Stretched Markov nature of single-file self-dynamics

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We study the generalized diffusion of a tagged particle in a one-dimensional fluid of hard-point particles. The dynamics of a single particle in its nonuniform, nondeterministic environment is assumed known. On eliminating suitably defined transients from the exact solution, we find a universal form for the tagged particle dynamics when written in terms of stretched space and time, appearing as the classical telegrapher's equation.

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I. INTRODUCTION

Single-file flow of (classically modeled) fluids in pores, a domain of considerable importance from biological to industrial physics [1,2], has come under increasing scrutiny, both theoretical [3–7] and experimental [8–10], of late. The prototype of self-diffusion of *impenetrable point particles*, on a one-dimensional (1D) infinite line, was solved, in various versions, many years ago [11–13]. However, going beyond the prototype in a reliable fashion requires, at the very least, understanding the dominant physical mechanisms in a concise quantitative fashion. This in turn requires knowledge of the response of the system to external probes that are sufficiently searching. Here, we will interpret this objective by positing a quite general single-particle stochastic dynamics, and then asking for the consequences of our idealized very strong interaction between the particles. By so doing, we will hope to recognize the dominant mechanisms alluded to above, allowing us to extrapolate from the prototype with some degree of confidence.

The questions being asked fall under the broad classification of few particle properties of interacting many-body systems, and hence under that of dimensional reduction. In preparation for the in-depth analysis of fluids in highly confining geometries, we have previously examined the diffusion of a single particle in a structured quasi-1D enclosure [14–16]. We have shown how the reduction of the full space to 1D longitudinal space can be carried out in conjunction with a reduction of solution space, equivalent to the elimination of transients (or loss of memory), resulting in a self-consistent low resolution 1D dynamics [16]. The explicit nature of the desired reduction in the many-particle case is not obvious, and here we will restrict our attention to a large class of initial conditions for which a reasonable transient elimination process can be carried out.

The basic information that we take as given is that of the stochastic sojourn of a single noninteracting particle in its environment, i.e.,

$$p_0(x,t;y,0) \tag{1.1}$$

is the probability density that a given particle is both: located at y at time 0 and at x at time t. From the viewpoint of Brownian motion or any of its extensions, this is perfectly well defined. In the context of pure inertial dynamics, this is not the case, since the initial velocity of the particle must be specified as well, and if distributed, should be regarded as quenched in any averaging process. The key to the solution of the multiparticle stochastic dynamics is the tacit assumption that there is no distinction between a pair of untagged point particles colliding, or passing through each other. This is literally true in systems of identical particles for inertial dynamics, or for Brownian dynamics with infinitesimal jumps, but corresponds to a specific assumption on the jump mechanism in the context of finite jumps. If this assumption is made, then since the order of hard tagged particles is invariant, we need only a formalism for identifying the jth particle, in order, and this is no problem.

Our conclusion will be that since the time scales of the mean particle dynamics of an isolated particle, and of one in an interacting system, are qualitatively separated, we can define a quasisteady state of tagged particle dynamics once local transients have disappeared. In this state, irrespective of the spatial nonuniformity of the equilibrium fluid we are dealing with, the particle self-dynamics takes on a stretched Markov form.

Our paper is organized as follows: In Sec. II, we present the generalized procedure for transforming the dynamics of a single untagged particle [expressed by definition (1.1)] to the self-dynamics of the particle, when immersed in the system of identical impenetrable particles. This transformation represents a kind of dimensional reduction, from the space of coordinates of all particles to the space of only the tagged particle. The results are formulas for the density and current density of the tagged particle conditioned on its initial location.

Section III is introducing "stretched" space-time coordinates F, Q and corresponding density and current density in this representation. The self-dynamics expressed in these coordinates appears to be very transparent and formally independent of the original dynamics of the untagged particle.

In Sec. IV we investigate properties of the stretched coordinates as functions of real time and space for two representative models of the single particle dynamics: pure inertial motion and diffusion. Our aim is to demonstrate that (at least) in these models, our surmises concerning the stretched (time) coordinate Q in the limit of large time, used in the definition of the "stretched" space-time, are satisfied.

In the final sections, we discuss the Markov nature of the self-dynamics, if studied in stretched coordinates, and its relation to the corresponding picture in real space-time, described by the Boltzmann equation for the inertial dynamics.

II. BASIC SELF-DYNAMICS

We will focus on

$$p(x,t;y,0), \tag{2.1}$$

the probability density that a specified tagged particle both starts at $(y,0)$ and propagates to (x,t). Our system consists of N particles $\{x_k(t)\}$, on a line of length L, and we will be interested in a suitable thermodynamic limit, consistent with any spatial inhomogeneity built into (1.1). Since the number of particles to the right of point x is given by $\Sigma_k\Theta[x_k(t)-x]$, where Θ is the Heaviside unit step function [and the value of $\Theta(0)$ is irrelevant] insertion of the Kronecker δ function $\delta_{Kr}(\Sigma_j\Theta[x_j(t)-x]-\Sigma_k\Theta[x_k(0)-y])$ imposes the condition that there are the same number of particles to the right of x at time t as there are to the right of y at time 0. Thus, in terms of the noninteracting trajectories $\{x_k(t)\}$ (and a Fourier representation of δ_{Kr}), we can follow a tagged particle, one of the N in the system, by evaluating

$$p(x,t;y,0) = \frac{1}{2\pi N}\int_{-\pi}^{\pi} d\phi \Bigg\langle \sum_{j,k} \delta[x_j(t)-x]\delta[x_k(0)-y] \times \exp\Bigg[i\phi\Bigg(\sum_l \Theta[x_l(t)-x] - \sum_m \Theta[x_m(0)-y]\Bigg)\Bigg]\Bigg\rangle, \tag{2.2}$$

$\langle\,\rangle$ means averaging over the probability $\Pi_i p_0[x_i(t),t;x_i(0),0]$.

Now we observe that $\exp[i\phi\Theta(\xi-x)]=1+(e^{i\phi}-1)\Theta(\xi-x)$, so that

$$\frac{\partial}{\partial x}\exp[i\phi\Theta(\xi-x)] = (1-e^{i\phi})\delta(\xi-x). \tag{2.3}$$

Hence, on inserting a constant so that the (principal part or real part) integral converges and limits can be interchanged, we have

$$p(x,t;y,0) = \frac{\partial^2}{\partial x\,\partial y}\frac{1}{4\pi N}\int_{-\pi}^{\pi}\Bigg\langle \exp\Bigg[i\phi\Bigg(\sum_j \Theta[x_j(t)-x] - \sum_j \Theta[x_j(0)-y]\Bigg)\Bigg] - 1\Bigg\rangle \frac{d\phi}{(1-\cos\phi)}. \tag{2.4}$$

But if we adopt initial conditions such that the $\{x_j(0)\}$ are independent and identically distributed, then this will hold for the $\{x_j(t)\}$ as well, and (2.4) separates at once into

$$p(x,t;y,0) = \frac{\partial^2}{\partial x\,\partial y}\frac{1}{4\pi N}\int_{-\pi}^{\pi}(\langle \exp i\phi(\Theta[X(t)-x] - \Theta[Y(t)-y])\rangle^N - 1)\frac{d\phi}{(1-\cos\phi)}. \tag{2.5}$$

We want to take the $N\to\infty$ limit of (2.5). For this purpose, we first write

$$p_0(x,t;y,0) = p_0(x,t|y,0)p_0(y,0), \tag{2.6}$$

and similarly for the fully interacting $p(x,t;y,0)$, where $p_0(y,0)$ is the probability density for a particle to be at y at time $t=0$, and $p_0(x,t|y,0)$ the associated conditional probability at (x,t). For N particles, the corresponding particle density is

$$n_0(y,0) = Np_0(y,0). \tag{2.7}$$

Then, since

$$e^{i\phi[\Theta(a)-\Theta(b)]} = 1 + (e^{i\phi}-1)\Theta(a)\Theta(-b) + (e^{-i\phi}-1)\Theta(-a)\Theta(b), \tag{2.8}$$

it follows that

$$\langle e^{i\phi(\Theta[X(t)-x]-\Theta[X(0)-y])}\rangle = 1 + \frac{1}{N}\int\int dXdYn_0(Y,0)p_0(X,t|Y,0) \times[(e^{i\phi}-1)\Theta(X-x)\Theta(y-Y) + (e^{-i\phi}-1)\Theta(x-X)\Theta(Y-y)]. \tag{2.9}$$

We can now indeed take the $N\to\infty$ limit in (2.5),

$$p(x,t|y,0) = \frac{1}{n_0(y,0)}\frac{\partial^2}{\partial x\,\partial y}\frac{1}{4\pi}\int_{-\pi}^{\pi}\frac{d\phi}{1-\cos\phi} \times\Bigg[\exp\Bigg((e^{i\phi}-1)\int_{-\infty}^{y}dY\int_x^{\infty}dXn_0(Y,0) \times p_0(X,t|Y,0) + (e^{-i\phi}-1)\int_y^{\infty}dY\int_{-\infty}^{x}dXn_0(Y,0) \times p_0(X,t|Y,0)\Bigg) - 1\Bigg]. \tag{2.10}$$

If we define

$$Q(x,t;y,0) = \Bigg(\int_{-\infty}^{x}dX\int_y^{\infty}dY + \int_x^{\infty}dX\int_{-\infty}^{y}dY\Bigg)n_0(X,t;Y,0),$$

$$W(x,t;y,0) = \Bigg(\int_{-\infty}^{x}dX\int_y^{\infty}dY - \int_x^{\infty}dX\int_{-\infty}^{y}dY\Bigg)n_0(X,t;Y,0), \tag{2.11}$$

and introduce the density $n(x,t;y,0)$ as in (2.7), we end up with the concise form

$$n(x,t;y,0) = \frac{\partial^2}{\partial x\,\partial y}\frac{1}{4\pi}\int_{-\pi}^{\pi}(\exp[Q(x,t;y,0)(\cos\phi-1) - iW(x,t;y,0)\sin\phi] - 1)\frac{d\phi}{1-\cos\phi}. \tag{2.12}$$

The current density corresponding to (2.12) is just as easily obtained. We need only replace $\Sigma_{j,k}\delta[x_j(t)-x]\delta[x_k(0)-y]$ in (2.2) by $\Sigma_{j,k}\dot{x}_j(t)\delta[x_j(t)-x]\delta[x_k(0)-y]$, and correspondingly replace (2.3) by

$$\frac{\partial}{\partial t}\exp(i\phi\Theta[\xi(t)-x]) = -(1-e^{i\phi})\dot{\xi}(t)\delta[\xi(t)-x]. \tag{2.13}$$

This results at once in

$$j(x,t;y,0) = -\frac{\partial^2}{\partial t\,\partial y}\frac{1}{4\pi}\int_{-\pi}^{\pi}(\exp[Q(x,t;y,0)(\cos\phi-1) - iW(x,t;y,0)\sin\phi]-1)\frac{d\phi}{1-\cos\phi}, \tag{2.14}$$

and of course the conservation equation

$$\frac{\partial}{\partial t}n(x,t;y,0) + \frac{\partial}{\partial x}j(x,t;y,0) = 0 \tag{2.15}$$

is immediately verified. An alternative representation is in terms of the cumulative density $B(x,t;y,0)$,

$$n(x,t;y,0) = \frac{\partial}{\partial x}B(x,t;y,0),$$

$$j(x,t;y,0) = -\frac{\partial}{\partial t}B(x,t;y,0), \tag{2.16}$$

where

$$B(x,t;y,0) = \frac{\partial}{\partial y}\frac{1}{4\pi}\int_{-\pi}^{\pi}(\exp[Q(x,t;y,0)(\cos\phi-1) - iW(x,t;y,0)\sin\phi]-1). \tag{2.17}$$

III. STRETCHED COORDINATE SELF-DYNAMICS

Observing that $\int_{-\infty}^{x}dX\int_{y}^{\infty}dY - \int_{x}^{\infty}dX\int_{-\infty}^{y}dY = \int_{-\infty}^{x}dX\int_{-\infty}^{\infty}dY - \int_{-\infty}^{\infty}dX\int_{-\infty}^{y}dY = \int_{-\infty}^{\infty}dX\int_{y}^{\infty}dY - \int_{x}^{\infty}dX\int_{-\infty}^{\infty}dY$, with due attention to the limits $\pm\infty$, we can rewrite W in (2.11) as

$$W(x,t;y,0) = \int_{-\infty}^{x}n_0(X,t)dX - \int_{-\infty}^{y}n_0(Y,0)dY = -\int_{x}^{\infty}n_0(X,t)dX + \int_{y}^{\infty}n_0(Y,0)dY. \tag{3.1}$$

Any average of the expressions in (3.1) is equally valid, but if the system has the same left and right limiting densities, the equal weight average

$$W(x,t;y,0) = F_0(x,t) - F_0(y,0),$$

where

$$F_0(x,t) = \frac{1}{2}\int_{-\infty}^{\infty}\mathrm{sgn}(x-X)n_0(X,t)dX \tag{3.2}$$

is easiest to manipulate on an infinite domain. In all cases, discretion is called for in taking the limits. However, what really matters is that

$$\frac{\partial}{\partial x}F_0(x,t) = n_0(x,t). \tag{3.3}$$

For the purposes of this initial study, we will assume that our (untagged) many-particle system is in steady state, so that (3.2) reduces to

$$W(x,t;y,0) = F_0(x) - F_0(y), \tag{3.4}$$

in obvious notation. The form of $Q(x,t;y,0)$ requires more detailed investigation, but as a tentative guess, to be verified in the sequel, we adopt the assumption that in the large-time limit,

$$Q(x,t;y,0) = Q(t) \tag{3.5}$$

depends only upon time. To the extent that (3.4) and (3.5) are valid, significant conclusions can be drawn. We introduce the "stretched" variables

$$Q(t) = Q, \quad F_0(x) = F, \quad F_0(y) = F', \tag{3.6}$$

and the conditional density and current density

$$n(x,t|y,0) = n(x,t;y,0)/n_0(y,0),$$

$$j(x,t|y,0) = j(x,t;y,0)/n_0(y,0), \tag{3.7}$$

as well as those normalized by their noninteracting images,

$$g(F,Q|F') = n(x,t|y,0)/n_0(x),$$

$$k(F,Q|F') = j(x,t|y,0)/\dot{Q}(t). \tag{3.8}$$

Equations (2.12) and (2.14) then translate to the universal dynamics and environment independent equations

$$g(F,Q|F') = \frac{\partial^2}{\partial F\,\partial F'}\int_{-\pi}^{\pi}(e^{(\cos\phi-1)Q-i\sin\phi\,(F-F')}-1)\frac{d\phi/4\pi}{1-\cos\phi} = \frac{1}{4\pi}\int_{-\pi}^{\pi}(1+\cos\phi)e^{(\cos\phi-1)Q-i\sin\phi\,(F-F')}d\phi, \tag{3.9}$$

$$k(F,Q|F') = -\frac{\partial^2}{\partial Q\,\partial F'}\int_{-\pi}^{\pi}(e^{(\cos\phi-1)Q-i\sin\phi\,(F-F')}-1)\frac{d\phi/4\pi}{1-\cos\phi} = \frac{1}{4\pi}\int_{-\pi}^{\pi}i\sin\phi\, e^{(\cos\phi-1)Q-i\sin\phi\,(F-F')}d\phi. \tag{3.10}$$

The integrations in (3.9) and (3.10) are routine, and are derivable at once from the well known equation

$$\frac{1}{2\pi}\int_{-\pi}^{\pi}e^{in\phi+Q\cos\phi-iW\sin\phi}d\phi = \left(\frac{Q+W}{Q-W}\right)^{n/2}I_n(\sqrt{Q^2-W^2}), \tag{3.11}$$

where I_n is the nth order modified Bessel function and n is an integer. Hence,

$$g = \frac{1}{2}e^{-Q}\left(I_0(\sqrt{Q^2-W^2}) + \frac{Q}{\sqrt{Q^2-W^2}}I_1(\sqrt{Q^2-W^2})\right),$$

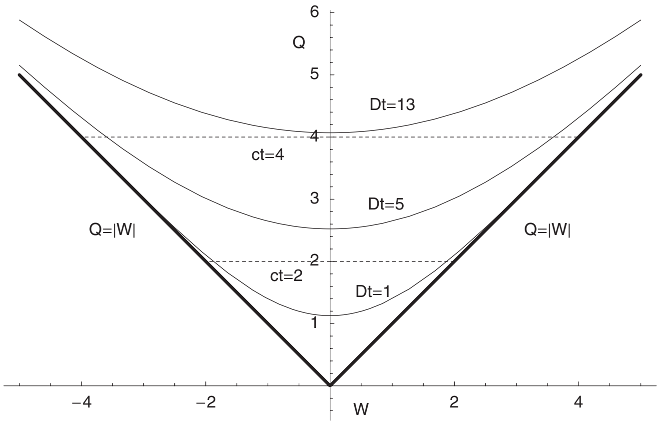

FIG. 1. Function Q depending on $W=n_0(x-y)$; here $n_0=1$. $Q=|W|$ is the lower bound of Q, corresponding to $Q(t=0)$ for any dynamics of the noninteracting particles. The full lines correspond to diffusion, Eq. (4.17), and the dashed lines are Q for the toy model of particles moving only with the velocities $v=\pm c$, formula (3.25).

$$k = \frac{W}{2\sqrt{Q^2 - W^2}} e^{-Q} I_1(\sqrt{Q^2 - W^2}). \tag{3.12}$$

The "stretched" density g and the current density k (3.12) are well defined for $|W|=|F-F'|\leq Q$. This restriction comes from the initial value of $Q(x,t;y,0)$ at time $t=0$,

$$Q(x,0;y,0) = \int_{\min(x,y)}^{\max(x,y)} n_0(\xi) d\xi = |F - F'|, \tag{3.13}$$

which can be easily verified using the relation inverse to (2.11),

$$n_0(x,t;y,0) = -\frac{1}{2}\frac{\partial^2}{\partial x\,\partial y} Q(x,t;y,0). \tag{3.14}$$

If applied on $Q(x,0;y,0)$ of (3.13),

$$-\frac{1}{2}\frac{\partial^2}{\partial x\,\partial y}|F_0(x) - F_0(y)| = \frac{1}{2}\frac{\partial}{\partial x}\left(\mathrm{sgn}(x-y)\frac{\partial F_0(y)}{\partial y}\right) = \delta(x-y) n_0(y), \tag{3.15}$$

which is $n_0(x,t;y,0)$ at $t=0$ for any dynamics of the untagged particles. For increasing $t>0$, the function $Q(x,t;y,0)$ at a fixed W also increases, satisfying according to (2.11) the condition $|W|<Q$ (see Fig. 1).

In the limit of large time t, which is of our main interest, Q is also large, and g and k according to (3.12) are negligible, except in the region $|W|\ll Q$. Here the asymptotic expansion of the Bessel functions can be used, giving

$$g \sim e^{-Q} I_0(\sqrt{Q^2 - W^2}) \sim \frac{1}{\sqrt{2\pi Q}} e^{-W^2/2Q}. \tag{3.16}$$

Using simple algebra in (3.9) and (3.10), one can show that the stretched density g and the corresponding current density k satisfy not only the "mass flow" conservation equation

$$\frac{\partial g}{\partial Q} + \frac{\partial k}{\partial F} = 0, \tag{3.17}$$

but also the "momentum flow" dynamics

$$\frac{\partial k}{\partial Q} + \frac{\partial g}{\partial F} = -2k, \tag{3.18}$$

with the initial conditions

$$g(F,Q|F') = \frac{Q+2}{4} e^{-Q}, \quad k(F,Q|F') = \frac{W}{4} e^{-Q}, \tag{3.19}$$

for $Q=|W|=|F-F'|$, corresponding to the limits of (3.12) at $t=0$.

Note that (3.17) and (3.18) combine to read

$$2\frac{\partial g}{\partial Q} + \frac{\partial^2 g}{\partial Q^2} - \frac{\partial^2 g}{\partial F^2} = 0, \tag{3.20}$$

the familiar "telegrapher's equation" of transmission line theory. (The same holds also for k.) In the short stretched-time period of rapid change, $\partial^2 g/\partial Q^2$ dominates over $\partial g/\partial Q$, so that

$$\frac{\partial^2 g}{\partial Q^2} = \frac{\partial^2 g}{\partial F^2}, \tag{3.21}$$

a constant stretched velocity wave front propagating at $|dF/dQ|=1$. But in the high Q asymptotic region, $\partial g/\partial Q$ dominates, and

$$2\frac{\partial g}{\partial Q} = \frac{\partial^2 g}{\partial F^2}, \tag{3.22}$$

a simple diffusion equation with diffusion constant 1/2, is satisfied by the asymptotic relation (3.16). Of course, this behavior is also obtainable from the explicit (3.9).

The assertion that $Q(x,t;y,0)=Q(t)$ is a function of time alone is an approximation or at best a limit, and so it is instructive to see its genesis in a simple solvable model. Consider then a point particle system under inertial dynamics, in equilibrium, at density n_0, with no external field. Since the velocity distribution cannot change under collision, we choose to restrict velocities to $v=\pm c$, equally occupied. The distribution of an arbitrary particle at velocity v has the dynamics

$$n_v(x,t;y,0) = \tfrac{1}{2} n_0 \delta(x-y-vt), \tag{3.23}$$

or averaging over the two values of v,

$$n_0(x,t;y,0) = \tfrac{1}{2} n_0[\delta(x-y-ct) + \delta(x-y+ct)]. \tag{3.24}$$

If follows from (2.11) that

$$Q(x,t;y,0) = n_0 \max(|x-y|, ct). \tag{3.25}$$

Anticipating, from (3.16), that self-dynamics in the interacting system will be diffusive, with $|x-y|\sim\sqrt{t}$, Eq. (3.25) then reduces to $Q(x,t;y,0)=n_0 ct$, the form desired. Note too, that under these circumstances, $\dot{Q}=n_0 c$, $F_0(x)-F_0(y)=n_0(x-y)$, so that $n(x,t;y,0)$ and $j(x,t;y,0)$ of a tagged particle satisfy

$$\frac{\partial n}{\partial t}+\frac{\partial j}{\partial x}=0, \quad \frac{\partial j}{\partial t}+c^2\frac{\partial n}{\partial x}=-2n_0 cj, \tag{3.26}$$

precisely (3.17) and (3.18), to within scaling.

IV. QUASISTEADY SELF-DYNAMICS

Now we must attend to the condition of validity of the stretched space-time description. From our discussion in the preceding paragraph, this will not hold until sufficient memory of the initial state [e.g., the $|x-y|$ term in (3.25)] has been lost, and so corresponds to a transient-reduced or quasisteady state. The precise definition of this situation is not obvious, but will become so as we specify the dynamics more explicitly. The determination of the crucial $Q(x,y,t)=Q(x,t;y,0)$ is in principle no problem at all, since only the stochastic dynamics of an isolated particle is to be examined. The model of a particle in a fixed external field $\varphi(x)$ under (Gaussian) white noise $f(t)$, coupled with a linear dissipation mechanism driving the system to thermal equilibrium at reciprocal temperature β, or to steady flow, is widely used and will be used here as well. We thus have the Langevin dynamics

$$m\dot{v}+\gamma v=-\varphi'(x)+f(t),$$

$$\dot{x}=v, \quad \langle f(t)\rangle=0, \quad \langle f(t)f(t')\rangle=2A^2\delta(t-t'), \tag{4.1}$$

giving rise to the Fokker-Planck (or Kramers) equation for the one-particle probability density, normalized to N particles,

$$\dot{n}_0(x,v,t)+vn_0'(x,v,t)-\frac{1}{m}\varphi'(x)\frac{\partial}{\partial v}n_0(x,v,t)$$
$$=D\frac{\partial}{\partial v}\left(m\beta v+\frac{\partial}{\partial v}\right)n_0(x,v,t),$$

$$n_0(x,v,0)=n_0(x)\delta(x-y)\sqrt{m\beta/2\pi}e^{-m\beta v^2/2}, \tag{4.2}$$

where $D=A^2/m^2$, $\beta=\gamma/A^2$.

Let us confine our attention to two extremes of (4.2) since they exemplify rather different situations. One extreme is that of $D=0$, purely inertial motion, so that the unmodified Liouville equation

$$\dot{n}_0(x,v,t)+vn_0'(x,v,t)-\frac{1}{m}\varphi'(x)\frac{\partial}{\partial v}n_0(x,v,t)=0,$$

$$n_0(x,v,0)=n_0(x)\delta(x-y)\sqrt{m\beta/2\pi}e^{-m\beta v^2/2}, \tag{4.3}$$

is relevant. To find the desired $n_0(x,t)$, we must as in (3.23) first find $n_0(x,v,t)$ and then integrate over v. It is simplest to make a direct average over trajectories. Specializing to the case of no net flow, the equilibrium distribution will be the canonical

$$n_0(x,v)=\frac{N}{Z}e^{-\beta E(x,v)}, \tag{4.4}$$

where $E(x,v)=mv^2/2+\varphi(x)$, $Z=\int\int e^{-\beta E(x,v)}dxdv$.

Suppose we denote by $X_\sigma[y,E(y,v),t]$ the pair of values ($\sigma=\mathrm{sgn}\, v$) of $x(t)$ under inertial dynamics starting at $x(0)=y$ with energy $E(y,v)$ where $v=v(0)$. Then

$$n_0(x,t;y,0)=\frac{N}{Z}\sum_\sigma \int\int \delta(X_\sigma[Y,E(Y,v),t]-x)$$
$$\times\delta(Y-y)e^{-\beta E(Y,v)}dYdv. \tag{4.5}$$

Since $\partial E/\partial v=mv$, we next transform from v to E,

$$n_0(x,t;y,0)=\frac{N}{mZ}\sum_\sigma \int\int \delta[X_\sigma(Y,E,t)-x]$$
$$\times\delta(Y-y)e^{-\beta E}dYdE/v_E(Y), \tag{4.6}$$

where $v_E(x)=\sqrt{2[E-\varphi(x)]/m}$. One more transformation: define $T_\alpha(x,y,E)$ as the time of travel from y to x at energy E, α indicating the αth route as one allows $\sigma=\pm 1$ as well as various numbers of reflections if E is lower than $\varphi_{\max}$. Hence,

$$T_\alpha(x,y,E)=\int_{y^{(\alpha)}}^{x}\frac{dz}{v_E(z)}, \tag{4.7}$$

where (α) denotes the αth trajectory from y to x. The important property of $T_\alpha(x,y,E)$ is that

$$|\partial T_\alpha(x,y,E)/\partial x|=1/v_E(x),$$

$$|\partial T_\alpha(x,y,E)/\partial y|=1/v_E(y), \tag{4.8}$$

so that we can rewrite (4.6) as

$$n_0(x,t;y,0)=\frac{N}{mZ}\sum_\alpha \int \delta[T_\alpha(x,y,E)-t]e^{-\beta E}dE/[v_E(x)v_E(y)], \tag{4.9}$$

from which

$$\dot{n}_0(x,t;y,0)=\frac{N}{mZ}\sum_\alpha \int \delta'[t-T_\alpha(x,y,E)]$$
$$\times e^{-\beta E}dE/[v_E(x)v_E(y)]. \tag{4.10}$$

Then, taking advantage of (4.8) once more, using (2.11), we conclude that

$$\dot{Q}(x,y,t)=\frac{2N}{mZ}\sum_\alpha \int \Theta[t-T_\alpha(x,y,E)]e^{-\beta E}dE \tag{4.11}$$

or, defining $E_\alpha(x,y,t)$ as the energy needed to traverse y to x along path α in time t, that

$$\dot{Q}(x,y,t)=\frac{2N}{mZ}\sum_\alpha \int \Theta[E-E_\alpha(x,y,t)]e^{-\beta E}dE$$
$$=\frac{2N}{\beta mZ}\sum_\alpha e^{-\beta E_\alpha(x,y,t)}. \tag{4.12}$$

The consequences of (4.12) are clear. If y and x are not in a common trough of the potential φ, they can be connected by a trajectory only if $E>\varphi_{\max}$, in which case there is only one trajectory. But then, large transit time can only be achieved if $E \to \varphi_{\max}$, and so we conclude that

$$\dot{Q}(x,y,t) \to \frac{2N}{\beta m Z} e^{-\beta \varphi_{\max}}, \tag{4.13}$$

which is independent of x and y.

We next turn to the other extreme of the Fokker-Planck equation, the highly overdamped pure diffusion in which inertia can be neglected, e.g., by taking $m=0$. Carrying this out in (4.2) is a bit delicate, but not so in (4.1), which can be written simply as

$$\gamma \dot{x} = -\varphi'(x) + f(t), \tag{4.14}$$

leading directly to the forced diffusion

$$\dot{n}_0(x,t;y,0) = D n_0''(x,t;y,0) + D \frac{\partial}{\partial x}[\beta \varphi'(x) n_0(x,t;y,0)],$$

$$n_0(x,t;y,0) = n_0(x)\delta(x-y). \tag{4.15}$$

Making use of (3.14), Eq. (4.15) can be converted to the more direct

$$\frac{1}{D}\dot{Q}(x,y,t) = e^{-\beta\varphi(x)} \frac{\partial}{\partial x} e^{\beta\varphi(x)} \frac{\partial}{\partial x} Q(x,y,t),$$

$$Q(x,y,0) = |W(x,y)| = |F_0(x) - F_0(y)|. \tag{4.16}$$

Equation (4.16) is best understood by first dropping the external field $\varphi(x)$, so that correspondingly $W(x,y)=n_0(x-y)$. We then have the immediate solution

$$Q(x,y,t) = n_0\left[(x-y)\mathrm{Erf}\left(\frac{x-y}{2\sqrt{Dt}}\right) + 2\sqrt{Dt/\pi}\, e^{-(x-y)^2/4Dt}\right],$$

where

$$\mathrm{Erf}(z) = \frac{2}{\sqrt{\pi}} \int_0^z e^{-\xi^2} d\xi, \tag{4.17}$$

divided into one term representing the decay of the initial isolated particle distribution, and one term representing the diffusive "filling-in" of the distribution. Suppose now that $(x-y)^2/4Dt \ll 1$, which is certainly the case for the resulting fluid, where we know that the distribution has a range scaling as $|x-y|/t^{1/4}$. Then (4.17) can be expanded in a $t^{1/2}$ Laurent series starting as

$$Q(x,y,t) = \frac{2}{\sqrt{\pi}} n_0 (Dt)^{1/2} + \frac{1}{2\sqrt{\pi}} n_0 (x-y)^2 (Dt)^{-1/2} + \cdots, \tag{4.18}$$

with a second to first term ratio of $\sim (x-y)^2/t$.

We expect the general qualitative form not to change under the imposition of an external field. Here, it is perhaps more illuminating to switch from x and y to the stretched $F=F_0(x)$, $F'=F_0(y)$. Since $dF/dx = n_0(x) = \tilde{n}_0(F)$ and $n_0(x)e^{\beta\varphi(x)}=\text{const}$, we have from (4.16),

$$\frac{1}{D}\dot{Q} = n_0(x)\frac{dF}{dx}\frac{\partial}{\partial F}\frac{1}{n_0(x)}\frac{dF}{dx}\frac{\partial}{\partial F} Q = \tilde{n}_0^2(F)\frac{\partial^2 Q}{\partial F^2}. \tag{4.19}$$

Now, supposing the expansion

$$Q(F,F',t) = a_0(F,F')(Dt)^{1/2} + a_1(F,F')(Dt)^{-1/2} + \cdots, \tag{4.20}$$

substituting into (4.19), and equating coefficients of $(Dt)^{1/2}$, $(Dt)^{-1/2}$, etc., results in

$$\tilde{n}_0^2(F)\frac{\partial^2}{\partial F^2} a_0 = 0,$$

$$\tilde{n}_0^2(F)\frac{\partial^2}{\partial F^2} a_1 = a_0/2, \tag{4.21}$$

$$\cdots.$$

The solution for the leading term is

$$a_0(F,F') = K(F') + K'(F')F = K_0 + K_1(F+F') + K_2 F F', \tag{4.22}$$

if the symmetry $Q(x,y,t)=Q(y,x,t)$ is taken into account. Because we deal with an infinite system with bounded potential $\varphi(x)$, the stretched coordinates F, F' are unbounded over the interval $(-\infty,\infty)$, and the constants K_1 and K_2 must be zero. The leading term $\sim (Dt)^{1/2}$, determining the asymptotic behavior of $Q(F,F',t)$ for large t does not depend algebraically on F and F'. In the case of zero potential, $K_0 = 2n_0/\sqrt{\pi}$, otherwise we determine this constant from (4.19), rewritten in the form

$$\left(\frac{\partial}{\partial t} - D\nu^2 \frac{\partial^2}{\partial F^2}\right) Q(F,F',t) = |F-F'|\delta(t) + D[\tilde{n}_0^2(F) - \nu^2]\frac{\partial^2}{\partial F^2} Q(F,F',t), \tag{4.23}$$

enabling us to use a perturbation approach. Here, ν represents a constant, which is then to be fixed by the following consideration.

The zeroth order of Q includes only the response to imposing the initial condition

$$Q_0(F,F',t) = \int G_0(F,t;F_1,t')\delta(t')|F_1 - F'| dF_1 dt' = 2\nu\sqrt{\frac{Dt}{\pi}} e^{-(F-F')^2/4D\nu^2 t} + (F-F')\mathrm{Erf}\left(\frac{F-F'}{2\nu\sqrt{Dt}}\right), \tag{4.24}$$

where

$$G_0(F,t;F't') = \frac{\Theta(t-t')}{2\nu\sqrt{\pi D(t-t')}} e^{-(F-F')^2/4D\nu^2(t-t')} \tag{4.25}$$

is the Green function of the left-hand side operator in (4.23).

Q_0 is of the same form as (4.17) for the particles in zero potential, with the stretched coordinates F, F' instead of x, y and with the diffusion constant D rescaled by the factor ν^2. The leading term $\sim(Dt)^{1/2}$ again comes from the exponential function in (4.24),

$$K_0 = 2\nu/\sqrt{\pi}. \tag{4.26}$$

This value includes all the contributions $\sim(Dt)^{1/2}$, if the perturbation corrections

$$D\int_0^t dt' \int G_0(F,t;F_1,t')[\tilde{n}_0^2(F_1) - \nu^2]\frac{\partial^2}{\partial F_1^2}Q(F_1,F',t')dF_1 \tag{4.27}$$

quench in the limit $t\to\infty$. This is the condition, which fixes ν. Taking only the first-order correction

$$\begin{aligned}Q_1 &= D\int_0^t dt' \int dF_1 G_0(F,t;F_1,t')[\tilde{n}_0^2(F_1) - \nu^2] \\ &\quad\times\frac{\partial^2}{\partial F_1^2}Q_0(F_1,F',t') \\ &= \int_0^t dt' \int dF_1 \frac{[\tilde{n}_0^2(F_1) - \nu^2]}{2\pi\nu^2\sqrt{t'(t-t')}} \\ &\quad\times e^{-(F-F_1)^2/4D\nu^2(t-t')-(F_1-F')^2/4D\nu^2t'} \\ &\to \frac{1}{2\nu^2}\int [\tilde{n}_0^2(F_1) - \nu^2]dF_1\end{aligned} \tag{4.28}$$

in the limit $t\to\infty$, so the condition $Q_1(t\to\infty)=0$ yields

$$\begin{aligned}\nu^2 &= \left(\int \tilde{n}_0^2(F)dF\right)\Big/\left(\int dF\right) \\ &= \left(\int n_0^3(x)dx\right)\Big/\left(\int n_0(x)dx\right);\end{aligned} \tag{4.29}$$

in the lowest order of perturbation, ν^2 is the averaged $\tilde{n}_0^2(F)$ over the range of the stretched coordinate F.

V. DISCUSSION

In the domain of validity of the $Q(t)$, $F_0(x)$, $F_0(y)$ description, the function $Q(t)$ also has direct physical meaning for self-motion in the interacting system. One question we might ask is that of the time dependence of the mean square tagged particle displacement, weighted by the probability of its initial location,

$$\langle[\Delta x(t)]^2\rangle = \int p_0(y)dy \int (x-y)^2 p(x,t|y,0)dx. \tag{5.1}$$

But let us instead examine the stretched time dependence of the squared stretched displacement,

$$\begin{aligned}\langle(\Delta F_0[x(t)])^2\rangle &= \int\int [F_0(x) - F_0(y)]^2 n(x,t;y,0)dxdy/N \\ &= \int\int [F_0(x) - F_0(y)]^2 n(x,t;y,0) \\ &\quad\times\frac{dF_0(x)dF_0(y)}{Nn_0(x)n_0(y)} \\ &= \int\int (F-F')^2 g(F,Q|F')dFdF'/N,\end{aligned} \tag{5.2}$$

in the notation of (3.8). Hence

$$\begin{aligned}&\frac{\partial}{\partial Q}\langle\{\Delta F_0[x(t)]\}^2\rangle \\ &\quad= -\int\int (F-F')^2\frac{\partial^2}{\partial F\,\partial F'} \\ &\qquad\times\int_{-\pi}^{\pi}\frac{d\phi}{4\pi N}e^{(\cos\phi-1)Q-i(F-F')\sin\phi}dFdF' \\ &\quad= \int\int\int_{-\pi}^{\pi}\frac{d\phi}{2\pi N}e^{(\cos\phi-1)Q+i(F'-F)\sin\phi}dFdF' \\ &\quad= \int\int_{-\pi}^{\pi}e^{(\cos\phi-1)Q+iF'\sin\phi}\delta(\phi)d\phi dF'/N = 1.\end{aligned} \tag{5.3}$$

Thus, to within an additive constant, Q is precisely $\langle(\Delta F_0[x(t)])^2\rangle$.

In the case of periodic potentials of period λ, when $\langle(x-y)^2\rangle$ becomes much larger than λ^2 in the large-time limit, we can approximate $F_0(x)-F_0(y)$ by $\langle n_0\rangle(x-y)$ with the equilibrium density $\langle n_0\rangle$ averaged over λ; hence

$$\begin{aligned}\frac{\partial}{\partial t}\langle[F_0(x) - F_0(y)]^2\rangle &= \dot{Q}\frac{\partial}{\partial Q}\langle[F_0(x) - F_0(y)]^2\rangle \\ &= \dot{Q} \simeq \langle n_0\rangle^2\frac{\partial}{\partial t}\langle(x-y)^2\rangle.\end{aligned} \tag{5.4}$$

This result explains subdiffusion observed in the systems of one-dimensional (1D) hard-point particles in a specific way: In real space-time, the asymptotic evolution of the mean squared displacement $\langle[x(t)-x(0)]^2\rangle\sim t^{\alpha}$ is influenced by the original dynamics of noninteracting particles, which is involved in $\dot{Q}$ in (5.4). It gives rise also to $\alpha\neq 1$, e.g., for diffusion, $Q\sim\sqrt{t}$, hence $\alpha=1/2$. On the other hand, in stretched coordinates, the evolution of the mean squared displacement $\langle(F-F')^2\rangle$ is asymptotically proportional to the stretched time Q, not depending on the original dynamics of the noninteracting particles. This expresses the effect of dominating collisions of particles in the large time limit—and in stretched space-time, there is no subdiffusion, but instead standard diffusion. Subdiffusion in real space can be then understood as a result of the nonlinear transformation from the *stretched* to the *real* coordinates, which is specific for each dynamics of the noninteracting particles.

Now, we focus on the relevant dynamical equations of our system in real (x,t) space. It is only necessary to rewrite their stretched space-time version (3.18), (3.19) for density and current density in physical space-time. We have

$$\begin{aligned}\frac{\partial}{\partial t}n(x,t;y,0) &= n_0(x)n_0(y)\frac{\partial}{\partial t}g(x,t;y,0)\\ &= n_0(x)n_0(y)\dot{Q}(t)\frac{\partial}{\partial Q}g(F,Q|F')\\ &= -n_0(x)n_0(y)\dot{Q}(t)\frac{\partial}{\partial F}k(F,Q|F')\\ &= -n_0(y)\dot{Q}(t)\frac{\partial}{\partial x}k(F,Q|F') = -\frac{\partial}{\partial x}j(x,t;y,0),\end{aligned} \tag{5.5}$$

just the expected mass conservation. Then, for momentum conservation,

$$\begin{aligned}\frac{\partial}{\partial t}j(x,t;y,0) &= n_0(y)\frac{\partial}{\partial t}[\dot{Q}(t)k(x,t;y,0)]\\ &= \ddot{Q}(t)n_0(y)k(x,t;y,0) + \dot{Q}(t)n_0(y)\frac{\partial}{\partial t}k(x,t;y,0)\\ &= [\ddot{Q}(t)/\dot{Q}(t)]j(x,t;y,0)\\ &\quad + \dot{Q}^2(t)n_0(y)\frac{\partial}{\partial Q}k(F,Q|F')\\ &= [\ddot{Q}(t)/\dot{Q}(t)]j(x,t;y,0) - \dot{Q}^2(t)n_0(y)\\ &\quad \times\left(2k(F,Q|F') + \frac{\partial}{\partial F}g(F,Q|F')\right)\\ &= \left(\frac{\ddot{Q}(t)}{\dot{Q}(t)} - 2\dot{Q}(t)\right)j(x,t;y,0)\\ &\quad - \frac{\dot{Q}^2(t)}{n_0(x)}\frac{\partial}{\partial x}\frac{n(x,t;y,0)}{n_0(x)}.\end{aligned} \tag{5.6}$$

Dropping implicit arguments, and observing that $n_0'/n_0 = -\beta\varphi'$, physical space-time dynamics now reads

$$\frac{\partial n}{\partial t} + \frac{\partial j}{\partial x} = 0,$$

$$\frac{\partial j}{\partial t} + \left(\frac{\dot{Q}}{n_0}\right)^2\frac{\partial n}{\partial x} = \left(\frac{\ddot{Q}}{\dot{Q}} - 2\dot{Q}\right)j - \beta\varphi'\left(\frac{\dot{Q}}{n_0}\right)^2 n. \tag{5.7}$$

It would be more than a bit valuable if we could find a simple physical approximation that gives rise to (5.7) without first obtaining the exact solution, for this could then be extrapolated to other than point cores on a line. As a hydrodynamic model, (5.7) is unusual, and so it is not clear how one would do this. For example, a first attempt for inertial dynamics would often take the form of a suitable Boltzmann equation. Here, this is particularly simple: we can imagine that we have an ideal gas fluid of phase-space density $f(x,v,t)=n_0(x)h_0(v)$. One particle is tagged, with a (self-) phase-space density $f_s(x,v,t)$ for the tag, and anytime that a tagged particle passes a fluid particle, the tag is transferred to the latter. Ignoring correlations (mean field) and tallying the rates of production and destruction of a tag moving at velocity v, we clearly have the augmented Liouville equation [the self-self collision term $f_s(x,v,t)f_s(x,v',t)$ cancels]

$$\begin{aligned}&\frac{\partial}{\partial t}f_s(x,v,t) + v\frac{\partial}{\partial x}f_s(x,v,t) - \frac{1}{m}\varphi'(x)\frac{\partial}{\partial v}f_s(x,v,t)\\ &\quad = \int |v-v'|[f_s(x,v',t)f(x,v,t) - f_s(x,v,t)f(x,v',t)]dv'\\ &\quad = n_0(x)\int |v-v'|[h_0(v)f_s(x,v',t) - h_0(v')f_s(x,v,t)]dv'.\end{aligned} \tag{5.8}$$

Define

$$n_s(x,t) = \int f_s(x,v,t)dv, \quad j_s(x,t) = \int vf_s(x,v,t)dv. \tag{5.9}$$

Then, integrating (5.8) over v gives us

$$\frac{\partial}{\partial t}n_s(x,t) + \frac{\partial}{\partial x}j_s(x,t) = 0, \tag{5.10}$$

as expected, while multiplying by v and integrating over v yields

$$\begin{aligned}&\frac{\partial}{\partial t}j_s(x,t) + \frac{\partial}{\partial x}\int v^2 f_s(x,v,t)dv\\ &\quad = \frac{1}{m}\varphi'(x)n_s(x,t)\\ &\qquad + n_0(x)\int\left(\int |v-v'|(v-v')h_0(v)dv\right)f_s(x,v',t)dv'.\end{aligned} \tag{5.11}$$

If we set

$$v^2(x,t) = \left(\int v^2 f_s(x,v,t)dv\right)\Bigg/\left(\int f_s(x,v,t)dv\right), \tag{5.12}$$

(5.11) can be also written as

$$\begin{aligned}&\frac{\partial}{\partial t}j_s(x,t) + v^2(x,t)\frac{\partial}{\partial x}n_s(x,t)dv\\ &\quad = \left(\frac{1}{m}\varphi'(x) - \frac{\partial}{\partial x}[v^2(x,t)]\right)n_s(x,t)\\ &\qquad + n_0(x)\int\left(\int |v-v'|(v-v')h_0(v)dv\right)f_s(x,v',t)dv',\end{aligned} \tag{5.13}$$

very much in the form of (5.7). The simplest model with only two velocities $v=\pm c$, introduced in Sec. III, exhibits exact correspondence between both descriptions. For zero potential, $\varphi(x)=0$, also $n_0(x)=n_0$ and $v^2(x,t)=\langle v^2\rangle$ are constant, and the distribution of velocities

$$h_0(v) = \tfrac{1}{2}[\delta(v-c) + \delta(v+c)], \tag{5.14}$$

corresponding to (3.23), enables us to express $f_s(x,v,t)$ from Eqs. (5.9) as

$$f_s(x,v,t) = \tfrac{1}{2}[\delta(v-c) + \delta(v+c)]\left(n_s(x,t) + \frac{1}{v}j_s(x,t)\right). \tag{5.15}$$

Substituting for (5.13), we recover

$$\frac{\partial}{\partial t}j_s(x,t) + c^2\frac{\partial}{\partial x}n_s(x,t) = -2n_0 c j_s(x,t), \tag{5.16}$$

which is exactly Eq. (3.26), the form of the space-time dynamics (5.7) for this simple model.

For the general distribution function $h_0(v)=h_0(-v)$ and zero potential φ, Q is calculated explicitly from (2.11),

$$Q(x,t;y,0) = 2n_0\left((x-y)\int_0^{(x-y)/t} h_0(v)dv + \int_{(x-y)/t}^{\infty} v t h_0(v)dv\right), \tag{5.17}$$

so its time derivatives are

$$\dot{Q} = 2n_0\int_{(x-y)/t}^{\infty} v h_0(v)dv \quad \text{and} \quad \ddot{Q} = 2n_0\frac{(x-y)^2}{t^3}h_0\left(\frac{x-y}{t}\right). \tag{5.18}$$

For a fixed $(x-y)^2/t$ and $t\to\infty$, $\ddot{Q}$ quenches and $\dot{Q}/n_0$ approaches the mean absolute velocity $\langle|v|\rangle$, corresponding exactly to the result (4.13) for the canonical equilibrium distribution (4.4). So the coefficient at $\partial n/\partial x$ is $\langle|v|\rangle^2$ in Eqs. (5.7), instead of $\langle v^2\rangle$ (5.12), as it comes out from the Boltzmann equation. Similar problems appear in comparison with $-2\dot{Q}j$ in (5.7) with the collision integral on the right-hand side of (5.13).

The Boltzmann equation gives a coarse picture, which is helpful to interpret the real space self-dynamics, expressed by Eqs. (5.7). However, a detailed correspondence, and the region of validity, of the mean field assumption, remain to be established.

VI. CONCLUSION

Our investigation of 1D systems of hard-point (impenetrable) particles, colliding elastically with their nearest neighbors, can be summarized as follows:

If the dynamics of a single noninteracting particle, expressed by the probability density $p_0(x,t;y,0)$ (1.1), is known, the probability density $p(x,t;y,0)$ (2.1) of a *tagged* particle, interacting with its neighbors, is calculable by the formula (2.10), a sort of rather complicated nonlinear transformation $p_0\to p$. This transformation supposes that the system is thermalized, and the density of anonymous neighbors does not depend on time, i.e., the transients are quenched. Then the transformation can be understood as a dimensional reduction of the full space of solutions of the many-particle dynamics onto the dynamics of only the tagged particle.

To understand the dynamics of the tagged particle in a more transparent way, we defined new "stretched" variables F, F', and Q, connected with the physical coordinates x, y, and t by the nonlinear transformation (3.2) and (2.11). While F, F' replaces the spatial coordinates, Q appears to depend on time alone in the limit $t\to\infty$ for infinite systems, i.e., F, $F'\in(-\infty,\infty)$, as we have shown for both inertial and diffusion dynamics of the isolated particles. In the stretched coordinates, the dynamics of the tagged particle can be expressed as simple differential equations (3.17) and (3.18) for the stretched density g and the current density k. If combined, they yield Eq. (3.20), the classical telegrapher's equation.

The dynamics of the tagged particle is universal in the stretched coordinates; it does not depend explicitly on the original dynamics of the single noninteracting particle p_0, which is effectively hidden only in the type of the nonlinear transformation between the *stretched* and *real space-time* coordinates. In the limit of large time, the stretched density evolves according to standard diffusion in the stretched coordinates F, F' and the stretched time Q, with the mean square stretched displacement obeying the classical Einstein formula $\langle(F-F')^2\rangle\simeq Q$. Thus, the subdiffusion observed in real space-time appears as a result of the nonlinear transformation from the stretched coordinates back to real space.

Finally, Eqs. (3.17) and (3.18) for the stretched density g and current density k, transformed to real space-time, give rise to the mass conservation law and the momentum conservation equation (5.7), involving corresponding collisions of the tagged particle with both of its neighbors. They play a dominant role in the limit of large time.

Our theory is based on the assumption that the colliding hard-point particles can be described as two noninteracting particles, exchanging only their labels (or tags). This is valid only for one-component systems in the form presented. Extension to mixtures with common dynamical parameters (mass in the inertial case, diffusivity in the diffusive case) is relatively simple, and will be reported in a future presentation. The unequal parameter case is significantly more difficult.

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