predicted from classical diffusion (governed by Fick's law). Examples found in nature include ion or water transport through pores in biological membranes [11], one-dimensional hopping conductivity [12], and channeling in zeolites [13]. SFD effects have also been studied in a number of experimental setups such as colloidal systems and ringlike constructions [14–18]. One of the most apparent characteristics of SFD is that the mean-square displacement (MSD) $\mathcal{S}(t) = \langle (y_T - y_{T,0})^2 \rangle$ of a tagged particle is in the long-time limit proportional to $t^{1/2}$ in an infinite system with a fixed particle concentration (angular brackets denote an average over initial positions and noise and y_T and $y_{T,0}$ are tagged particle positions at times t and $t=0$, respectively). Also, the conditional probability density function (PDF) for the tagged particle position (tPDF) is Gaussian.

The first theoretical study showing the $t^{1/2}$ law of the MSD and that the tPDF is Gaussian is in Ref. [19]. Subsequent studies, proving the MSD law in alternative ways, are found in [20–23]. Simple arguments to its origin are presented in [24–26], one of which [26] uses a simple relationship between the displacement of a single particle and particle density fluctuations, with the latter known to be the same as for independent particles [19,27]. The $t^{1/2}$ law and Gaussian behavior have, in the long-time limit, been shown to be of general validity for identical strongly overdamped particles interacting via any short-range potential in which

mutual passage is forbidden [28]. A generalized central limit theorem for tagged particle motion has also been proven [29]. More recent work includes [30] where particles interacting via a screened Coulomb potential (i.e., not perfectly hard core) were studied numerically (see also [31]), [32] deals with SFD in an external potential, and [33–35] address SFD dynamics with different diffusion constants. A phenomenological Langevin formulation of SFD was presented in [36].

Although much work has been dedicated to single-file systems, to our knowledge, very few exact results for finite systems with finite-sized particles have been obtained. The one exception is [37] where the PDF for N point particles diffusing on a finite one-dimensional line was derived. However, simplified expressions for the tPDF was only considered in the thermodynamic limit ($N, L \to \infty$, where L denotes the system length and the concentration $\varrho = N/L$ is kept fixed). In this paper, we go beyond previous studies in the following ways: first, finite-sized particles are considered and we show that the N-particle probability density function (NPDF) can be written as a Bethe ansatz solution. We obtain an exact expression for the tPDF in terms of Jacobi polynomials (or hypergeometric functions), which reduces to that in [37] for the case of point particles. Second, we perform a (nonstandard) large-N analysis of the tPDF, keeping the system size L finite. The expression for $\rho_{\mathcal{T}}(y_{\mathcal{T}}, t | y_{\mathcal{T},0})$ in the many-particle limit is presented compactly in terms of modified Bessel functions. An analysis of the tPDF reveals the existence of three dynamical regimes for a particle located roughly in the middle of the system: (A) short times, $t \ll \tau_{\mathrm{coll}} = 1/(\varrho^2 D)$, where τ_{coll} denotes the collision time and D is the diffusion constant. In this limit the tagged particle undergoes standard Brownian motion with a MSD $\mathcal{S}(t) \sim t$; (B) for intermediate times, $\tau_{\mathrm{coll}} \ll t \ll \tau_{\mathrm{eq}}$, where $\tau_{\mathrm{eq}} = L^2/D$ is the equilibrium time, we get a SFD regime where $\mathcal{S}(t) \sim t^{1/2}$; (C) for long times, $t \gg \tau_{\mathrm{eq}}$, an equilibrium tPDF of polynomial type is found. Notably, only regimes (A) and (B) exist in infinite systems.

This paper has the following organization. Section II contains the formulation of the problem and a mapping onto a point-particle system. The tPDF is also formally stated in terms of the NPDF to which governing dynamical equations are introduced. In Sec. III, we provide the solution to the equations of motion for the NPDF using a coordinate Bethe ansatz. In Sec. IV the initial coordinates as well as the coordinates for all particles except the tagged one are integrated out in order to obtain an exact expression for the tPDF. Also, asymptotic results for large N for the tPDF are derived. In Sec. V the asymptotic large-N expression for the tPDF is expanded for short and long times, and three different time regimes (A)–(C) (see above) are identified. More technical details are given in the appendixes. A brief summary of some of our results, corroborated with Gillespie simulations (Monte Carlo type), can be found in [38].

II. PROBLEM DEFINITION

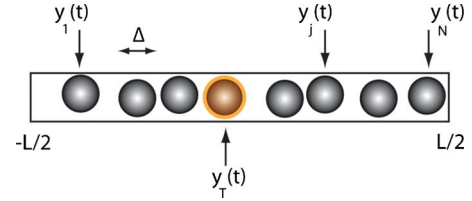In this paper we consider a system of N identical hard-core interacting particles, each with a diffusion constant

FIG. 1. (Color online) Cartoon of the problem considered here: N particles of linear size Δ diffusing is a one-dimensional system of length L. The particles have center-of-mass coordinates y_j and initial positions $y_{j,0}$ ($j = 1, \ldots, N$) and are unable to overtake. This implies that $y_{j+1} \geq y_j + \Delta$ ($j = 1, \ldots, N-1$) for all times. Also, the particles cannot diffuse out of the box, i.e., $y_1 > -L/2 + \Delta/2$ and $y_N < L/2 - \Delta/2$.

D and a linear size Δ, diffusing in a finite one-dimensional system extending from $-L/2$ to $L/2$. A schematic cartoon is depicted in Fig. 1. The particles each have center of mass (CM) and initial coordinates $\vec{y} = (y_1, \ldots, y_N)$ and $\vec{y}_0 = (y_{1,0}, \ldots, y_{N,0})$, respectively. Due to the hard-core interaction, the particles cannot pass each other and retain their order at all times, i.e., $y_{j+1} \geq y_j + \Delta$ for $j = 1, \ldots, N-1$. The ends of the system are reflecting (the particles cannot escape), i.e., $y_1 > -(L-\Delta)/2$ and $y_N < (L-\Delta)/2$.

The diffusion of finite-sized particles can be mapped onto a point-particle problem. Introducing the rescaled effective system length

$$\ell = L - N\Delta, \tag{1}$$

and making the coordinate transformation

$$x_j = y_j - j\Delta + \frac{N+1}{2}\Delta,$$

$$x_{j,0} = y_{j,0} - j\Delta + \frac{N+1}{2}\Delta, \tag{2}$$

it leads to

$$\mathcal{R}: -\ell/2 < x_1 < x_2 \ldots < x_N < \ell/2, \tag{3}$$

where $\mathcal{R}$ denotes the phase space spanned by Eq. (3). The phase space $\mathcal{R}_0$ is also introduced for the initial coordinates which satisfy $-\ell/2 < x_{1,0} < x_{2,0} \ldots < x_{N,0} < \ell/2$. For convenience, we also introduce the shorthand notations $\vec{x} = (x_1, \ldots, x_N)$ and $\vec{x}_0 = (x_{1,0}, \ldots, x_{N,0})$. Equations (1) and (2) map *exactly* the problem of N finite-sized hard-core particles in a box of length L onto a N point-particle problem in a box of length ℓ.

The main quantity of interest in this study is the tPDF $\rho_{\mathcal{T}}(x_{\mathcal{T}}, t | x_{\mathcal{T},0})$ that is the probability density that a tagged particle $\mathcal{T}$ ($\mathcal{T} = 1, \ldots, N$) is at position $x_{\mathcal{T}}$ at time t, given that it was at $x_{\mathcal{T},0}$ at $t = 0$ [an ensemble average over the initial (equilibrium) distribution of the surrounding $N-1$ particles is implicit]. The equilibrium tPDF is straightforwardly calculated from the ergodicity principle: all points in the allowed phase space $\mathcal{R}$ are equally probable. This leads the equilibrium NPDF

$$\mathcal{P}^{\mathrm{eq}}(\vec{x}) = \frac{N!}{\ell^N} \prod_{i=1}^{N-1} \theta(x_{i+1} - x_i), \qquad (4)$$

where $\theta(z)$ is the Heaviside step function; $\theta(z) = 1$ for $z > 0$ and zero elsewhere. Using an extended phase-space integration technique (see Appendix C) it is easy to verify that $\int_{\mathcal{R}} dx_1 \cdots dx_N \, \mathcal{P}^{\mathrm{eq}}(\vec{x}) = 1$. Integrating Eq. (4) over all coordinates leaving out one, x_T, gives the tPDF

$$\rho_T^{\mathrm{eg}}(x_T) = \int_{\mathcal{R}} dx_1' \cdots dx_N' \, \delta(x_T - x_T') \mathcal{P}^{\mathrm{eq}}(\vec{x}')$$

$$= \frac{N!}{\ell^N} \frac{1}{N_L! \, N_R!} \int_{-\ell/2}^{x_T} dx_1' \cdots \int_{-\ell/2}^{x_T} dx_{T-1}'$$

$$\times \int_{x_T}^{\ell/2} dx_{T+1}' \cdots \int_{x_T}^{\ell/2} dx_N'$$

$$= \frac{1}{\ell^N} \frac{N!}{N_L! \, N_R!} \left(\frac{\ell}{2} + x_T\right)^{N_L} \left(\frac{\ell}{2} - x_T\right)^{N_R}, \qquad (5)$$

where $\delta(z)$ is the Dirac delta function and N_L (N_R) is the number of particles to the left (right) of the tagged particle ($N = N_L + N_R + 1$). In the remaining part of this section, we show how to calculate the complete time evolution of the tPDF from the many-particle NPDF.

In order to obtain $\rho_T(x_T, t | x_{T,0})$ one needs to first introduce the N-particle *joint* probability density $\mathcal{P}(\vec{x}, t; \vec{x}_0)$, which gives the probability density that the system is in a state $\vec{x}$ *and* that it initially was in a state $\vec{x}_0$. The joint probability density for the tagged particle $\rho_T(x_T, t; x_{T,0})$ is simply obtained from the joint NPDF by integration over $\mathcal{R}$ and $\mathcal{R}_0$: $\rho_T(x_T, t; x_{T,0}) = \int_{\mathcal{R}} dx_1' \cdots dx_N' \int_{\mathcal{R}0} dx_{1,0}' \cdots dx_{N,0}' \, \delta(x_T - x_T') \delta(x_{T,0} - x_{T,0}') \mathcal{P}(\vec{x}', t; \vec{x}_0')$. Relating the conditional and joint probability densities using Bayes' rule [39], i.e., $\mathcal{P}(\vec{x}, t; \vec{x}_0) = \mathcal{P}(\vec{x}, t | \vec{x}_0) \mathcal{P}^{\mathrm{eq}}(\vec{x}_0)$ and $\rho_T(x_T, t; x_{T,0}) = \rho_T(x_T, t | x_{T,0}) \rho^{\mathrm{eq}}(x_{T,0})$, leads to

$$\rho_T(x_T, t | x_{T,0}) = \frac{1}{\rho^{\mathrm{eq}}(x_{T,0})} \int_{\mathcal{R}} dx_1' \cdots dx_N' \, \delta(x_T - x_T')$$

$$\times \int_{\mathcal{R}0} dx_{1,0}' \cdots dx_{N,0}' \, \delta(x_{T,0} - x_{T,0}')$$

$$\times \mathcal{P}(\vec{x}', t | \vec{x}_0') P^{\mathrm{eq}}(\vec{x}_0'), \qquad (6)$$

where $\rho_T^{\mathrm{eg}}(x_{T,0})$ is given in Eq. (5).

In order to get the tPDF using Eq. (6), we need to calculate the NPDF $\mathcal{P}(\vec{x}, t | \vec{x}_0)$. It is governed by the diffusion equation

$$\frac{\partial \mathcal{P}(\vec{x}, t | \vec{x}_0)}{\partial t} = D\left(\frac{\partial^2}{\partial x_1^2} + \frac{\partial^2}{\partial x_2^2} + \cdots + \frac{\partial^2}{\partial x_N^2}\right) \mathcal{P}(\vec{x}, t | \vec{x}_0), \quad (7)$$

for $\vec{x} \in \mathcal{R}$ [$\mathcal{P}(\vec{x}, t | \vec{x}_0) \equiv 0$ outside $\mathcal{R}$]. The equation certifying that neighboring particles cannot overtake reads

$$D\left(\frac{\partial}{\partial x_{i+1}} - \frac{\partial}{\partial x_i}\right) \mathcal{P}(\vec{x}, t | \vec{x}_0)|_{x_{i+1} = x_i} = 0. \qquad (8)$$

Also, reflecting boundaries are placed at the system ends,

$$D \left. \frac{\partial \mathcal{P}(\vec{x}, t | \vec{x}_0)}{\partial x_1} \right|_{x_1 = -\ell/2} = 0, \qquad (9)$$

$$D \left. \frac{\partial \mathcal{P}(\vec{x}, t | \vec{x}_0)}{\partial x_N} \right|_{x_N = \ell/2} = 0, \qquad (10)$$

making sure that the particles are restricted to $[-\ell/2, \ell/2]$ at all times. Finally, the initial condition is

$$\mathcal{P}(\vec{x}, 0 | \vec{x}_0) = \delta(x_1 - x_{1,0}) \cdots \delta(x_N - x_{N,0}). \qquad (11)$$

Summarizing this section, the problem of N hard-core interacting particles of size Δ diffusing in a one-dimensional system of a finite length L was mapped onto a point-particle problem using relationships (1) and (2). The dynamics of the NPDF is governed by Eqs. (7)–(10). Once they are solved (topic of Sec. III), the tPDF can be calculated via Eq. (6) (as demonstrated in Sec. IV).

III. *N*PDF AS A COORDINATE BETHE ANSATZ

In this section we obtain the NPDF for the diffusion problem defined in previous section using a coordinate Bethe ansatz. The Bethe ansatz has been proven useful in solving a large variety of interacting particle problems since its introduction by Bethe in 1931 (see [40] for a review). The Bethe ansatz solution for the present problem reads

$$\mathcal{P}(\vec{x}, t | \vec{x}_0) = \int_{-\infty}^{\infty} \frac{dk_1}{2\pi} \int_{-\infty}^{\infty} \frac{dk_2}{2\pi} \cdots \int_{-\infty}^{\infty} \frac{dk_N}{2\pi} e^{-E(k_1, \ldots, k_N)t}$$

$$\times \Pi_{j=1}^{N} \phi(k_j, x_{j,0}) [e^{ik_1 x_1 + ik_2 x_2 + ik_3 x_3 + \cdots + ik_N x_N}$$

$$+ S_{21} e^{ik_2 x_1 + ik_1 x_2 + ik_3 x_3 + \cdots + ik_N x_N}$$

$$+ S_{32} S_{31} e^{ik_2 x_1 + ik_3 x_2 + k_1 x_3 + \cdots + ik_N x_N}$$

$$+ \text{all other permut. of } \{k_1, k_2, \ldots, k_N\}],$$

$$(12)$$

where $E(k_1, \ldots, k_N)$ is the dispersion relation, S_{ij} are the scattering coefficients, and $\phi(k_j, x_{j,0})$ denotes a function containing boundary and initial conditions. Each one of these quantities is described below.

The dispersion relation has the form

$$E(k_1, \ldots, k_n) = D(k_1^2 + \cdots + k_N^2), \qquad (13)$$

and relates "energy" to the momenta $k_1, \ldots, k_N$. Equation (13) is obtained by inserting the Bethe ansatz (12) into the equation of motion (7).

The scattering coefficients S_{ij} describe pairwise particle interactions and are in general functions of the momentum variables k_i and k_j, $S_{ij} = S(k_i, k_j)$. They are, however, independent of the initial positions of the particles. In Appendix A it is demonstrated that the scattering coefficients making sure that the particles cannot pass each other [i.e., satisfying Eq. (8)] are given by

$$S_{ij} = 1, \qquad (14)$$

which means that they are independent of momenta and correspond to perfect reflection. For noninteracting particles

$S_{ij}=0$, which reduces the Bethe ansatz to a standard Fourier transform.

The quantity $\phi(k_j, x_{j,0})$ contains information about the initial and boundary conditions of the problem, which are here defined by Eqs. (9)–(11). The form of $\phi(k_j, x_{j,0})$ satisfying these relationships is given by

$$\phi(k_j, x_{j,0}) = 2 \cos[k_j(x_{j,0} + \ell/2)] \sum_{m=-\infty}^{\infty} e^{ik_j(2m+1/2)\ell}, \quad (15)$$

which is shown explicitly in Appendix A. Notably, for an infinite system we have $\phi(k_j, x_{j,0}) = e^{-ik_j x_{j,0}}$ [41,42].

It is interesting to note that for SFD systems described by Eqs. (12)–(15) any *macroscopic* quantity that is invariant under interchange of any two particle positions, $x_i \leftrightarrow x_j$, takes the same value as for a system of noninteracting particles. This is in marked contrast to *microscopic* quantities such as the tPDF which in general behave very differently for single-file and independent particle systems. In Appendix F we use the Bethe ansatz to explicitly calculate two macroscopic quantities, the dynamic structure factor and the center-of-mass PDF, and show that they agree with standard results for independent particle systems.

Integration over momenta in Eq. (12) [using Eqs. (13)–(15)] leads to the *N*PDF

$$
\begin{aligned}
\mathcal{P}(\vec{x}, t | \vec{x}_0) = {} & \psi(x_1, x_{1,0}; t) \psi(x_2, x_{2,0}; t) \cdots \psi(x_N, x_{N,0}; t) \\
& + \psi(x_1, x_{2,0}; t) \psi(x_2, x_{1,0}; t) \cdots \psi(x_N, x_{N,0}; t) \\
& + \text{all other permut. of } \{x_{1,0}, x_{2,0}, \ldots, x_{N,0}\},
\end{aligned}
$$
(16)

where

$$
\begin{aligned}
\psi(x_i, x_{j,0}; t) = {} & \frac{1}{(4\pi Dt)^{1/2}} \sum_{m=-\infty}^{\infty} \left\{ \exp\left[-\frac{(x_i - x_{j,0} + 2m\ell)^2}{4Dt} \right] \right. \\
& \left. + \exp\left[-\frac{[x_i + x_{j,0} + (2m+1)\ell]^2}{4Dt} \right] \right\}
\end{aligned}
$$
(17)

is obtained from the inverse Fourier transform $(2\pi)^{-1} \int_{-\infty}^{\infty} dk_j \, \phi(k_j, x_{j,0}) e^{-Dk_j^2 t} e^{ik_j x_i}$. We point out that $\psi(x_i, x_{j,0}; t)$ is the single-particle PDF for a particle in confined in a box of length ℓ.

The single-particle PDF given in Eq. (17) is, however, not convenient for analyzing the long-time limit $t \to \infty$. In order to get a more suitable expression we seek instead the eigenmode expansion of $\psi(x_i, x_{j,0}; t)$, which can be done in a variety of ways. Here, we use Bromwich integration. The Laplace transform of Eq. (17) is (see Appendix B)

$$
\begin{aligned}
\psi(x_i, x_{j,0}; s) = {} & \int_0^{\infty} dt \, e^{-st} \psi(x_i, x_{j,0}; t) \\
= {} & \frac{1}{\sqrt{4Ds} \, \sinh(\ell\sqrt{s/D})} \{\cosh[(x_i + x_{j,0})\sqrt{s/D}] \\
& + \cosh[(\ell - |x_{j,0} - x_i|)\sqrt{s/D}]\}.
\end{aligned}
$$
(18)

The sought eigenvalue expansion is obtained as a sum of residues of $\psi(x_i, x_{j,0}; s)$ (see, e.g., Ref. [43]) and reads

$$\psi(x_i, x_{j,0}; t) = \frac{1}{\ell} \left[1 + \sum_{m=1}^{\infty} \mathcal{G}_m(x_i, x_{j,0}) \mathcal{E}_m(t) \right], \quad (19)$$

where

$$
\begin{aligned}
\mathcal{G}_m(x_i, x_{j,0}) = {} & \nu_m^{(+)} \cos\left(\frac{m\pi x_i}{\ell}\right) \cos\left(\frac{m\pi x_{j,0}}{\ell}\right) \\
& + \nu_m^{(-)} \sin\left(\frac{m\pi x_i}{\ell}\right) \sin\left(\frac{m\pi x_{j,0}}{\ell}\right),
\end{aligned}
$$
(20)

$$\mathcal{E}_m(t) = e^{-(m\pi)^2 Dt/\ell^2}, \quad (21)$$

$$\nu_m^{(\pm)} = 1 \pm (-1)^m. \quad (22)$$

Elementary trigonometric identities [44] were used to bring $\mathcal{G}_m(x_i, x_{j,0})$ onto the form in Eq. (20). Equations (19)–(22) agrees with well-known results [45]. The single-particle PDF (19) is more convenient for obtaining the long-time limit as well as for numerical computations compared to Eq. (17).

In summary, the many-particle *N*PDF for excluding particles of size Δ diffusing in a finite interval of length L with reflecting boundaries is given by Eqs. (16) and (19) [or Eq. (17)] combined with the mapping equations (1) and (2). For point particles ($\Delta = 0$) these results agree with those presented in [37] where a different approach was used [46]. Based on the explicit expression of our *N*PDF, we will in the following section address the tPDF.

IV. tPDF—EXACT AND LARGE *N* RESULTS

In this section, we calculate the tPDF (6) by integrating out the coordinates and initial positions of all nontagged particles from the *N*PDF given in Eq. (16) [47]. As is shown in detail in Appendix C we can, due to the property that $\mathcal{P}(\vec{x}, t | \vec{x}_0)$ is invariant under permutations of $x_i \leftrightarrow x_j$, extend the integration from $\mathcal{R}$ to the hypercubes $x_j \in [-\ell/2, x_{\mathcal{T}}]$ ($j = 1, \ldots, \mathcal{T}-1$) and $x_j \in [x_{\mathcal{T}}, \ell/2]$ ($j = \mathcal{T}+1, \ldots, N$). A similar procedure holds for integration over $\mathcal{R}_0$ (initial positions). Using the extended phase-space technique, Eq. (6) becomes

$$
\begin{aligned}
\rho_{\mathcal{T}}(x_{\mathcal{T}}, t | x_{\mathcal{T},0}) = {} & \frac{f_L^{N_L} f_R^{N_R}}{N_L! \, N_R!} \int_{-\ell/2}^{x_{\mathcal{T}}} dx_1 \cdots \int_{-\ell/2}^{x_{\mathcal{T}}} dx_{\mathcal{T}-1} \int_{x_{\mathcal{T}}}^{\ell/2} dx_{\mathcal{T}+1} \cdots \\
& \times \int_{x_{\mathcal{T}}}^{\ell/2} dx_N \int_{-\ell/2}^{x_{\mathcal{T},0}} dx_{1,0} \cdots \int_{-\ell/2}^{x_{\mathcal{T},0}} dx_{\mathcal{T}-1,0} \\
& \times \int_{x_{\mathcal{T},0}}^{\ell/2} dx_{\mathcal{T}+1,0} \cdots \int_{x_{\mathcal{T},0}}^{\ell/2} dx_{N,0} \, \mathcal{P}(\vec{x}, t | \vec{x}_0),
\end{aligned}
$$
(23)

where

$$f_L = (\ell/2 + x_{\mathcal{T},0})^{-1}, \quad f_R = (\ell/2 - x_{\mathcal{T},0})^{-1}. \quad (24)$$

Using a similar combinatorial analysis to the one in Ref. [37], we arrive at Eq. (D1) (see Appendix D). The tPDF is, however, more conveniently expressed in terms of Jacobi polynomials [44], $P_n^{(\alpha,\beta)}(z)$. Using the identities $P_n^{(\alpha,\beta)}(z) = (n+\alpha)! (n+\beta)! / [n! (n+\alpha+\beta)!][(z-1)/2]^{-a} P_{n+\alpha}^{(-\alpha,\beta)}(z)$ and $P_n^{(\alpha,\beta)}(-z) = (-1)^n P_n^{(\beta,\alpha)}(z)$ [48] leads to

$$\rho(x_T,t|x_{T,0}) = \frac{(N_L + N_R - 1)!}{N_L! \, N_R!} (\psi_L^L)^{N_L} (\psi_R^R)^{N_R}$$

$$\times \left\{ (N_L + N_R) \psi \Phi(0,0,0;\xi) \right.$$

$$+ N_L^2 \frac{\psi^L \psi_L}{\psi_L^L} \Phi(1,0,0;\xi) + N_R^2 \frac{\psi^R \psi_R}{\psi_R^R} \Phi(0,1,0;\xi)$$

$$\left. + N_L N_R \left[\frac{\psi^R \psi_L}{\psi_L^R} + \frac{\psi^L \psi_R}{\psi_R^L} \right] \Phi(0,0,1;\xi) \right\}, \quad (25)$$

where

$$\Phi(a,b,c;\xi) = \frac{[N_L - (a+c)]! \, (N_R - b)!}{[N_L + N_R - (a+b+c)]!} \xi^c (1-\xi)^{N_L - (a+c)}$$

$$\times P_{N_L - (a+c)}^{(c, N_R - N_L + a - b)} \left(\frac{1+\xi}{1-\xi} \right), \quad (26)$$

$$\xi = \frac{\psi_R^L \psi_L^R}{\psi_L^L \psi_R^R}, \quad (27)$$

were introduced. The quantities ψ_L, ψ_L^L, etc. are defined in Eq. (D3) and are integrals of the one-particle propagator $\psi = \psi(x_i, x_{j,0}; t)$ [49]. For the general case we have $\xi \in [0, 1]$ [50]. By using limiting results of ψ_L^L, ψ_R^R, ψ_L^L, and ψ_R^L from Appendix E, one concludes that $\xi \to 0$ for short times ($t \to 0$), and $\xi \to 1$ in the long-time limit ($t \to \infty$). It is also possible using standard relations for the Jacobi polynomials [44] to express $\Phi(a,b,c;\xi)$ as a Gauss hypergeometric function $_2F_1(\alpha, \beta, \gamma; z)$,

$$\Phi(a,b,c;\xi) = {}_2F_1(-N_L + a, -N_R + b, -[N_L + N_R] + a + b$$

$$+ c; 1 - \xi), \quad (28)$$

which is convenient for obtaining the long-time behavior as will be seen in the next section.

Finally, we need to find explicit expressions for the integrals of $\psi(x_i, x_{j,0}; t)$ [Eq. (D3)]. Integrating Eq. (19) [or integrating $\psi(x_i, x_{j,0}; s)$ prior to Laplace inversion (see Appendix E)] yields (arguments are left implicit)

$$\psi_L^L = \frac{1}{2} + \frac{x_T}{\ell} + \left(\frac{1}{2} + \frac{x_{T,0}}{\ell} \right)^{-1} \sum_{m=1}^{\infty} K_m \mathcal{E}_m(t),$$

$$\psi_R^R = \frac{1}{2} - \frac{x_T}{\ell} + \left(\frac{1}{2} - \frac{x_{T,0}}{\ell} \right)^{-1} \sum_{m=1}^{\infty} K_m \mathcal{E}_m(t),$$

$$\psi^L = \frac{1}{2} + \frac{x_T}{\ell} + \sum_{m=1}^{\infty} J_m(x_T, x_{T,0}) \mathcal{E}_m(t),$$

$$\psi_L = \frac{1}{\ell} \left[1 + \left(\frac{1}{2} + \frac{x_{T,0}}{\ell} \right)^{-1} \sum_{m=1}^{\infty} J_m(x_{T,0}, x_T) \mathcal{E}_m(t) \right],$$

$$\psi_R = \frac{1}{\ell} \left[1 - \left(\frac{1}{2} - \frac{x_{T,0}}{l} \right)^{-1} \sum_{m=1}^{\infty} J_m(x_{T,0}, x_T) \mathcal{E}_m(t) \right],$$

$$\psi^R = 1 - \psi^L, \quad \psi_L^R = 1 - \psi_L^L, \quad \psi_R^L = 1 - \psi_R^R, \quad (29)$$

with

$$K_m = \frac{1}{(m\pi)^2} \left[\nu_m^{(+)} \sin\left(\frac{m\pi x_T}{\ell} \right) \sin\left(\frac{m\pi x_{T,0}}{\ell} \right) \right.$$

$$\left. + \nu_m^{(-)} \cos\left(\frac{m\pi x_T}{\ell} \right) \cos\left(\frac{m\pi x_{T,0}}{\ell} \right) \right], \quad (30)$$

$$J_m(z,z') = \frac{1}{m\pi} \left[\nu_m^{(+)} \sin\left(\frac{m\pi z}{\ell} \right) \cos\left(\frac{m\pi z'}{\ell} \right) \right.$$

$$\left. - \nu_m^{(-)} \cos\left(\frac{m\pi z}{\ell} \right) \sin\left(\frac{m\pi z'}{\ell} \right) \right], \quad (31)$$

where $\mathcal{E}_m(t)$ and $\nu_m^{(\pm)}$ are given by Eqs. (21) and (22), respectively. To summarize, the complete expression for the tagged particle PDF is given by Eqs. (25)–(27), (29), and (30) together with Eqs. (1) and (2) for the case of finite-sized particles. The expressions for $\rho_T(x_T, t|x_{T,0})$ can straightforwardly be computed numerically; our MATLAB implementation is available upon request.

In the remaining part of this section we derive the tagged particle PDF $\rho_T(x_T, t|x_{T,0})$ valid for a large N and (finite) system size ℓ. This large-N expansion will be used in the next section for identifying different time regimes and to obtain $\rho_T(x_T, t|x_{T,0})$ for short and intermediate times. From Eq. (26) we note that the argument in the Jacobi polynomial, $P_n^{(\alpha,\beta)}(z)$, is in the interval $z \in [1, \infty)$ (since $\xi \in [0, 1]$) and that the number of particles is related to the order n. A large-N expansion of $\Phi(a,b,c;\xi)$ therefore amounts to find a large order n expansion valid for $z \in [1, \infty)$ (i.e., for all times) for the Jacobi polynomial. One such expansion was derived in [51] (see also [52,53]), and applying it to Eq. (26) yields

$$\Phi(a,b,c;\xi) \approx [N - (a+b+c)]^{1/2} \xi^{(2c-1)/4} (2\pi\zeta)^{1/2}$$

$$\times \left(\frac{1-\xi}{4} \right)^{[N-(a+b+c)]/2} I_c\{[N-(a+b+c)]\zeta\}$$

$$\times [1 + A(\zeta)], \quad (32)$$

where [54]

$$\zeta = \frac{1}{2} \ln\left[\frac{1 + \sqrt{\xi}}{1 - \sqrt{\xi}} \right], \quad (33)$$

and $I_\alpha(z)$ is the modified Bessel function of the first kind of order α. Stirling's formula [44] was also used to approximate factorials involving N_L and N_R. The correction term appearing in Eq. (32) is

$$A(\zeta) = \frac{B_0(\zeta)}{N - (a+b+c)} \frac{I_{c+1}\{[N-(a+b+c)]\zeta\}}{I_c\{[N-(a+b+c)]\zeta\}},$$

$$B_0(\zeta) = \frac{1}{2}\left\{ (c^2 - 1/4)\left(\frac{1}{\zeta} - \coth \zeta \right) \right.$$
$$\left. - [(\delta_N + a - b)^2 - 1/4]\tanh(\zeta) \right\}, \quad (34)$$

where $\delta_N = N_R - N_L$ was introduced. The expression for $A(\zeta)$ was found by explicitly evaluating an integral in Ref. [51], and it is a straightforward matter to show that the correction term $A(\zeta)$ is indeed always small for all $\xi \in [0,1]$ provided that $1/N$, $|\delta_N|/N \ll 1$. Inserting Eq. (32) in Eq. (25) and using the same approximations as above, we obtain our final large-N result for the tPDF,

$$\rho_T(x_T,t|x_{T,0}) = (\psi_L^L)^{(N-\delta_N-1)/2}(\psi_R^R)^{(N+\delta_N-1)/2}$$
$$\times (1-\xi)^{(N-1)/2}\left(\frac{\zeta}{\sqrt{\xi}} \right)^{1/2}\left\{ (1-\xi)^{1/2}\psi I_0[N\zeta] \right.$$
$$+ \frac{N}{2}\left(\frac{\psi^L\psi_L}{\psi_L^L} + \frac{\psi^R\psi_R}{\psi_R^R} \right)I_0[N\zeta]$$
$$\left. + \frac{N}{2}\sqrt{\xi}\left(\frac{\psi^R\psi_L}{\psi_L^R} + \frac{\psi^L\psi_R}{\psi_R^L} \right)I_1[N\zeta] \right\}. \quad (35)$$

We point out that this expression, in contrast to previous asymptotic expressions [20,22,37], is valid for a finite box of size ℓ, assuming only that the number of particles is large $N \gg 1$ and that the tagged particle is approximately in the center of the system: $|\delta_N|/N \ll 1$.

V. THREE DIFFERENT TIME REGIMES

In this section we show that, for large N, the finite SFD system considered here has three different time regimes to which expressions for $\rho_T(x_T,t|x_{T,0})$ are derived. Mathematically, the different cases appear due to the magnitude of $N\zeta$ [found in the argument of the Bessel functions in Eq. (35)], and if ζ is small or large. Utilizing Eqs. (E14) and (33), these cases can be turned into different time regimes if introducing the collision time

$$\tau_{coll} = \frac{1}{\varrho^2 D}, \quad (36)$$

where $\varrho = N/\ell$ is the concentration of particles, and the equilibrium time

$$\tau_{eq} = \frac{\ell^2}{D}. \quad (37)$$

For a particle located roughly in the middle, $|\delta_N|/N \ll 1$ [i.e., Eq. (35) applies], the three cases are given by (A) *short* times, $N\zeta \ll 1$, i.e., $t \ll \tau_{coll}, \tau_{eq}$; (B) *intermediate* times, $\zeta \ll 1$ and $N\zeta \gg 1$, corresponding to $\tau_{coll} \ll t \ll \tau_{eq}$; and (C) *long* times, $\zeta \gg 1$, i.e., $t \gg \tau_{coll}, \tau_{eq}$.

Time regimes (A)–(C) are analyzed in detail below.

A. Short times, $t \ll \tau_{coll}, \tau_{eq}$

For short times we have $N\zeta \ll 1$ and may therefore use the approximations $I_\alpha(z)|_{z\ll 1} \approx (z/2)^\alpha/\Gamma(\alpha+1)$ [44], $\zeta \approx \sqrt{\xi}$, and

$\xi \ll 1$. In this limit, one finds that the first term in Eq. (35) dominates which in combination with Eq. (2) leads to

$$\rho_T(y_T,t|y_{T,0}) = (4\pi Dt)^{-1/2}\exp\left[-\frac{(y_T - y_{T,0})^2}{4Dt} \right], \quad (38)$$

for which the MSD is

$$\mathcal{S}(t) = 2Dt. \quad (39)$$

In the short-time regime, almost no collisions with the neighboring particles (nor the box walls) have occurred and the tPDF is therefore a Gaussian with width $2Dt$ as for a free particle in an infinite one-dimensional system.

B. Intermediate times, $\tau_{coll} \ll t \ll \tau_{eq}$

In the intermediate-time regime the tagged particle has collided many times with its neighbors but not yet reached its equilibrium tPDF. For this regime, where $\zeta \ll 1$ but $N\zeta \gg 1$, we get the tPDF as follows. First, the first term in Eq. (35) is neglected (this is checked at the end of the calculation). Second, the Bessel function is approximated with $I_\alpha(z)|_{z\gg 1} \approx e^z/\sqrt{2\pi z}$. A straightforward expansion of Eq. (35) for ψ_L^R, $\psi_R^L \ll 1$ (i.e., $\sqrt{\xi} \ll 1$), together with Stirling's formula, gives

$$\rho_T(y_T,t|y_{T,0}) \approx \frac{1}{2}e^{-\delta_N(\psi_R^L - \psi_R^R)}\sqrt{\frac{N}{2\pi}}(\psi_R^L\psi_R^R)^{-1/4}e^{-(N/2)(\sqrt{\psi_R^L} - \sqrt{\psi_L^R})^2}$$
$$\times \left[\psi^L\psi_L + \psi^R\psi_R + \psi^R\psi_L\left(\frac{\psi_R^L}{\psi_L^R} \right)^{1/2} \right.$$
$$\left. + \psi^L\psi_R\left(\frac{\psi_L^R}{\psi_R^L} \right)^{1/2} \right]. \quad (40)$$

If we furthermore assume that the average of the absolute value of $\eta = (x_T - x_{T,0})/\sqrt{4Dt}$ is small (which is checked after the calculation), Eq. (E15) may be used which in combination with Eqs. (1), (2), and (40), keeping only lowest order terms in η, leads to the SFD result,

$$\rho_T(y_T,t|y_{T,0}) = \frac{1}{\sqrt{2\pi}}\left(\frac{1}{\frac{4Dt}{\pi}\left(\frac{1-\varrho\Delta}{\varrho} \right)^2} \right)^{1/4}$$
$$\times \exp\left[-\frac{(y_T - y_{T,0})^2}{2\sqrt{\frac{4Dt}{\pi}\left(\frac{1-\varrho\Delta}{\varrho} \right)^2}} \right], \quad (41)$$

where the MSD is

$$\mathcal{S}(t) = \frac{1-\varrho\Delta}{\varrho}\sqrt{\frac{4Dt}{\pi}}. \quad (42)$$

Equation (42) justifies the assumption that the expectation value of $|\eta|$ is a small number. Also, comparing the magnitude of the first term in Eq. (35) with respect to the second and the third shows indeed that our first assumption above was correct [55]. For point particles $\Delta = 0$, Eq. (41) agrees

with standard results [20,37], in which $N, L \to \infty$ while keeping the concentration ϱ fixed. The result above shows that SFD behavior appears also in a finite system with reflecting ends, as an intermediate regime (for a particle roughly in the middle). In addition, note that the simple rescaling $\varrho \to \varrho/(1-\varrho\Delta)$ takes us from previous point-particle results to those of finite-sized particles.

C. Long times, $t \gg \tau_{eq}$

In the long-time limit we have $\zeta \gg 1$, for which the tPDF can be obtained exactly for arbitrary N. Using the exact expression for $\rho_{\mathcal{T}}(x_{\mathcal{T}}, t | x_{\mathcal{T},0})$ found in Eqs. (25) and (28), together with $_2F_1(\alpha, \beta, \gamma; z=0)=1$ [44] and Eq. (E7) [also using Eqs. (1) and (2)] gives

$$\rho_{\mathcal{T}}^{eq}(y_{\mathcal{T}}) = \frac{1}{(L-N\Delta)^N} \frac{(N_L+N_R+1)!}{N_L! N_R!}$$
$$\times \left(\frac{L}{2}+y_{\mathcal{T}}-\Delta(1/2+N_l)\right)^{N_L}\left(\frac{L}{2}-y_{\mathcal{T}}-\Delta(1/2+N_R)\right)^{N_R}$$
(43)

where $\rho_{\mathcal{T}}^{eq}(y_{\mathcal{T}}) = \rho_{\mathcal{T}}(y_{\mathcal{T}}, t \to \infty | y_{\mathcal{T},0})$. This equation agrees with the equilibrium tPDF given in Eq. (5) (for $\Delta=0$), as it should [56]. The results above show the consistency of our analysis and illustrate the ergodicity of the finite SFD system. Calculating the second moment of the equilibrium tPDF, $\mathcal{S}(t \to \infty) = \mathcal{S}_{eq}$, gives

$$\mathcal{S}_{eq} = \left(\frac{1}{4}\right)^{N_R+1}\left(\frac{L-N\Delta}{2}\right)^2 \frac{\Gamma(1/2)\Gamma(2[N_R+1])}{\Gamma(N_R+1)\Gamma(N_R+5/2)}, \quad (44)$$

for $N_L=N_R$ where $\Gamma(z)$ is the gamma function. For $N \gg 1$ we can simplify the expression for the equilibrium tPDF as well as $\mathcal{S}_{eq}$. If a symmetric file is assumed, i.e., $N_L=N_R$ and $\mathcal{T} = (N+1)/2$, an asymptotic expansion of $\rho_{\mathcal{T}}^{eq}(y_{\mathcal{T}})$ (using Stirling's approximation [44]) gives the Gaussian PDF

$$\rho_{\mathcal{T}}^{eq}(y_{\mathcal{T}}) \approx \sqrt{\frac{2N}{\pi} \frac{1}{(L-N\Delta)^2}} \exp\left[-2N\left(\frac{y_{\mathcal{T}}}{L-N\Delta}\right)^2\right],$$
(45)

from which we read off that

$$\mathcal{S}_{eq} \approx \frac{(L-N\Delta)^2}{4N}. \quad (46)$$

Equation (46) can also be found directly from a large-N expansion of Eq. (44) using Stirling's formula and assuming $N \approx 2N_R$. We point out that $\rho_{\mathcal{T}}^{eq}(y_{\mathcal{T}}) \to 0$ for $N, L \to \infty$ even if the concentration $\varrho=N/L$ is kept fixed. This is consistent with the long-time limit of Eq. (41), which indeed goes to zero for large times. Finally, the analysis in this subsection also gives an estimate on the time required to reach equilibrium, namely, $t \gg \tau_{eq}$.

VI. CONCLUSIONS AND OUTLOOK

In this study we have solved exactly a nonequilibrium statistical-mechanics problem: diffusion of N hard-core interacting particles of size Δ which are unable to pass each other

in a one-dimensional system of length L with reflecting boundaries. In particular, we obtained an exact expression for the probability density function $\rho_{\mathcal{T}}(y_{\mathcal{T}}, t | y_{\mathcal{T},0})$ (denoted as tPDF) that a tagged particle $\mathcal{T}$ is at position $y_{\mathcal{T}}$ at time t given that it at time $t=0$ was at position $y_{\mathcal{T},0}$. We derived the tPDF by first finding the N-particle probability density function (NPDF) via the Bethe ansatz, and then integrating out the coordinates and taking the average over the initial positions of all particles except one. The exact expression for $\rho_{\mathcal{T}}(y_{\mathcal{T}}, t | y_{\mathcal{T},0})$ is found in Eqs. (1), (2), (25), and (26) and constitutes the main result of the paper. For a large number of particles and for a tagged particle located roughly in the middle of the system, an asymptotic expansion of the tPDF was derived [see Eq. (35)]. Based on this equation, we found three time regimes of interest: (A) for short times, i.e., times much smaller than the collision time $t \ll \tau_{coll}=1/(\varrho^2 D)$, where $\varrho=N/L$ is the particle number concentration, the tPDF coincides with the Gaussian probability density function that characterizes a free particle [Eq. (38)]. (B) For intermediate times $t \gg \tau_{coll}$, but much smaller than the equilibrium time $t \ll \tau_{eq}=L^2/D$, a subdiffusive single-file regime was found in which the tPDF is a Gaussian with an associated MSD proportional to $t^{1/2}$ [Eq. (41)]. (C) For times exceeding the equilibrium time $t \gg \tau_{eq}$, the tPDF approaches a probability density of polynomial type [Eq. (43)].

We point out that the subdiffusive behavior for a tagged particle in time regime (B) is of fractional Brownian motion type [33,57,58] rather than that of continuous-time random walks (CTRWs) characterized by heavy-tailed waiting time densities [59–61]. For such CTRW processes the probability density function is not a Gaussian as for the current system. Further comparison between subdiffusion in single-file systems and that occurring in CTRW theory was pursued numerically in [62].

The Bethe ansatz is often employed in quantum mechanics when many-body systems are studied (e.g., quantum spin chains) [40,63], and also for stochastic many-particle lattice problems [64,65]. We hope that the theoretical analysis based on the Bethe ansatz presented here will stimulate further progress in the field of single-file diffusion and that of interacting random walkers. For instance, it would be interesting to see whether our analysis could be extended to derive exact results also for particles interacting through potentials other than hard-core type [31], and for particles having different diffusion constants [34].

From the applied point of view, our exact expression for the tPDF covers all time regimes and is straightforward to implement for numerical computations. Therefore, we believe that our explicit formula for $\rho_{\mathcal{T}}(y_{\mathcal{T}}, t | y_{\mathcal{T},0})$, as well as the approximate results for regimes (A)–(C), will be useful for experimentalists (see, for instance, [18]) seeking to extract system parameters such as the particle size Δ, the system size L, the particle's diffusion constants (D), and the number (N_L and N_R) of particles to the left and right of the tagged particle.

We finally note that the use of fluorescently labeled (tagged) particles is of much use for studying biological systems. The understanding of how the motion of such particles correlates with its environment is therefore the key for grasping the behavior of such systems in a quantitative fashion.

ACKNOWLEDGMENTS

APPENDIX A: BETHE ANSATZ

In this section we show that the Bethe ansatz, Eq. (12), is a solution to the problem defined by Eqs. (7)–(11). First, it is demonstrated that Eq. (12) satisfies the boundary conditions at the ends of the box. Second, we show that the requirement that the particles are unable to pass each other is satisfied by setting the scattering coefficients to unity. Finally, it is demonstrated that Eq. (12) also satisfies the initial condition.

1. Boundary conditions at the ends of the box

In this subsection it is proven that Eq. (12) satisfies the reflecting boundary conditions (9) and (10) at $\pm\ell/2$ with an appropriate choice for $\phi(k_j, x_{j,0})$ [Eq. (15)]. The scattering coefficients are set to $S_{ij}=1$, which is proven to be correct in the following subsection. First, we define the function

$$\lambda(k,z) = \phi(k,z)e^{-ik\ell/2} = 2\cos[k(z+\ell/2)]\sum_{m=-\infty}^{\infty}e^{-2ikm\ell},$$

(A1)

which has the symmetry relation

$$\lambda(k,z) = \lambda(-k,z). \tag{A2}$$

By taking the derivative of Eq. (12) with respect to x_1 and evaluating at the left boundary $x_1=-\ell/2$ give

$$\left.\frac{\partial\mathcal{P}(\vec{x},t|\vec{x}_0)}{\partial x_1}\right|_{x_1=-\ell/2} = \int_{-\infty}^{\infty}\frac{dk_1}{2\pi}\cdots\int_{-\infty}^{\infty}\frac{dk_N}{2\pi}e^{-D(k_1^2+\cdots+k_N^2)t}\Pi_{j=1}^N\phi(k_j,x_{j,0})[ik_1 e^{ik_1 x_1}(e^{ik_2 x_2+\cdots+ik_N x_N}+\text{perm. of }\{k_2,\ldots,k_N\})$$

$$+\cdots+ik_i e^{ik_i x_1}(e^{ik_2 x_2+\cdots+ik_i x_i+\cdots+ik_N x_N}+\text{perm. of }\{k_2,\ldots,k_{i-1},k_{i+1},\ldots,k_N\})+\cdots+ik_N e^{ik_N x_1}(e^{ik_2 x_2+\cdots+ik_1 x_N}$$

$$+\text{perm. of }\{k_1,\ldots,k_{N-1}\})]_{x_1=-\ell/2}$$

$$=\int_{-\infty}^{\infty}\frac{dk_2}{2\pi}\cdots\int_{-\infty}^{\infty}\frac{dk_N}{2\pi}e^{-D(k_2^2+\cdots+k_N^2)t}\Pi_{j=2}^N\phi(k_j,x_{j,0})\int_{-\infty}^{\infty}\frac{dk_1}{2\pi}(ik_1)e^{-Dk_1^2 t}\lambda(k_1,x_{1,0})$$

$$+\cdots+\int_{-\infty}^{\infty}\frac{dk_1}{2\pi}\cdots\int_{-\infty}^{\infty}\frac{dk_{i-1}}{2\pi}\int_{-\infty}^{\infty}\frac{dk_{i+1}}{2\pi}\cdots\int_{-\infty}^{\infty}\frac{dk_N}{2\pi}e^{-D(k_1^2+\cdots+k_{i-1}^2+k_{i+1}^2+\cdots+k_N^2)t}\Pi_{j=1,j\neq i}^N\phi(k_j,x_{j,0})$$

$$\times\int_{-\infty}^{\infty}\frac{dk_i}{2\pi}(ik_i)e^{-Dk_i^2 t}\lambda(k_i,x_{i,0})+\cdots+\int_{-\infty}^{\infty}\frac{dk_1}{2\pi}\cdots\int_{-\infty}^{\infty}\frac{dk_{N-1}}{2\pi}e^{-D(k_1^2+\cdots+k_{N-1}^2)t}\Pi_{j=1}^{N-1}\phi(k_j,x_{j,0})$$

$$\times\int_{-\infty}^{\infty}\frac{dk_N}{2\pi}(ik_N)e^{-Dk_N^2 t}\lambda(k_N,x_{N,0})=0,$$

(A3)

where $\int_{-\infty}^{\infty}dk_i\,k_i e^{-Dk_i^2 t}\lambda(k_i,x_{i,0})=0$ [odd integrand; see Eq. (A2)] was used in the last step. Note that this calculation does not rely on any specific form of $\phi(k_j,x_{j,0})$. It is only required that the symmetry relation (A2) holds. Furthermore, the dispersion relation $E(\vec{k})=D(k_1^2+\cdots+k_N^2)$ was also used in the above derivation. However, it would work equally well for any dispersion relation as long as $E(\vec{k})=\sum_i E(k_i)$ with $E(k_i)=E(-k_i)$ is valid.

A similar analysis as just presented shows that the Bethe ansatz solution also satisfies the reflecting condition at $+\ell/2$ [Eq. (10)]. In fact, since the Bethe ansatz is in-variant under the coordinate transformation $x_i\leftrightarrow x_j$, it gives $[\partial\mathcal{P}(\vec{x},t|\vec{x}_0)/\partial x_j]_{x_j=\pm\ell/2}=0$ for *all* x_j.

2. Single-file condition: Particles are unable to overtake

In this subsection it is shown that the condition that the particles are unable to pass each other [Eq. (8)] is satisfied for scattering coefficients given by $S_{ij}=1$ in the Bethe ansatz solution (12). We start off by expressing $\mathcal{P}(\vec{x},t|\vec{x}_0)$ in two alternative ways:

$$\mathcal{P}(\vec{x},t|\vec{x}_0) = \int_{-\infty}^{\infty} \frac{dk_1}{2\pi} \int_{-\infty}^{\infty} \frac{dk_2}{2\pi} \cdots \int_{-\infty}^{\infty} \frac{dk_N}{2\pi} e^{-D(k_1^2+\cdots+k_N^2)t} \Pi_{j=1}^N \phi(k_j,x_{j,0}) [e^{ik_1 x_j}(e^{ik_j x_1+\cdots+ik_{j-1}x_{j-1}+ik_{j+1}x_{j+1}+ik_{j+2}x_{j+2}+\cdots+ik_N x_N}$$

$$+ \text{ all other permut. of } \{k_2,\ldots,k_N\}) + e^{ik_2 x_j}(e^{ik_1 x_1+ik_j x_2+\cdots+ik_{j-1}x_{j-1}+ik_{j+1}x_{j+1}+ik_{j+2}x_{j+2}+\cdots+ik_N x_N}$$

$$+ \text{ all other permut. of } \{k_1,k_3,\ldots,k_N\}) + \cdots + e^{ik_N x_j}(e^{ik_1 x_1+\cdots+ik_{j-1}x_{j-1}+ik_{j+1}x_{j+1}+ik_{j+2}x_{j+2}+\cdots+ik_j x_N}$$

$$+ \text{ all other permut. of } \{k_1,\ldots,k_{N-1}\})] \tag{A4}$$

and

$$\mathcal{P}(\vec{x},t|\vec{x}_0) = \int_{-\infty}^{\infty} \frac{dk_1}{2\pi} \int_{-\infty}^{\infty} \frac{dk_2}{2\pi} \cdots \int_{-\infty}^{\infty} \frac{dk_N}{2\pi} e^{-D(k_1^2+\cdots+k_N^2)t} \Pi_{j=1}^N \phi(k_j,x_{j,0}) [e^{ik_1 x_{j+1}}(e^{ik_{j+1}x_1+\cdots+ik_{j-1}x_{j-1}+ik_j x_j+ik_{j+2}x_{j+2}+\cdots+ik_N x_N}$$

$$+ \text{ all other permut. of } \{k_2,\ldots,k_N\}) + e^{ik_2 x_{j+1}}(e^{ik_1 x_1+ik_{j+1}x_2+\cdots+ik_{j-1}x_{j-1}+ik_j x_j+ik_{j+2}x_{j+2}+\cdots+ik_N x_N}$$

$$+ \text{ all other permut. of } \{k_1,k_3,\ldots,k_N\}) + \cdots + e^{ik_N x_{j+1}}(e^{ik_1 x_1+\cdots+ik_{j-1}x_{j-1}+ik_j x_j+ik_{j+2}x_{j+2}+\cdots+ik_{j+1}x_N}$$

$$+ \text{ all other permut. of } \{k_1,\ldots,k_{N-1}\})]. \tag{A5}$$

Using the above equations one finds

$$\left(\frac{\partial \mathcal{P}(\vec{x},t|\vec{x}_0)}{\partial x_{j+1}} - \frac{\partial \mathcal{P}(\vec{x},t|\vec{x}_0)}{\partial x_j}\right)\bigg|_{x_{j+1}=x_j} = \int_{-\infty}^{\infty} \frac{dk_1}{2\pi} \int_{-\infty}^{\infty} \frac{dk_2}{2\pi} \cdots \int_{-\infty}^{\infty} \frac{dk_N}{2\pi} e^{-D(k_1^2,\ldots,k_N^2)t} \Pi_{j=1}^N \phi(k_j,x_{j,0})$$

$$\times [ik_1 e^{ik_1 x_j}(e^{ik_{j+1}x_1+\cdots+ik_{j-1}x_{j-1}+ik_j x_{j+1}+ik_{j+2}x_{j+2}+\cdots+ik_N x_N}$$

$$- e^{ik_j x_1+\cdots+ik_{j-1}x_{j-1}+ik_{j+1}x_{j+1}+ik_{j+2}x_{j+2}+\cdots+ik_N x_N} + \text{ all other permut. of } \{k_2,\ldots,k_N\})$$

$$+ ik_2 e^{ik_2 x_j}(e^{ik_1 x_1+ik_{j+1}x_2+\cdots+ik_{j-1}x_{j-1}+ik_j x_{j+1}+ik_{j+2}x_{j+2}+\cdots+ik_N x_N}$$

$$- e^{ik_1 x_1+ik_j x_2+\cdots+ik_{j-1}x_{j-1}+ik_{j+1}x_{j+1}+ik_{j+2}x_{j+2}+\cdots+ik_N x_N} + \text{ all other permut. of } \{k_1,k_3,\ldots,k_N\})$$

$$+ \cdots + ik_N e^{ik_N x_j}(e^{ik_1 x_1+\cdots+ik_{j-1}x_{j-1}+ik_j x_{j+1}+ik_{j+2}x_{j+2}+\cdots+ik_{j+1}x_N}$$

$$- e^{ik_1 x_1+\cdots+ik_{j-1}x_{j-1}+ik_{j+1}x_{j+1}+ik_{j+2}x_{j+2}+\cdots+ik_j x_N} + \text{ all other permut. of } \{k_1,\ldots,k_{N-1}\})] = 0, \tag{A6}$$

where it was used that each parenthesis is identically zero due to the cancellation of the $2(N-1)!$ terms after permutation over all allowed momenta. Note that this derivation is independent of the choice of $\phi(k_j,x_{j,0})$ and $E(\vec{k})$.

3. Initial condition

In this subsection we show that the Bethe ansatz (12) agrees with the initial condition (11) when $t \to 0$. By defining

$$\Omega(x,y) = \int_{-\infty}^{\infty} \frac{dk_j}{2\pi} e^{ik_j x} \phi(k_j,y), \tag{A7}$$

Eq. (12) reads

$$\mathcal{P}(\vec{x},t \to 0|\vec{x}_0) = \Omega(x_1,x_{1,0})\Omega(x_2,x_{2,0}) \cdots \Omega(x_N,x_{N,0})$$

$$+ \Omega(x_1,x_{2,0})\Omega(x_2,x_{1,0}) \cdots \Omega(x_N,x_{N,0})$$

$$+ \text{ all other permut. of } \{x_{1,0},\ldots,x_{N,0}\}. \tag{A8}$$

Using the explicit expression for $\phi(k,y)$ found in Eq. (15) and that $\delta(x-z) = (2\pi)^{-1} \int_{-\infty}^{\infty} dk \, e^{ik(x-z)}$ leads to

$$\Omega(x,y) = \sum_{m=-\infty}^{\infty} \delta(x-y+2m\ell) + \delta(x+y+[2m+1]\ell). \tag{A9}$$

For all $m \neq 0$ the δ functions are nonzero for coordinates lying outside of $\mathcal{R}$ and $\mathcal{R}_0$ where, per definition, $\mathcal{P}(\vec{x},t|\vec{x}_0) \equiv 0$ (see discussion in Sec. II). For $m=0$, it is only the first δ function in the sum, $\delta(x-y)$, that contributes to the NPDF. Furthermore, since all terms except the first one in Eq. (A8) are zero due to the fact that $\mathcal{P}(\vec{x},t|\vec{x}_0)=0$ outside $\mathcal{R}$, one obtains

$$\mathcal{P}(\vec{x},t \to 0|\vec{x}_0) = \delta(x-x_0) \cdots \delta(x_N - x_{N,0}) \tag{A10}$$

as $t \to 0$, which is the desired result.

APPENDIX B: LAPLACE TRANSFORM OF $\psi(x_i,x_{j,0};t)$

In this section it is shown explicitly how one can go from the one-particle PDF $\psi(x_i,x_{j,0};t)$ for a particle in a box expressed in terms of Gaussians [Eq. (17)], to the eigenmode expansion [Eqs. (19)–(22)] used in this paper. First, the summation in Eq. (17) is divided schematically into

$\Sigma_{m=-\infty}^{\infty} f_m = f_{m=0} + \Sigma_{m=1}^{\infty}[f_m + f_{-m}]$. Then, using the Laplace transform $\mathcal{L}[(\pi t)^{-1/2} e^{-a/(4t)}] = s^{-1/2} e^{-a\sqrt{s}}$ $(a > 0)$ [44] one finds

$$\psi(x_i, x_{j,0}; s) = \mathcal{Q}(s) + \frac{e^{-(x_i + x_{j,0} + \ell)\sqrt{s/D}}}{\sqrt{4Ds}}$$
$$+ \left[\frac{e^{-(x_i - x_{j,0})\sqrt{s/D}} + e^{(x_i - x_{j,0})\sqrt{s/D}}}{\sqrt{4Ds}} \right.$$
$$+ \left. \frac{e^{-(x_i + x_{j,0} + \ell)\sqrt{s/D}} + e^{(x_i + x_{j,0} + \ell)\sqrt{s/D}}}{\sqrt{4Ds}} \right] \sum_{m=1}^{\infty} e^{-2m\ell\sqrt{s/D}},$$
(B1)

where

$$\mathcal{Q}(s) = \begin{cases} (4Ds)^{-1/2} e^{-(x_i - x_{j,0})\sqrt{s/D}}, & x_i \ge x_{j,0} \\ (4Ds)^{-1/2} e^{-(x_{j,0} - x_i)\sqrt{s/D}}, & x_i \le x_{j,0}. \end{cases}$$
(B2)

Considering the cases $x_i > x_{j,0}$ and $x_i < x_{j,0}$ separately, and that $\Sigma_{m=1}^{\infty} e^{-2m\ell\sqrt{s/D}} = (e^{2\ell\sqrt{s/D}} - 1)^{-1}$, leads to
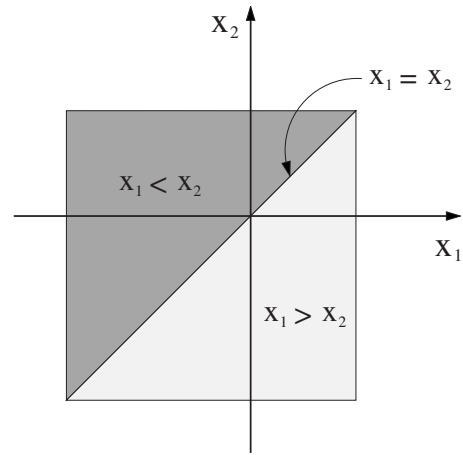
FIG. 2. Integration area (the darker upper area, $x_1 < x_2$) for the integral defined in Eq. (C2). For any function which is symmetric under $x_1 \leftrightarrow x_2$ the integration over the lower triangle ($x_1 > x_2$) yields the same result as integration over the same function over the upper triangle ($x_1 < x_2$). One may therefore extend the integration area to the full rectangle above provided one divides the corresponding result by 2.

$$\psi(x_i, x_{j,0}; s) = \frac{1}{\sqrt{sD} \, \sinh[\ell\sqrt{s/D}]} \begin{cases} \cosh[(\ell/2 + x_i)\sqrt{s/D}] \cosh[(\ell/2 - x_{j,0})\sqrt{s/D}], & x_i \le x_{j0} \\ \cosh[(\ell/2 - x_i)\sqrt{s/D}] \cosh[(\ell/2 + x_{j,0})\sqrt{s/D}], & x_i \ge x_{j,0}, \end{cases} \qquad (B3)$$

which after elementary trigonometric manipulations result in Eq. (18).

APPENDIX C: EXTENDED PHASE-SPACE INTEGRATION

When the tPDF is integrated out from the *N*PDF we need to resolve the following type of integral:

$$\mathcal{I}(x_{\mathcal{T}}) = \int_{\mathcal{R} \backslash x_{\mathcal{T}}} dx'_1 \cdots dx'_{\mathcal{T}-1} dx'_{\mathcal{T}+1} \cdots dx'_N \, \mathcal{P}(\vec{x}', t | \vec{x}_0) \quad \text{(C1)}$$

over the region $\mathcal{R}$ [Eq. (3)] with the tagged particle coordinate $x_{\mathcal{T}}$ left out. As pointed previously in the paper, the Bethe ansatz solution [Eq. (12)] is symmetric under the transformation $x_i \leftrightarrow x_j$ when all scattering coefficients are given by $S_{ij} = 1$. This allows the integration of $\mathcal{P}(\vec{x}, t | \vec{x}_0)$ in Eq. (C1) to be extended to the whole hyperspace $x_j \in [-\ell/2, x_{\mathcal{T}}]$, $j = 1, \ldots, \mathcal{T} - 1$ and $x_j \in [x_{\mathcal{T}}, \ell/2]$, $j = \mathcal{T}+1, \ldots, N$. This is most easily demonstrated in an example which then is extended to the general situation. Consider the case of three particles where particle 3 is tagged $\mathcal{T} = 3$,

$$\mathcal{I}(x_3) = \int_{-\ell/2 < x_1 < x_2 < x_3 < \ell/2} dx_1 dx_2 \, \mathcal{P}(x_1, x_2, x_3, t | \vec{x}_0).$$
(C2)

The integration area in the (x_1, x_2) plane is sketched in Fig. 2 (upper dark triangle). Since $\mathcal{P}(\vec{x}, t | \vec{x}_0)$ is invariant under $x_1 \leftrightarrow x_2$, integration over the lower triangle gives the same result, i.e.,

$$\mathcal{I}(x_3) = \int_{-\ell/2 < x_2 < x_1 < x_3 < \ell/2} dx_1 dx_2 \, \mathcal{P}(x_1, x_2, x_3, t | \vec{x}_0).$$
(C3)

If Eqs. (C2) and (C3) are added, $\mathcal{I}(x_3)$ can be expressed as an integral over the full rectangle

$$\mathcal{I}(x_3) = \frac{1}{2} \int_{-\ell/2}^{x_{\mathcal{T}}} dx_1 \int_{-\ell/2}^{x_{\mathcal{T}}} dx_2 \, \mathcal{P}(x_1, x_2, x_3, t | \vec{x}_0). \quad \text{(C4)}$$

For the general case, the integration can be extended for any particle number to the left of the tagged particle. This means that it is possible to go from integration over the phase space $-\ell/2 < x_1 < \ldots < x_{\mathcal{T}-1} < x_{\mathcal{T}}$ to $-\ell/2 < x_j < x_{\mathcal{T}}$ for $j = 1, \ldots, \mathcal{T} - 1$ provided that we divide by $N_L!$. This holds also for N_R particles to the right and Eq. (C1) can in general be written as

$$\mathcal{I}(x_T) = \frac{1}{N_L! \, N_R!} \int_{-\ell/2}^{x_T} dx_1 \int_{-\ell/2}^{x_T} dx_2 \cdots$$

$$\times \int_{-\ell/2}^{x_T} dx_{T-1} \int_{x_T}^{\ell/2} dx_{T+1} \cdots \int_{x_T}^{\ell/2} dx_N \, \mathcal{P}(\vec{x}, t | \vec{x}_0).$$

(C5)

Since $\mathcal{P}(\vec{x}, t | \vec{x}_0)$ is also invariant under $x_{i,0} \leftrightarrow x_{j,0}$, a similar

extended phase-space technique is valid for integrations over the initial particle positions $\mathcal{R}_0$.

APPENDIX D: FROM THE *N*PDF TO THE tPDF

In this appendix the tPDF is obtained from integral (6) using the Bethe ansatz *N*PDF (16) explicitly. A similar combinatorial analysis to that found in [37] gives

$$\rho(x_T, t | x_{T,0}) = \frac{1}{N_L! \, N_R!} \left\{ \sum_{q=0}^{\min\{N_L, N_R\}} H^0(q) (\psi_L^L)^{N_L - q} (\psi_R^L)^q \psi (\psi_L^R)^q (\psi_R^R)^{N_R - q} + \sum_{q=0}^{\min\{N_L - 1, N_R\}} H_L^L(q) (\psi_L^L)^{N_L - q - 1} (\psi_R^L)^q \psi^L \psi_L (\psi_L^R)^q (\psi_R^R)^{N_R - q} \right.$$

$$+ \sum_{q=0}^{\min\{N_L, N_R - 1\}} H_R^R(q) (\psi_L^L)^{N_L - q} (\psi_R^L)^q \psi^R \psi_R (\psi_L^R)^q (\psi_R^R)^{N_R - q - 1} + \sum_{q=0}^{\min\{N_L - 1, N_R - 1\}} H_L^R(q)$$

$$\times (\psi_L^L)^{N_L - q - 1} (\psi_R^L)^{q+1} \psi^R \psi_L (\psi_L^R)^q (\psi_R^R)^{N_R - q - 1} + \sum_{q=0}^{\min\{N_L - 1, N_R - 1\}} H_R^L(q) (\psi_L^L)^{N_L - q - 1} (\psi_R^L)^q \psi^L \psi_R (\psi_L^R)^{q+1} (\psi_R^R)^{N_R - q - 1} \right\}, \quad (D1)$$

with the combinatorial factors

$$H^0(q) = \binom{N_L}{q} \binom{N_R}{q} N_L! \, N_R!,$$

$$H_L^L(q) = \binom{N_L - 1}{q} \binom{N_R}{q} N_L! \, N_R! \, N_L,$$

$$H_R^R(q) = \binom{N_L}{q} \binom{N_R - 1}{q} N_L! \, N_R! \, N_R,$$

$$H_L^R(q) = \binom{N_L - 1}{q} \binom{N_R}{q+1} N_L! \, N_R! \, N_L,$$

$$H_R^L(q) = \binom{N_L}{q+1} \binom{N_R - 1}{q} N_L! \, N_R! \, N_R, \quad (D2)$$

and integrals (leaving arguments $x_{T,0}$ and x_T implicit)

$$\psi_L^L(t) = f_L \int_{-\ell/2}^{x_T} dx_i \int_{-\ell/2}^{x_{T,0}} dx_{j,0} \, \psi(x_i, x_{j,0}; t),$$

$$\psi_R^R(t) = f_R \int_{x_T}^{\ell/2} dx_i \int_{x_{T,0}}^{\ell/2} dx_{j,0} \, \psi(x_i, x_{j,0}; t),$$

$$\psi_L^R(t) = f_L \int_{x_T}^{\ell/2} dx_i \int_{-\ell/2}^{x_{T,0}} dx_{j,0} \, \psi(x_i, x_{j,0}; t),$$

$$\psi_R^L(t) = f_R \int_{-\ell/2}^{x_T} dx_i \int_{x_{T,0}}^{\ell/2} dx_{j,0} \, \psi(x_i, x_{j,0}; t)$$

$$\psi^L(t) = \int_{-\ell/2}^{x_T} dx_i \, \psi(x_i, x_{j,0}; t),$$

$$\psi^R(t) = \int_{x_T}^{\ell/2} dx_i \, \psi(x_i, x_{j,0}, t),$$

$$\psi_L(t) = f_L \int_{-\ell/2}^{x_{T,0}} dx_{j,0} \, \psi(x_j, x_{j,0}; t),$$

$$\psi_R(t) = f_R \int_{x_{T,0}}^{\ell/2} dx_{j,0} \, \psi(x_j, x_{j,0}; t). \quad (D3)$$

The prefactors f_L and f_R are found in Eq. (24) and correspond to uniform distributions to the left and right of the tagged particle according to which the surrounding particles are initially placed. They appear when integrals over initial coordinates are performed. Also, it is easy to see from normalization that $\psi^L(t) + \psi^R(t) = 1$, $\psi_L^L(t) + \psi_L^R(t) = 1$, and $\psi_R^R(t) + \psi_R^L(t) = 1$.

If considering a single particle in a box of length ℓ, the integrals defined in Eq. (D3) are easily interpreted as follows. First, ψ_L^L (ψ_R^R) is the probability that a single particle is to the left (right) of x_T at time t given that it started, with an equal probability, anywhere to the left (right) of $x_{T,0}$. Similar interpretations hold also for ψ_L^R and ψ_R^L. The quantity ψ_L (ψ_R) is the probability that a single particle is at position x_T given that the particle started somewhere to the left (right) of $x_{T,0}$. Finally, ψ^L (ψ^R) is the probability that a single particle is to the left (right) of x_T at time t given that it started at position $x_{T,0}$.

APPENDIX E: INTEGRALS OF $\psi(x_i, x_{j,0}; s)$ IN LAPLACE SPACE

In this appendix, exact expressions as well as limiting forms for the integrals appearing in Eq. (D3) are given in the Laplace domain. Using the Laplace-transformed one-particle PDF $\psi(x_i, x_{j,0}; s)$ found in Eq. (B3), the integrals defined in Eq. (D3) (with time t replaced with Laplace variable s, and x_T and $x_{T,0}$ left out) are given by

$$\psi^L(s) = \frac{1}{s\,\sinh[\ell\sqrt{s/D}]} \begin{cases} \sinh[(\ell/2 + x_T)\sqrt{s/D}]\cosh[(\ell/2 - x_{T,0})\sqrt{s/D}], & x_T \leq x_{T,0} \\ \sinh[\ell\sqrt{s/D}] - \sinh[(\ell/2 - x_T)\sqrt{s/D}]\cosh[(\ell/2 + x_{T,0})\sqrt{s/D}], & x_T \geq x_{T,0}, \end{cases} \tag{E1}$$

$$\psi_L(s) = \frac{f_L}{s\,\sinh[\ell\sqrt{s/D}]} \begin{cases} \sinh[\ell\sqrt{s/D}] - \cosh[(\ell/2 + x_T)\sqrt{s/D}]\sinh[(\ell/2 - x_{T,0})\sqrt{s/D}], & x_T \leq x_{T,0} \\ \cosh[(\ell/2 - x_T)\sqrt{s/D}]\sinh[(\ell/2 + x_{T,0})\sqrt{s/D}], & x_T \geq x_{T,0}, \end{cases} \tag{E2}$$

$$\psi_R(s) = \frac{f_R}{s\,\sinh[\ell\sqrt{s/D}]} \begin{cases} \cosh[(\ell/2 + x_T)\sqrt{s/D}]\sinh[(\ell/2 - x_{T,0})\sqrt{s/D}], & x_T \leq x_{T,0} \\ \sinh[\ell\sqrt{s/D}] - \cosh[(\ell/2 - x_T)\sqrt{s/D}]\sinh[(\ell/2 + x_{T,0})\sqrt{s/D}], & x_T \geq x_{T,0}, \end{cases} \tag{E3}$$

$$\psi_L^L(s) = \frac{1}{s\,\sinh[\ell\sqrt{s/D}]} \begin{cases} [1 - (x_{T,0} - x_T)f_L]\sinh[\ell\sqrt{s/D}] - f_L\sqrt{\frac{D}{s}}\,\sinh[(\ell/2 + x_T)\sqrt{s/D}]\sinh[(\ell/2 - x_{T,0})\sqrt{s/D}], & x_T \leq x_{T,0} \\ \sinh[\ell\sqrt{s/D}] - f_L\sqrt{\frac{D}{s}}\,\sinh[(\ell/2 - x_T)\sqrt{s/D}]\sinh[(\ell/2 + x_{T,0})\sqrt{s/D}], & x_T \geq x_{T,0}, \end{cases} \tag{E4}$$

$$\psi_R^R(s) = \frac{1}{s\,\sinh[\ell\sqrt{s/D}]} \begin{cases} \sinh[\ell\sqrt{s/D}] - f_R\sqrt{\frac{D}{s}}\,\sinh[(\ell/2 + x_T)\sqrt{s/D}]\sinh[(\ell/2 - x_{T,0})\sqrt{s/D}], & x_T \leq x_{T,0} \\ [1 - (x_T - x_{T,0})f_R]\sinh[\ell\sqrt{s/D}] - f_R\sqrt{\frac{D}{s}}\,\sinh[(\ell/2 - x_T)\sqrt{s/D}]\sinh[(\ell/2 + x_{T,0})\sqrt{s/D}], & x_T \geq x_{T,0}. \end{cases} \tag{E5}$$

The remaining three integrals follow from the normalization conditions (arguments are left implicit)

$$\psi^L + \psi^R = \frac{1}{s}, \quad \psi_L^L + \psi_L^R = \frac{1}{s}, \quad \psi_R^R + \psi_R^L = \frac{1}{s}. \tag{E6}$$

The Laplace inversion of the above relationships, using, e.g., residue calculus [43], gives Eq. (29). In the following subsections we give asymptotic results in the (1) long- and (2) short-time limits for the expressions above.

1. Long-time behavior

The long-time behavior of Eqs. (E1)–(E16) is obtained from a series expansion for $\ell\sqrt{s/D} \ll 1$ and reads (arguments are left implicit)

$$\psi = \psi_L = \psi_R = \frac{1}{s\ell}, \quad \psi^L = \psi_L^L = \psi_R^L = \frac{1}{s}\left(\frac{1}{2} + \frac{x_T}{\ell}\right),$$

$$\psi^R = \psi_R^R = \psi_L^R = \frac{1}{s}\left(\frac{1}{2} - \frac{x_T}{\ell}\right). \tag{E7}$$

The inverse transforms are found from $\mathcal{L}^{-1}(s^{-1}) = 1$ [44].

2. Short-time behavior

Short times is defined here as $(\ell \pm x_T)\sqrt{s/D}, \ (\ell \pm x_{T,0})\sqrt{s/D} \gg 1$, i.e., times shorter than the time it takes to diffuse across the entire box. The short-time behavior of Eqs. (E1)–(E16) is given by

$$\psi^L(s) \approx \begin{cases} \dfrac{1}{2s} e^{-(x_{T,0}-x_T)\sqrt{s/D}}, & x_T \le x_{T,0} \\[2ex] \dfrac{1}{s}\left(1 - \dfrac{1}{2}e^{-(x_T-x_{T,0})\sqrt{s/D}}\right), & x_T \ge x_{T,0}, \end{cases} \tag{E8}$$

$$\psi_L(s) \approx \begin{cases} \dfrac{f_L}{s}\left(1 - \dfrac{1}{2}e^{-(x_{T,0}-x_T)\sqrt{s/D}}\right), & x_T \le x_{T,0} \\[2ex] \dfrac{f_L}{2s} e^{-(x_T-x_{T,0})\sqrt{s/D}}, & x_T \ge x_{T,0}, \end{cases} \tag{E9}$$

$$\psi_R(s) \approx \begin{cases} \dfrac{f_R}{2s} e^{-(x_{T,0}-x_T)\sqrt{s/D}}, & x_T \le x_{T,0} \\[2ex] \dfrac{f_R}{s}\left(1 - \dfrac{1}{2}e^{-(x_T-x_{T,0})\sqrt{s/D}}\right), & x_T \ge x_{T,0}, \end{cases} \tag{E10}$$

$$\psi_L^L(s) \approx \begin{cases} \dfrac{1}{s}\left(1 - (x_{T,0}-x_T)f_L - \dfrac{f_L}{2}\sqrt{\dfrac{D}{s}}\,e^{-(x_{T,0}-x_T)\sqrt{s/D}}\right), & x_T \le x_{T,0} \\[2ex] \dfrac{1}{s}\left(1 - \dfrac{f_L}{2}\sqrt{\dfrac{D}{s}}\,e^{-(x_T-x_{T,0})\sqrt{s/D}}\right), & x_T \ge x_{T,0}, \end{cases} \tag{E11}$$

$$\psi_R^R(s) \approx \begin{cases} \dfrac{1}{s}\left(1 - \dfrac{f_R}{2}\sqrt{\dfrac{D}{s}}\,e^{-(x_{T,0}-x_T)\sqrt{s/D}}\right), & x_T \le x_{T,0} \\[2ex] \dfrac{1}{s}\left(1 - (x_T-x_{T,0})f_R - \dfrac{f_R}{2}\sqrt{\dfrac{D}{s}}\,e^{-(x_T-x_{T,0})\sqrt{s/D}}\right), & x_T \ge x_{T,0}. \end{cases} \tag{E12}$$

The remaining integrals follow from Eq. (E16).

Equations (E9)–(E12) can be inverted exactly into time domain. Using standard formulas [44] and introducing

$$\eta = \frac{x_T - x_{T,0}}{\sqrt{4Dt}}, \tag{E13}$$

it leads to

$$\psi_L(t) = \frac{f_L}{2}(1 - \mathrm{erf}\,\eta), \quad \psi_R(t) = \frac{f_R}{2}(1 + \mathrm{erf}\,\eta),$$

$$\psi^L(t) = \frac{1}{2}(1 + \mathrm{erf}\,\eta), \quad \psi^R(t) = \frac{1}{2}(1 - \mathrm{erf}\,\eta),$$

$$\psi_L^L(t) = 1 - \frac{f_L}{2}\sqrt{\frac{4Dt}{\pi}}[e^{-\eta^2} + \sqrt{\pi}\,\eta(\mathrm{erf}\,\eta - 1)],$$

$$\psi_R^R(t) = 1 - \frac{f_R}{2}\sqrt{\frac{4Dt}{\pi}}[e^{-\eta^2} + \sqrt{\pi}\,\eta(\mathrm{erf}\,\eta + 1)], \tag{E14}$$

where $\mathrm{erf}\,z$ is the error function [44]. The expressions above are valid for times such that $4Dt/(\ell/2 \pm x_{T,0})^2 \ll 1$ and $4Dt/(\ell/2 \pm x_T)^2 \ll 1$. Expanding the result in Eq. (E14) for small η and using the normalization conditions (E6) yield

$$\psi_L(t) = \frac{f_L}{2}\left(1 - \frac{2\eta}{\sqrt{\pi}}\right), \quad \psi_R(t) = \frac{f_R}{2}\left(1 + \frac{2\eta}{\sqrt{\pi}}\right),$$

$$\psi^L(t) = \frac{1}{2}\left(1 + \frac{2\eta}{\sqrt{\pi}}\right), \quad \psi^R(t) = \frac{1}{2}\left(1 - \frac{2\eta}{\sqrt{\pi}}\right),$$

$$\psi_L^R(t) = \frac{f_L}{2}\sqrt{\frac{4Dt}{\pi}}(1 - \sqrt{\pi}\,\eta),$$

$$\psi_R^L(t) = \frac{f_R}{2}\sqrt{\frac{4Dt}{\pi}}(1 + \sqrt{\pi}\,\eta), \tag{E15}$$

and (arguments are left implicit)

$$\psi^L + \psi^R = 1, \quad \psi_L^L + \psi_L^R = 1, \quad \psi_R^R + \psi_R^L = 1. \tag{E16}$$

The limit where $t \to 0$ limit ($s \to \infty$) is most conveniently found from Eqs. (E1)–(E16) which, in combination with $\mathcal{L}^{-1}(s^{-1}) = 1$, read

$$\psi^L(t \to 0) = \begin{cases} 0, & x_T \le x_{T,0} \\ 1, & x_T \ge x_{T,0}, \end{cases} \tag{E17}$$

$$\psi_L(t \to 0) = \begin{cases} f_L, & x_T \le x_{T,0} \\ 0, & x_T \ge x_{T,0}, \end{cases} \tag{E18}$$

$$\psi_R(t \to 0) = \begin{cases} 0, & x_T \le x_{T,0} \\ f_R, & x_T \ge x_{T,0}, \end{cases} \tag{E19}$$

$$\psi_L^L(t \to 0) = \begin{cases} 1 - (x_{T,0} - x_T)f_L, & x_T \le x_{T,0} \\ 1, & x_T \ge x_{T,0} \end{cases} \tag{E20}$$

$$\psi_R^R(t \to 0) = \begin{cases} 1, & x_T \le x_{T,0} \\ 1 - (x_T - x_{T,0})f_R, & x_T \ge x_{T,0}, \end{cases} \tag{E21}$$

Again, the remaining integrals follow from the normalization condition (E16).

APPENDIX F: MACROSCOPIC DYNAMICS—THE DYNAMIC STRUCTURE FACTOR AND CENTER-OF-MASS MOTION

Macroscopic quantities for a single-file system are the same as for a system consisting of noninteracting particles [19,27]. By "macroscopic" we here refer to any quantity which is invariant under $x_i \to x_j$, i.e., any one which does not "notice" if two particles are interchanged in the system. In this appendix we explicitly evaluate two such macroscopic quantities: (1) the dynamic structure factor and (2) the PDF for the center-of-mass coordinate. We demonstrate that indeed they agree with known results for noninteracting systems.

1. Dynamic structure factor

The dynamic structure factor is tractable via scattering experiments (see, e.g., Ref. [66]) and is widely used in condensed-matter physics and crystallography. Considering a set of noise-driven stochastic trajectories $X_1(t), \ldots, X_N(t)$, the dynamic structure factor is [67]

$$S(Q,t) = \frac{1}{N} \sum_{i,j} \langle e^{iQ[X_i(t) - X_{j,0}]} \rangle, \tag{F1}$$

where the angular brackets denote an average over different realizations of the noise. In terms of the NPDF and the equilibrium NPDF (see Sec. II), it is given by

$$S(Q,t) = \frac{1}{N} \int_{\mathcal{R}} dx_1 \cdots dx_N \int_{\mathcal{R}_0} dx_{1,0} \cdots dx_{N,0}$$
$$\times \sum_{i,j} e^{iQ(x_i - x_{j,0})} \mathcal{P}(\vec{x}, t | \vec{x}_0) \mathcal{P}^{\mathrm{eq}}(\vec{x}_0), \tag{F2}$$

where we averaged over the (equilibrium) initial positions. Since the integrand above is invariant under $x_i \leftrightarrow x_j$, we can apply the technique explained in Appendix C to extend the integrations over coordinates as well as initial positions to $[-\ell/2, \ell/2]$, which leads to

$$S(Q,t) = \frac{1}{N} \frac{1}{N!} \frac{1}{\ell^N} \int_{-\ell/2}^{\ell/2} dx_1 \int_{-\ell/2}^{\ell/2} dx_2 \cdots \int_{-\ell/2}^{\ell/2} dx_N \int_{-\ell/2}^{\ell/2} dx_{1,0}$$
$$\times \int_{-\ell/2}^{\ell/2} dx_{2,0} \cdots \int_{-\ell/2}^{\ell/2} dx_{N,0} \sum_{i,j} e^{iQ(x_i - x_{j,0})} \mathcal{P}(\vec{x}, t | \vec{x}_0), \tag{F3}$$

where also Eq. (4) was used. Inserting explicitly the NPDF from Eq. (16) yields

$$S(Q,t) = \frac{1}{N} \frac{1}{N!} \frac{1}{\ell^N} \int_{-\ell/2}^{\ell/2} dx_1 \int_{-\ell/2}^{\ell/2} dx_2 \cdots \int_{-\ell/2}^{\ell/2} dx_N \int_{-\ell/2}^{\ell/2} dx_{1,0}$$
$$\times \int_{-\ell/2}^{\ell/2} dx_{2,0} \cdots \int_{-\ell/2}^{\ell/2} dx_{N,0} \left[\left(\sum_{i=1}^{N} e^{iQ(x_i - x_{i,0})} \right. \right.$$
$$\left. + \sum_{i,j,i \ne j} e^{iQ(x_i - x_{j,0})} \right)$$
$$\times \psi(x_1, x_{1,0}; t) \psi(x_2, x_{2,0}; t) \cdots \psi(x_N, x_{N,0}; t)$$
$$\left. + \text{remaining } N! - 1 \text{ terms} \right]. \tag{F4}$$

Defining

$$C(Q) = \frac{1}{\ell} \int_{-\ell/2}^{\ell/2} dx_i \int_{-\ell/2}^{\ell/2} dx_{j,0} \ \psi(x_i, x_{j,0}; t) e^{iQ(x_i - x_{j,0})}, $$

$$F(Q) = \frac{1}{\ell^2} \int_{-\ell/2}^{\ell/2} dx_i \int_{-\ell/2}^{\ell/2} dx_{j,0} \int_{-\ell/2}^{\ell/2} dx_k \int_{-\ell/2}^{\ell/2} dx_{l,0}$$
$$\times \psi(x_i, x_{j,0}; t) \psi(x_k, x_{l,0}; t) e^{iQ(x_i - x_{l,0})}, \tag{F5}$$

and noticing that all the $N!$ terms corresponding to permutations of the initial particle positions in Eq. (F4) give the same contribution lead to

$$S(Q,t) = C(Q)C(0)^{N-1} + (N-1)F(Q)C(0)^{N-2}. \tag{F6}$$

This result is identical to that of noninteracting particles (obtained, e.g., by putting, $S_{ij} \equiv 0$, in the Bethe ansatz (12) and allowing the particles to be in the full phase space $x_j \in [-\ell/2, \ell/2]$). The expression above is simplified by noticing that $C(0) = 1$ due to the normalization of $\psi(x_i, x_{j,0}; t)$.

As an example, we consider the case $\ell \to \infty$ and $\Delta = 0$ where $\psi(x_i, x_{j,0}; t) = (4\pi D t)^{-1/2} \exp[-(x_i - x_{j,0})^2/(4Dt)]$ can be used. A straightforward calculation of Eq. (F5) for this case gives

$$C(Q) = e^{-DQ^2 t}, \tag{F7}$$

$$F(Q) = \frac{2\pi}{\ell} \delta(Q) e^{-DQ^2 t}, \tag{F8}$$

where $\delta(z) = (2\pi)^{-1} \int_{-\infty}^{\infty} d\alpha \ e^{i\alpha z}$ was used. Inserting the results above into Eq. (F6) gives

$$S(Q,t) = e^{-DQ^2 t}, \quad Q \neq 0, \tag{F9}$$

which is in agreement with standard results for noninteracting particles in one dimension (see, e.g., Ref. [68]).

2. Center-of-mass dynamics

The probability density function for the CM coordinate X is given by [69]

$$P(X,t|\vec{x}_0) = \int_{\mathcal{R}} dx_1 dx_2 \cdots dx_N$$
$$\times \delta\left(X - \frac{x_1 + x_2 + \cdots + x_N}{N} \right) P(\vec{x},t|\vec{x}_0), \tag{F10}$$

where the NPDF $P(\vec{x},t|\vec{x}_0)$ is given in Eq. (12), and the integration region $\mathcal{R}$ is defined in Eq. (3). Since the integrand is invariant under $x_i \leftrightarrow x_j$, it is possible to extend the integration region to $x_j \in [-\ell/2, \ell/2]$ (provided we divide by $N!$), as was done in the previous subsection. Also, using the integral representation of the δ function from previous subsection, Eq. (F10) can be rewritten as

$$P(X,t|\vec{x}_0) = \frac{1}{N!} \int_{-\infty}^{\infty} \frac{dQ}{2\pi} \int_{-\ell/2}^{\ell/2} dx_1 \cdots \int_{-\ell/2}^{\ell/2} dx_N$$
$$\times \exp\left[iQ\left(X - \frac{x_1 + x_2 + \cdots + x_N}{N} \right) \right] P(\vec{x},t|\vec{x}_0). \tag{F11}$$

Combining this equation with Eqs. (12) and (13) and defining $g(k_j,Q) = \int_{-\ell/2}^{\ell/2} dx_i\, e^{ix_i(k_j - Q/N)}$ give

$$P(X,t|\vec{x}_0) = \int_{-\infty}^{\infty} \frac{dQ}{2\pi} e^{iQX} \int_{-\infty}^{\infty} \frac{dk_1}{2\pi} \cdots \int_{-\infty}^{\infty} \frac{dk_N}{2\pi} e^{-D(k_1^2 + \cdots + k_N^2)t}$$
$$\times \phi(k_1, x_{1,0}) \cdots \phi(k_N, x_{N,0}) g(k_1, Q) \cdots g(k_N, Q). \tag{F12}$$

Integrating over k_j leads to

$$P(X,t|\vec{x}_0) = \int_{-\infty}^{\infty} \frac{dQ}{2\pi} e^{iQX} h(Q,x_{1,0}) \cdots h(Q,x_{N,0}), \tag{F13}$$

where

$$h(Q,x_{j0}) = \int_{-\infty}^{\infty} \frac{dk_j}{2\pi} e^{-Dk_j^2 t} \phi(k_j, x_{j0}) g(k_j, Q)$$
$$= \int_{-\ell/2}^{\ell/2} dx_i \int_{-\infty}^{\infty} \frac{dk_j}{2\pi} e^{-Dk_j^2 t} \phi(k_j, x_{j,0}) e^{ix_i(k_j - Q/N)}. \tag{F14}$$

The result in Eq. (F13) is identical to that of noninteracting particles, as can be shown straightforwardly by setting $S_{ij} \equiv 0$ in Eq. (12) and not restricting the particles to the phase-space region $\mathcal{R}$.

As an example, Eq. (F13) is evaluated for an infinite system ($\ell \to \infty$) and $\Delta = 0$, where $\phi(k_j, x_{j,0}) = e^{-ik_j x_{j,0}}$. For this case Eq. (F14) becomes

$$h(Q,x_{j,0}) = \exp\left(-\frac{Q^2 Dt}{N^2} - \frac{ix_{j,0}Q}{N} \right), \tag{F15}$$

which when inserted in Eq. (F13) and integrated over Q gives the well-known Gaussian for the CM,

$$P(X,t|\vec{x}_0) = \frac{1}{(4\pi D_{CM}t)^{1/2}} \exp\left[-\frac{(X - X_{CM}^0)^2}{4D_{CM}t} \right], \tag{F16}$$

where $X_{CM}^0 = (\Sigma_{i=1}^N x_{i,0})/N$ and $D_{CM} = D/N$ denote the CM initial position and the diffusion constant, respectively.

[1] M. J. Rust, M. Bates, and X. W. Zhuang, Nat. Methods **3**, 793 (2006).

[2] G.-W. Li, O. G. Berg, and J. Elf, Nat. Phys. **5**, 294 (2009).

[3] Y. M. Wang, R. H. Austin, and E. C. Cox, Phys. Rev. Lett. **97**, 048302 (2006).

[4] K. Luby-Phelps, Int. Rev. Cytol. **192**, 189 (1999).

[5] R. J. Ellis and A. P. Milton, Nature (London) **425**, 27 (2003).

[6] N. Mitarai, K. Sneppen, and S. Pedersen, J. Mol. Biol. **382**, 236 (2008).

[7] S. E. Halford and J. F. Marko, Nucleic Acids Res. **32**, 3040 (2004).

[8] M. A. Lomholt, T. Ambjörnsson, and R. Metzler, Phys. Rev. Lett. **95**, 260603 (2005).

[9] C. Dekker, Nat. Nanotechnol. **2**, 209 (2007).

[10] A. Karlsson, R. Karlsson, M. Karlsson, A. S. Cans, A. Strömberg, F. Ryttsen, and O. Orwar, Nature (London) **409**, 150 (2001).

[11] A. L. Hodgkin and R. D. Keynes, J. Physiol. (London) **128**, 28 (1955).

[12] P. M. Richards, Phys. Rev. B **16**, 1393 (1977).

[13] V. Kukla, J. Kornatowski, D. Demuth, I. Girnus, H. Pfeifer, L. Rees, S. Schunk, K. Unger, and J. Kärger, Science **272**, 702 (1996).

[14] Q. H. Wei, C. Bechinger, and P. Leiderer, Science **287**, 625 (2000).

[15] G. Coupier, M. Saint Jean, and C. Guthmann, Phys. Rev. E **73**, 031112 (2006).

[16] G. Coupier, M. S. Jean, and C. Guthmann, EPL **77**, 60001 (2007).

[17] C. Lutz, M. Kollmann, and C. Bechinger, Phys. Rev. Lett. **93**, 026001 (2004).

[18] B. Lin, M. Meron, B. Cui, S. A. Rice, and H. Diamant, Phys. Rev. Lett. **94**, 216001 (2005).

[19] T. E. Harris, J. Appl. Probab. **2**, 323 (1965).

[20] D. G. Levitt, Phys. Rev. A **8**, 3050 (1973).

[21] H. van Beijeren, K. W. Kehr, and R. Kutner, Phys. Rev. B **28**,

5711 (1983).

[22] K. Hahn and J. Kärger, J. Phys. A **28**, 3061 (1995).

[23] R. Arratia, Ann. Probab. **11**, 362 (1983).

[24] J. K. Percus, Phys. Rev. A **9**, 557 (1974).

[25] J. Kärger, Phys. Rev. E **47**, 1427 (1993).

[26] S. Alexander and P. Pincus, Phys. Rev. B **18**, 2011 (1978).

[27] R. Kutner, Phys. Lett. **81A**, 239 (1981).

[28] M. Kollmann, Phys. Rev. Lett. **90**, 180602 (2003).

[29] M. D. Jara and C. Landim, Ann. I.H.P. Probab. Stat. **42**, 567 (2006).

[30] K. Nelissen, V. R. Misko, and F. M. Peeters, EPL **80**, 56004 (2007).

[31] T. Ambjörnsson and R. J. Silbey, J. Chem. Phys. **129**, 165103 (2008).

[32] E. Barkai and R. J. Silbey, Phys. Rev. Lett. **102**, 050602 (2009).

[33] P. Gonçalves and M. Jara, J. Stat. Phys. **132**, 1135 (2008).

[34] T. Ambjörnsson, L. Lizana, M. A. Lomholt, and R. J. Silbey, J. Chem. Phys. **129**, 185106 (2008).

[35] C. Aslangul, J. Phys. A **33**, 851 (2000).

[36] A. Taloni and M. A. Lomholt, Phys. Rev. E **78**, 051116 (2008).

[37] C. Rödenbeck, J. Kärger, and K. Hahn, Phys. Rev. E **57**, 4382 (1998).

[38] L. Lizana and T. Ambjörnsson, Phys. Rev. Lett. **100**, 200601 (2008).

[39] N. G. van Kampen, *Stochastic Processes in Physics and Chemistry* (Elsevier, Amsterdam, 2007).

[40] M. T. Batchelor, Phys. Today **60**(1), 36 (2007).

[41] The Bethe ansatz solution for particles jumping on a *infinite lattice* was given in [65]. Our solution for the infinite system, Eqs. (12)–(14) and $\phi(k_j, x_{j,0}) = e^{-ik_j x_{j,0}}$, can be obtained from the solution in [65] by the replacements $\int_0^{2\pi} dk_j/2\pi \to \int_{-\infty}^{\infty} dk_j/2\pi$ and by expanding the energy $E(k_1, \ldots, k_N)$ and the scattering coefficients S_{ij} in a power series in momenta to lowest order.

[42] The Bethe ansatz solution is often written in terms of discrete wave vectors [64]. Using the Poisson summation formula gives the identity $\sum_{m=-\infty}^{\infty} e^{2imk_j\ell} = (\pi/\ell)\sum_{m=-\infty}^{\infty} \delta(k_j + m\pi/\ell)$, from which the Bethe ansatz solution, Eqs. (12)–(15), can be rewritten in term of discrete wave vectors $m_j\pi/\ell$ ($m_j = -\infty, \ldots, -1, 0, 1, \ldots, \infty$) if desired.

[43] A. D. Wunsch, *Complex Application*, 2nd ed. (Addison-Wesley, Reading, MA, 1994).

[44] Milton Abramowitz and Irene A. Stegun, *Handbook of Mathematical Functions with Formulas, Graphs, and Mathematical Tables* (Dover, New York, 1964).

[45] H. S. Carslaw and J. C. Jaeger, *Conduction of Heat in Solids* (Oxford University Press, Oxford, 1959).

[46] Note that our convention, with coordinates in the range $[-L/2, L/2]$, is different to Ref. [37] where the left (right) end of the system is at 0 (L).

[47] Alternatively, one may be interested in the tPDF for a *fixed* initial particle distribution $\vec{x}_0$: $\tilde{\rho}_{\mathcal{T}}(x_{\mathcal{T}}, t | \vec{x}_0) = \int_{\mathcal{R}} dx_1' \cdots dx_N' \, \delta(x_{\mathcal{T}} - x_{\mathcal{T}}')\mathcal{P}(\vec{x}', t | \vec{x}_0)$. For the case where all particles start at the *same* position a straightforward integration yields, using Eq. (16), a result for $\tilde{\rho}_{\mathcal{T}}(x_{\mathcal{T}}, t | \vec{x}_0)$ which in the limit $\ell \to \infty$ is identical to that obtained in [69], as it should.

[48] G. Szegö, *Orthogonal Polynomials* (American Mathematical Society, New York, 1959).

[49] The expression for the tPDF, Eq. (25), is (for $\Delta = 0$) related to Eq. (61) in [37] via elementary recursion relations for the Jacobi polynomial [44].

[50] The variable ξ defined in Eq. (27) is related to the variable y in Ref. [37] according to $\xi = 1/y$.

[51] D. Elliott, Math. Comput. **25**, 309 (1971).

[52] F. W. J. Olver, Philos. Trans. R. Soc. London, Ser. A **247**, 307 (1954).

[53] F. W. J. Olver, Philos. Trans. R. Soc. London, Ser. A **249**, 65 (1956).

[54] We inverted the definition (see Ref. [51]) $\cosh 2\zeta = (1 + \xi)/(1 - \xi)$ to arrive at Eq. (33).

[55] In more detail, in arriving at the SFD expression (41) for $\rho_{\mathcal{T}}(y_{\mathcal{T}}, t | y_{\mathcal{T},0})$ we assumed $1/N \ll 1$, $\delta_N/N \ll 1$, $(4Dt)/(\ell/2 \pm x_{\mathcal{T}})^2 \ll 1$, $(4Dt)/(\ell/2 \pm x_{\mathcal{T},0})^2 \ll 1$, $|\eta| \ll 1$, $x_{\mathcal{T},0}/\ell \ll 1$, and $|\delta_N(x_{\mathcal{T}} - x_{\mathcal{T},0})|/\ell \ll 1$.

[56] The result in Eq. (43) (large N) can also be obtain from Eq. (35). Using $I_\alpha(z)|_{z \gg 1} \approx e^z/\sqrt{2\pi z}$ (but *not* assuming that ψ_L^R, ψ_R^L are small like in Sec. V B) one shows that the large-N long-time result ($\xi \to 1$), as determined by Eq. (35), agrees with Eq. (43).

[57] E. Lutz, Phys. Rev. E **64**, 051106 (2001).

[58] L. Lizana, T. Ambjörnsson, A. Taloni, E. Barkai, and M. Lomholt, e-print arXiv:0909.0881.

[59] J. Klafter, A. Blumen, and M. F. Shlesinger, Phys. Rev. A **35**, 3081 (1987).

[60] R. Metzler and J. Klafter, Phys. Rep. **339**, 1 (2000).

[61] R. Metzler and J. Klafter, J. Phys. A **37**, R161 (2004).

[62] F. Marchesoni and A. Taloni, Phys. Rev. Lett. **97**, 106101 (2006).

[63] H. B. Thacker, Rev. Mod. Phys. **53**, 253 (1981).

[64] O. Golinelli and K. Mallick, J. Phys. A **39**, 12679 (2006).

[65] G. M. Schutz, J. Stat. Phys. **88**, 427 (1997).

[66] B. J. Berne and R. Pecora, *Dynamic Light Scattering with Applications in Chemistry, Biology and Physics* (Dover, New York, 2003).

[67] M. Doi and S. F. Edwards, *The Theory of Polymer Dynamics* (Oxford University Press, Oxford, 1986).

[68] N. A. Clark, Am. J. Phys. **38**, 575 (1970).

[69] C. Aslangul, EPL **44**, 284 (1998).