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Single-file diffusion with random diffusion constants

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Abstract. The single-file problem of N particles in one spatial dimension is analysed, when each particle has a randomly distributed diffusion constant D sampled in a density $\rho(D)$. The averaged one-particle distributions of the edge particles and the asymptotic ($N \gg 1$) behaviours of their transport coefficients (anomalous velocity and diffusion constant) are strongly dependent on the D-distribution law, broad or narrow. When ρ is exponential, it is shown that the average one-particle front for the edge particles does not shrink when N becomes very large, in contrast to the pure (non-disordered) case. In addition, when ρ is a broad law, the same occurs for the averaged front, which can even have infinite mean and variance. On the other hand, it is shown that the central particle, dynamically trapped by all others as it is, follows a narrow distribution, which is a Gaussian (with a diffusion constant scaling as N^{-1}) when the fractional moment $\langle D^{-1/2}\rangle$ exists and is finite; otherwise ($\rho(D) \propto D^{\alpha-1}$, $\alpha \leqslant \frac{1}{2}$), this density is, far from the origin, a stretched exponential with an exponent in the range $]0, 2]$; then the effective diffusion constant scales as $N^{-\beta}$, with $\beta = 1/(2\alpha)$.

1. Introduction

The single-file diffusion problem is encountered in various fields (one-dimensional hopping conductivity [1], ion transport in biological membranes [2, 3], channelling in zeolithes [4]). Generally speaking, this is modelled by a set of N diffusing particles on the line with hard-core repulsion; due to such an interaction, any initial ordering is preserved in the course of time and the particles can be, once for all, labelled $1, 2, \ldots, N$ from left to right. When a strong bias is added, this model can be considered as the space-continuous version of the asymmetric exclusion model [5] for which exact results have been obtained in the past years ([6] and references therein).

As in [7], the case will be considered where, at the initial time, these particles form a compact cluster centred at the origin; the solution for an arbitrary initial condition has been given in [8], using the reflection principle. In addition, in contrast to the standard model in which all the particles have the same diffusion constant D, it is here assumed that the particle i has a random D_i, chosen independently of all the others in a given distribution law $\rho(D)$. The latter can always be written as follows:

$$\rho(D) = \frac{1}{D_0} r\left(\frac{D}{D_0}\right) \tag{1.1}$$

where D_0 denotes a specific value of the diffusion constant (e.g. the average value) and $r(\xi)$ a positive function normalized to unity:

$$\int_0^{+\infty} r(\xi)\mathrm{d}\xi = 1. \tag{1.2}$$

On a physical level, a random diffusion constant D can arise in various ways. For instance, by Stokes law and the Einstein relation, it can result from a random radius; more directly, this also happens for particles having random masses.

The main purpose of this paper is to analyse how the choice of the distribution r modifies the large-N dependence of the transport coefficients for one particle of the cluster and, more generally, to find out the density probability of its coordinate in the presence of random-diffusion constants. More specifically, focus will be given on edge particles and on the one which (for N odd) is at the middle of the cluster; for the 'pure' case (all the particles have the same D), asymptotic laws ($N \gg 1$) have been given in [7]. Among other results, it was shown that increasing N yields a narrowing of the one-particle probability distributions, as a result of the 'pressure' exerted by other particles on a given one. This will be shown not to be true in all cases when the D are randomly sampled. As a rule, if the middle particle is most often insensitive to disorder—provided that the average $\langle D^{-1/2}\rangle$ exists and is finite—it will be shown that the distribution for the side particles strongly depends on the latter, going from narrow to broad laws.

2. Basic relations

For a given configuration $\Omega = \{D_1, D_2, \ldots, D_N\}$, the diffusion equation here is

$$\frac{\partial}{\partial t} p_{\mathrm{C}}(x_1, x_2, \ldots, x_N; t) = \sum_{n=1}^{N} D_n \frac{\partial^2}{\partial x_n^2} p_{\mathrm{C}}(x_1, x_2, \ldots, x_N; t) \qquad (x_1 < x_2 < \cdots < x_N). \tag{2.1}$$

As a consequence of the hard-core repulsion and of the above-mentioned initial condition, the solution has the expression

$$p_{\mathrm{C}}(x_1, x_2, \ldots, x_N; t) = C_N(\Omega) \prod_{n=1}^{N} \frac{\mathrm{e}^{-x_n^2/(4D_n t)}}{\sqrt{4\pi D_n t}} \prod_{n=1}^{N-1} Y(x_{n+1} - x_n). \tag{2.2}$$

In (2.2), Y is the Heaviside unit step function ($Y(x) = 1$ if $x > 0$, 0 otherwise), and $C_N(\Omega)$ is the normalization constant. As can be seen by explicit calculations for small values of N, $C_N(\Omega)$ is (except for $N = 2$) a non-trivial function of the D_ns. As an example, for $N = 4$, one finds

$$C_N(D_1, D_2, D_3, D_4) = \frac{8\pi}{\arcsin \frac{D_1 D_2 + D_2 D_3 + D_3 D_1 - D_2^2}{D_1 D_2 + D_2 D_3 + D_3 D_1 + D_2^2} + \arcsin \frac{D_2 D_3 + D_3 D_4 + D_4 D_2 - D_3^2}{D_2 D_3 + D_3 D_4 + D_4 D_2 + D_3^2}}. \tag{2.3}$$

Unfortunately, no simple recursion relation exists between C_N and C_{N+1}, which, for instance, would allow us to analyse the possible self-averaging properties of the normalization constant in the limit of large N. Due to this normalization problem, it seems hopeless to obtain a tractable form of p_{C} for N arbitrary. This problem, well known in the physics of disordered systems, is sometimes referred to as the 'denominator problem' and is at the origin of the distinction between annealed and quenched quantities.

On the other hand, one can consider the set of all the initial states obtained by exchanging the particles, i.e. obtained by acting with the $N!$ permutations P_λ on the diffusion constants D'_n and subsequently take the arithmetical mean of all the $N!$ corresponding N-body probabilities. In some way, this 'shuffling' *looks like* averaging over the initial conditions for a given sampling of the D'_n. This yields the following distribution:

$$p(x_1, x_2, \ldots, x_N; t) = C_N \left[\frac{1}{N!} \sum_{\lambda=1}^{N!} \mathcal{P}_\lambda \prod_{n=1}^{N} \frac{\mathrm{e}^{-x_n^2/(4D_n t)}}{\sqrt{4\pi D_n t}} \right] \prod_{n=1}^{N-1} Y(x_{n+1} - x_n). \tag{2.4}$$

Now, the quantity in brackets is by construction a symmetric function of all the coordinates; due to this fact, the integrations can now be straightforwardly performed and the new normalization constant C_N in (2.4) is readily seen to be equal to $N!$ for each configuration Ω. All the quantities calculated with the distribution (2.4) can be said of the annealed type and their precise relation with quantities obtained without shuffling is, at this point, an open interesting question.

Since the D are assumed to be statistically independent, the various averages can now be readily performed; the N-particle front averaged over all possible configurations turns out to be

$$\langle p(x_1, x_2, \ldots, x_N; t)\rangle = N! \prod_{n=1}^{N} \langle G(x_n, t)\rangle \prod_{n=1}^{N-1} Y(x_{n+1} - x_n) \tag{2.5}$$

where $\langle G(x_n, t)\rangle$ is the average of the Gaussian distribution with the density $\rho(D)$:

$$\langle G(x_n, t)\rangle = \int_0^{+\infty} \mathrm{d}D\, \rho(D) \frac{\mathrm{e}^{-x_n^2/(4Dt)}}{\sqrt{4\pi Dt}} \equiv \frac{1}{(4D_0 t)^{1/2}} f(u_n) \tag{2.6}$$

with

$$f(u) = \frac{1}{\pi^{1/2}} \int_0^{+\infty} \mathrm{d}\xi\, \xi^{-1/2} r(\xi) \mathrm{e}^{-u^2/\xi} \qquad u_n = \frac{x_n}{(4D_0 t)^{1/2}}. \tag{2.7}$$

f is an even positive function normalized to $\frac{1}{2}$ on the interval $[0, +\infty]$.

From (2.5), all the one-particle averaged fronts can be formally obtained by integrating over all x but one:

$$\langle p_n^{(1)}(x_n; t)\rangle = \left(\prod_{m=1, m\neq n}^{N} \int_{-\infty}^{+\infty} \mathrm{d}x_m \right) \langle p(x_1, x_2, \ldots, x_N; t)\rangle. \tag{2.8}$$

One then finds that

$$\langle p_n^{(1)}(x; t)\rangle = \frac{N!}{(n-1)!(N-n)!} \left[\frac{1 + I(u)}{2}\right]^{n-1} \left[\frac{1 - I(u)}{2}\right]^{N-n} \frac{1}{(4D_0 t)^{1/2}} f(u) \qquad \left(u = \frac{x}{(4D_0 t)^{1/2}}\right) \tag{2.9}$$

where $I(u)$ is defined by

$$I(u) = 2\int_0^u \mathrm{d}u'\, f(u') = \int_0^{+\infty} \mathrm{d}\xi\, r(\xi) \Phi(u/\sqrt{\xi}) \equiv \langle \Phi(u/(\sqrt{\xi})\rangle \tag{2.10}$$

where Φ denotes the probability integral [9]. In (2.9), the two factors $[1 \pm I(u)]/2$ represent the steric effects on the nth particle due to all other ones. $I(u)$ is a non-decreasing odd function such that $I(\pm\infty) = \pm 1$ (for the pure case, one simply has $I(u) = \Phi(u)$). For the edge particles ($n = 1$ or $n = N$), $\langle p_n^{(1)}(x; t)\rangle$ can be given a form occurring also in the theory of extreme events [10], namely

$$\langle p_{1,N}^{(1)}(x; t)\rangle = \pm \frac{1}{(4D_0 t)^{1/2}} \frac{\mathrm{d}}{\mathrm{d}u} P_\pm(u) \qquad P_\pm(u) = \left[\frac{1 \pm I(u)}{2}\right]^N. \tag{2.11}$$

The $-$ sign (respectively $+$) refers to the left particle ($n = 1$) (respectively right particle ($n = N$)). In any case, the following relation holds true:

$$\langle p_1^{(1)}(x; t)\rangle = \langle p_N^{(1)}(-x; t)\rangle. \tag{2.12}$$

For n arbitrary, (2.11) generalizes into

$$\langle p_n^{(1)}(x; t)\rangle = \frac{1}{(4D_0 t)^{1/2}} C_N^n \left[\frac{\mathrm{d}}{\mathrm{d}u} \left(\frac{1 + I(u)}{2}\right)^n\right] \left(\frac{1 - I(u)}{2}\right)^{N-n}. \tag{2.13}$$

For the particle which is at the centre of the cluster (N odd), one has

$$\langle p^{(1)}_{(N+1)/2}(x;t)\rangle = \frac{1}{(4D_0t)^{1/2}}\frac{N!}{\{[(N-1)/2]!\}^2}\left[\frac{1-I^2(u)}{4}\right]^{(N-1)/2} f(u) \tag{2.14}$$

or, equivalently, from (2.13)

$$\langle p^{(1)}_{(N+1)/2}(x;t)\rangle = \frac{1}{(4D_0t)^{1/2}} C_N^{(N+1)/2}\left[\frac{\mathrm{d}}{\mathrm{d}u}\left(\frac{1+I(u)}{2}\right)^{(N+1)/2}\right]\left(\frac{1-I(u)}{2}\right)^{(N-1)/2}. \tag{2.15}$$

In the following sections, the above equations will be used with different choices for the distribution $r(\xi)$, taken in a set of common probability densities. Exact asymptotic results for large N can be obtained due to the fact that, for $N \gg 1$, the steric factors $\{\frac{1}{2}[1 \pm I(u)]\}^n$ display a rather sharp variation.

Generally speaking, the one-particle transport coefficients can be found from the behaviour at small k of the characteristic function $\Pi_n(K)$:

$$\Pi_n(K) = \int_{-\infty}^{+\infty} \mathrm{d}x\, \mathrm{e}^{\mathrm{i}kx}\langle p^{(1)}_n(x;t)\rangle \qquad \left(K = k\sqrt{4D_0t}\right). \tag{2.16}$$

The transport properties of the nth particle subjected to the random field of all the others are essentially described by the two first cumulants:

$$\langle x_n\rangle(t) = V_{1/2,n}(N)\sqrt{t} \qquad \Delta x_n^2 \equiv \langle x_n^2\rangle(t) - [\langle x_n\rangle(t)]^2 = 2\mathcal{D}_n(N)t. \tag{2.17}$$

The above time dependences come from the fact that the only available length scale is $(D_0t)^{1/2}$, so that $\langle x^\lambda\rangle \propto t^{\lambda/2}$ at all times and for any λ. Thus, at any time, the drift is always anomalous (no velocity) and the mean square displacement always has a purely diffusive motion. The following relations are trivially verified:

$$\langle x_1\rangle(t) = -\langle x_N\rangle(t) \qquad \Delta x_1^2(t) = \Delta x_N^2(t). \tag{2.18}$$

In addition to the one-particle transport coefficients, statistical correlations between the particles can be analysed. For definiteness, focus will be given on the correlations between the two edge particles, altogether contained in the two-body density:

$$\langle p^{(2)}_{1,N}(x_1,x_N)\rangle = \left(\prod_{m=2}^{N-1}\int_{-\infty}^{+\infty}\mathrm{d}x_m\right)\langle p(x_1,x_2,\ldots,x_N;t)\rangle. \tag{2.19}$$

Using (2.5)–(2.7), one finds that

$$\langle p^{(2)}_{1,N}(x_1,x_N;t)\rangle = \frac{1}{4D_0t}N(N-1)\left[\frac{I(u_N)-I(u_1)}{2}\right]^{N-2} f(u_1)f(u_N)Y(u_N-u_1). \tag{2.20}$$

3. Exponential distribution

As a first simple example, let us choose

$$\rho(D) = \frac{1}{D_0}\mathrm{e}^{-D/D_0}. \tag{3.1}$$

Here, D_0 is the expectation value of D. From (2.7) and (2.10), one readily obtains

$$f(u) = \mathrm{e}^{-2|u|} \qquad I(u) = \mathrm{sgn}u(1-\mathrm{e}^{-2|u|}). \tag{3.2}$$

The reduced densities for the edge particles density can now be explicitly calculated from (2.11) with

$$P_-(u) = \begin{cases} 2^{-N}\mathrm{e}^{-2Nu} & \text{if } u \geqslant 0 \\ (1-\frac{1}{2}\mathrm{e}^{-2|u|})^N & \text{if } u \leqslant 0 \end{cases} \tag{3.3}$$

and $P_+(u) = P_-(-u)$. From (3.3), the generating functions $\Pi_{1,\,N}(K)$ (2.16) for the edge particles are found as

$$\Pi_1(K) = 1 + \mathrm{i}K\left[\frac{1}{2^N(N-\mathrm{i}K)} + \sum_{p=1}^{N} C_N^p \frac{(-1)^p}{p+\mathrm{i}K}\right] \qquad \Pi_N(K) = \Pi_1^*(K). \tag{3.4}$$

Now, by expanding $\Pi_{1,N}$ in the vicinity of $K = 0$, and by coming back to the x-variable, one obtains

$$\langle x_N\rangle(t) = -\langle x_1\rangle(t) = [\ln(N/2) + C + \mathrm{O}(2^{-N})]\sqrt{D_0 t} \equiv V_{1/2,\mathrm{edge}}(N)\sqrt{D_0 t} \tag{3.5}$$

where C is the Euler constant ($C = 0.577\ldots$). The mean square displacements are

$$\Delta x_N^2 = \Delta x_1^2 = \left[\frac{\pi^2}{6} + \mathrm{O}(2^{-N})\right] D_0 t \equiv 2\mathcal{D}_{\mathrm{edge}}(N)t. \tag{3.6}$$

As compared with the pure case, the large-N behaviour of the transport coefficients is frankly different. When all the particles have the same diffusion constant, one has [7]

$$V_{1/2,\mathrm{edge}}^{(\mathrm{pure})}(N) \propto (\ln N)^{\frac{1}{2}} \qquad \mathcal{D}_{\mathrm{edge}}^{(\mathrm{pure})}(N) \propto (\ln N)^{-1}. \tag{3.7}$$

By contrast, for exponentially distributed random D, the anomalous drift coefficient increases like $\ln N$, whereas the effective diffusion constant $\mathcal{D}_{\mathrm{edge}}(N)$ tends towards a *finite* (non-vanishing) value. Note that the height of the maximum also saturates and does not go to zero for N infinite. Overall, the effect of an exponential disorder is rather subtle: most particles of the cluster have a rather small D, so that the pressure they exert on the edge ones is smaller than in the pure case; on the other hand, large D forces the packet to move with a 'velocity' which increases more rapidly with N than in the pure case. The interplay of these facts produces a distribution having finite height and width at infinite N. This is illustrated in figure 1, which clearly shows the width and height saturation when N becomes very large, as quantitatively described in (3.6). It is readily seen that the value of $\langle p_{1,N}^{(1)}\rangle$ at its maximum is close to $(2/\mathrm{e}) \propto N^0$.

For $N \gg 1$, the abscissae of the edge particles are approximately distributed according to

$$\langle p_N^{(1)}(x;t)\rangle \simeq Y(u)\frac{N}{(4D_0 t)^{1/2}}\mathrm{e}^{-(N/2)\mathrm{e}^{-2u}}\mathrm{e}^{-2u} \qquad \langle p_1^{(1)}(x;t)\rangle = \langle p_N^{(1)}(-x;t)\rangle. \tag{3.8}$$

These functions are exponentially small ($\sim\mathrm{e}^{-N}$) near $|u| = 0$ and display a plain exponential decay ($\sim\mathrm{e}^{-2|u|}$) for $|u| \gg \ln[(N/2)^{1/2}]$. $\langle p_N^{(1)}\rangle$ is maximum for $u = u_{\max} = \frac{1}{2}\ln(N/2)$; this shows that the corresponding $x_{\max}$ coincides with $\pm\langle x_N\rangle$ (see (3.5)). The approximate expressions (3.8) are hardly distinguishable from their exact counterparts as soon as N is greater than a rather small number ($\simeq$50) and can be rewritten in terms of the proper shifted (but here not rescaled) variable X:

$$\begin{aligned}&\langle p_N^{(1)}(x;t)\rangle \simeq Y(x)\frac{1}{(D_0 t)^{1/2}}\mathrm{e}^{-\mathrm{e}^{-X}}\mathrm{e}^{-X} \qquad X = \frac{x - x_{\max}}{(D_0 t)^{1/2}}\\ &x_{\max} = (D_0 t)^{1/2}\ln(N/2).\end{aligned} \tag{3.9}$$

The statistical correlations between the two edge particles are most simply measured by the correlator C_{1N}:

$$C_{1N} = \langle x_1 x_N\rangle - \langle x_1\rangle\langle x_N\rangle \tag{3.10}$$

which, due to scaling in space, varies linearly in time. C_{1N} can be found by using (2.20) and (3.2); for $N \gg 1$, a little algebra yields

$$C_{1N} = 4D_0 t[\ln^2(N/2) + \mathrm{O}(\ln N)]. \tag{3.11}$$

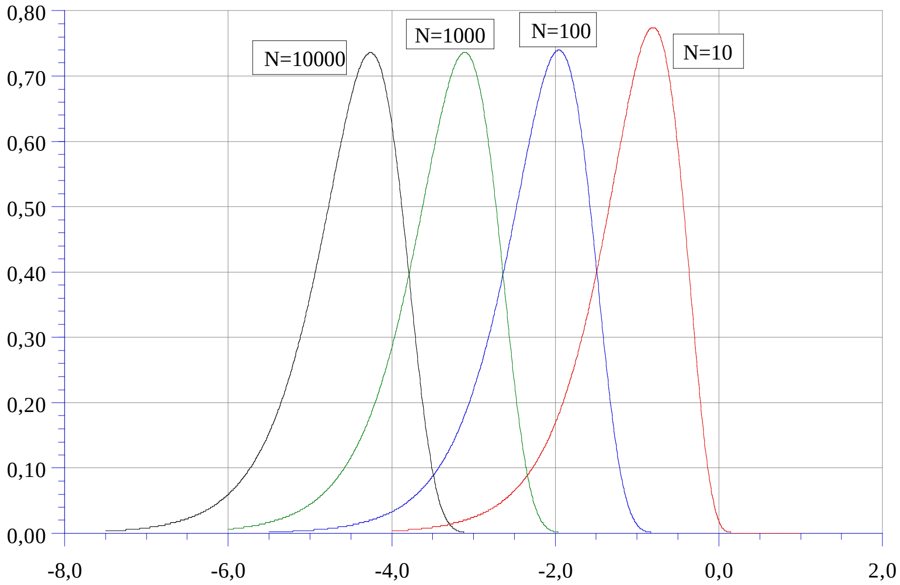

Figure 1. Exact averaged front $\langle p_1^{(1)}(x;t)\rangle$ for the left particle with exponentially distributed diffusion constants; the abscissa is the dimensionless variable $u = x/(4D_0t)^{1/2}$. Each curve is labelled by the number of particles in the cluster.

By (3.6), this implies that the normalized ratio $C_{1N}/\Delta x^2_{1,N}$—which is constant in time—has a logarithmic increase with N:

$$\frac{C_{1N}}{\Delta x^2_{1,N}} \simeq \frac{6}{\pi^2}\ln^2(N/2). \tag{3.12}$$

Although the numerator and the denominator of the ratio have separately different behaviours as compared with the pure case, the ratio still has a $\sim(\ln N)^2$ increase with N, exactly as in this latter case [7].

For the particle located at the middle of the cluster, the expression (2.15) becomes

$$\langle p^{(1)}_{(N+1)/2}(x;t)\rangle = \frac{1}{(4D_0t)^{1/2}} C_N^{(N+1)/2}\left[\left(1-\frac{1}{2}\mathrm{e}^{-2|u|}\right)\frac{1}{2}\mathrm{e}^{-2|u|}\right]^{(N-1)/2} \mathrm{e}^{-2|u|}. \tag{3.13}$$

From (3.13), the following large-N expression of the mean square dispersion is obtained:

$$\Delta x^2_{(N+1)/2}(x;t) = \frac{1}{2}D_0tC_N^{(N+1)/2}\left[B\left(\frac{N+1}{2},\frac{N+1}{2}\right) - 4B\left(\frac{N+3}{2},\frac{N+3}{2}\right)\right] \tag{3.14}$$

where B denotes the Euler beta-function [9]. Expansion for large-N yields

$$\Delta x^2_{(N+1)/2}(x;t) \simeq \frac{1}{N}D_0t \tag{3.15}$$

and provides the asymptotic dependence of the diffusion constant

$$\mathcal{D}_{\mathrm{middle}}(N) \simeq \frac{1}{2N}D_0. \tag{3.16}$$

This behaviour is the same as for the pure case [7]. Thus, for the exponential distribution, the transport coefficient of the central particle is essentially unaltered by disorder—as shown below this is also true for any r density having $\langle D^{-1/2}\rangle$ finite. The asymptotic density of the middle particle is obtained from (3.13) as

$$\langle p^{(1)}_{(N+1)/2}(x;t)\rangle \simeq \left(\frac{N}{2\pi D_0 t}\right)^{1/2} \mathrm{e}^{-2(|u|+Nu^2)}. \tag{3.17}$$

This function is normalized to unity up to N^{-1} terms. Apart from the cusp at $u = 0$ and outside the region $|u| \leqslant 1/N$, this is essentially a Gaussian distribution, exactly as in the pure case. For large N, the cusp can even be ignored and the distribution looks like a Gaussian everywhere.

In fact, it can now be stated the conditions for the stochastic dynamics of the central particle to be unaffected by disorder; such a particle is stymied in some way due to other particles and it can be suspected that strong steric effects most often dominate, except perhaps when the distribution $\rho(D)$ gives a high probability to find very small D. The analysis goes as follows. For $N \gg 1$, it is readily seen that the distribution (2.14) assumes non-negligible values only for $|u| \ll 1$. This in turn allows us to replace $I(u)$ by its small-u expansion; from (2.10) and (2.6), $f(0)$ exists and is finite provided that $\rho(D)$ is bounded by $D^{-\beta}(\beta < \frac{1}{2})$ for $D \to 0$. This means that when ρ diverges at small D, this divergence is not too severe, which implies that finding a small D has not such a great probability. With this assumption, one has

$$I(u) \simeq 2uf(0) \qquad f(0) = \frac{1}{\pi}\int_0^{+\infty} \mathrm{d}\xi\, \xi^{-1/2} r(\xi) \equiv \frac{1}{\pi}\left\langle\left(\frac{D_0}{D}\right)^{1/2}\right\rangle. \tag{3.18}$$

Using the Stirling formula, and expanding $\mathrm{e}^{[(N-1)/2]\ln[1-4u^2 f^2(0)]}$, one eventually gets the asymptotic approximation:

$$\langle p^{(1)}_{(N+1)/2}(x;t)\rangle \simeq \left(\frac{N}{2\pi D_0 t}\right)^{1/2} f(0)\mathrm{e}^{-2Nf^2(0)u^2}. \tag{3.19}$$

Note that the approximation automatically generates a properly normalized density. So, for any $\rho(D)$ such that $\lim_{D\to 0}[D^{1/2}\rho(D)] = 0$, the middle particle is essentially distributed according a normal law, the width of which decreasing as $N^{-1/2}$, up to unessential numerical factors. The expression (3.19) can be written as a universal law in termsw of the proper scaled variable X:

$$\langle p^{(1)}_{(N+1)/2}(x;t)\rangle \simeq \left(\frac{N}{\pi t}\right)^{1/2} \langle D^{-1/2}\rangle \frac{\mathrm{e}^{-X^2/2}}{(2\pi)^{1/2}} \qquad X = x\left(\frac{N}{\pi t}\right)^{1/2}\langle D^{-1/2}\rangle \tag{3.20}$$

expressing as a whole the irrelevance of details about the D distributions for the central particle when $\rho(D)$ is bounded near $D = 0$ as stated above, which entails that the fractional moment $\langle D^{-1/2}\rangle$ exists and is finite. The opposite case is treated in the next section which deals with the Gamma distribution.

4. Gamma distribution

As another example—which in fact contains the exponential distribution as a particular case—let us choose a Gamma distribution:

$$\rho(D) = \frac{1}{\Gamma(\alpha)D_0^{\alpha}} D^{\alpha-1}\mathrm{e}^{-D/D_0} \qquad (\alpha > 0). \tag{4.1}$$

With (4.1), the expectation values of D and D^2 are respectively equal to αD_0 and $\alpha(\alpha+1)D_0^2$. The exponential distribution is recovered by setting $\alpha = 1$, whereas the pure case can be obtained by taking the limit $\alpha \to \infty$, $D_0 \to 0$, $\alpha D_0 = \text{const}$. The f function (2.7) is

$$f(u) = \frac{2}{\sqrt{\pi}\,\Gamma(\alpha)}|u|^{\alpha-\frac{1}{2}} K_{\alpha-\frac{1}{2}}(2|u|) \tag{4.2}$$

where $K_{\alpha-\frac{1}{2}}$ is the Bessel function of imaginary argument [9]. $f(0)$ exists and is finite if $\alpha > \frac{1}{2}$:

$$f(0) = \frac{1}{\sqrt{\pi}} \frac{\Gamma(\alpha + \frac{1}{2})}{(\alpha - \frac{1}{2})\Gamma(\alpha)} \qquad (\alpha > \tfrac{1}{2}). \tag{4.3}$$

The large-N approximation of the one-particle densities can be obtained along the same lines as in the previous section, by using the approximate expression:

$$I(u) \simeq 1 - \frac{1}{\Gamma(\alpha)}|u|^{\alpha-1}\mathrm{e}^{-2|u|} \qquad (|u| \gg 1). \tag{4.4}$$

Let us first consider the right particle; one has

$$\langle p_N^{(1)}(x;t)\rangle \simeq Y(u)\frac{1}{(4D_0t)^{1/2}}\frac{N}{\Gamma(\alpha)}\mathrm{e}^{-\frac{N}{2\Gamma(\alpha)}u^{\alpha-1}\mathrm{e}^{-2u}}u^{\alpha-1}\mathrm{e}^{-2u}. \tag{4.5}$$

When $\alpha < 1$, i.e. when ρ diverges at small D, $\langle p_N^{(1)}\rangle$ is exponentially small near $x = 0$. On the contrary, for $\alpha > 1$, $\langle p_N^{(1)}\rangle$ strictly vanishes as $u^{\alpha-1}$, but this behaviour is realized on a very small interval, namely $u < N^{-1/(\alpha-1)}$, beyond which $\langle p_N^{(1)}\rangle$ remains exponentially small. On the other hand, at large u, $\langle p_N^{(1)}\rangle$ has essentially an exponential decay, so that all the average values $\langle x_N^m\rangle$ exist and are finite. $\langle p_N^{(1)}\rangle$ is maximum at $u_{\max}$:

$$u_{\max} \simeq \frac{1}{2}\ln\frac{N}{2\Gamma(\alpha)}. \tag{4.6}$$

Again, $x_{\max} = (4D_0t)^{1/2}u_{\max}$ is the relevant rescaled variable, since (4.5) can be rewritten as follows:

$$\langle p_N^{(1)}(x;t)\rangle \simeq Y(u)\frac{1}{(D_0t)^{1/2}}\mathrm{e}^{-(u/u_{\max})^{\alpha-1}\mathrm{e}^{-2(u/u_{\max})}}(u/u_{\max})^{\alpha-1}\mathrm{e}^{-2(u/u_{\max})}. \tag{4.7}$$

This readily gives $\langle p_N^{(1)}\rangle_{\max} \propto N^0$ which in turns allows us to guess that, as for the exponential case, one has $\langle x_N\rangle \propto \ln N$ and $\langle \Delta x_{1,N}^2\rangle \propto N^0$; it thus turns out that detailed calculations for $\alpha \neq 1$ are indeed of little interest. Up to unessential numerical factors, the large-N asymptotic laws all belong to the same class for Gamma-distributed diffusion constants, the behaviours being rather easily obtained by considering the simpler exponential case $\alpha = 1$; the same obviously holds for statistical correlations between edge particles.

For the central particle, one has to distinguish the two cases $\alpha > \frac{1}{2}$ and $\alpha < \frac{1}{2}$. Due to (4.3), the first one is described by the general expression (3.20). By contrast, for $\alpha < \frac{1}{2}$, one has

$$f(u) \simeq \frac{2^{2\alpha-1}}{\Gamma(2\alpha)\cos\alpha\pi}|u|^{2\alpha-1} \qquad (|u| \ll 1). \tag{4.8}$$

This in turns entails that

$$I(u) \simeq \frac{2^{2\alpha}}{\Gamma(2\alpha+1)\cos\alpha\pi}|u|^{2\alpha} \qquad (|u| \ll 1). \tag{4.9}$$

As a consequence, one obtains

$$\langle p_{(N+1)/2}^{(1)}(x;t)\rangle \simeq \frac{\alpha A}{(D_0t)^{1/2}}\sqrt{\frac{2N}{\pi}}\mathrm{e}^{-(N/2)A^2|u|^{4\alpha}}|u|^{2\alpha-1} \qquad A = \frac{1}{\sqrt{\pi}}\frac{\Gamma(\frac{1}{2}-\alpha)}{\alpha\Gamma(\alpha)}. \tag{4.10}$$

This shows that when the probability is very high to find quite small diffusion constants, the distribution for the central particle diverges at $x = 0$ (but is clearly integrable) and is essentially a stretched exponential when $|u|$ is large (see figure 2):

$$\langle p_{(N+1)/2}^{(1)}(x;t)\rangle \propto \begin{cases} |u|^{-(1-2\alpha)} & \text{if} \quad |u| \ll 1 \\ \mathrm{e}^{-C|u|^{4\alpha}} & \text{if} \quad |u| \gg 1. \end{cases} \tag{4.11}$$

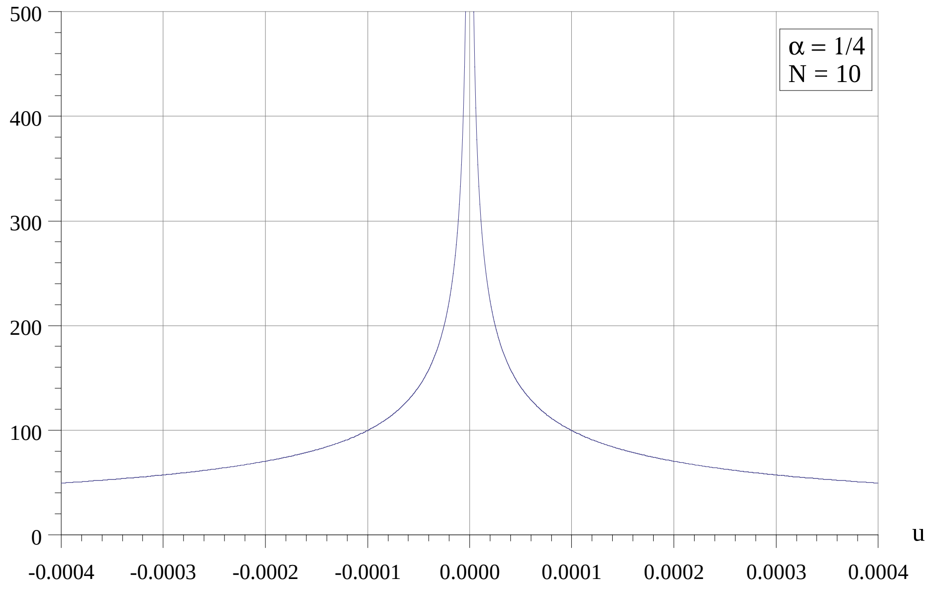

Figure 2. Averaged front $\langle p^{(1)}_{(N+1)/2}(x;t)\rangle$ of the central particle (4.10) for a cluster of ten particles when the diffusion constants are distributed according to (4.1) with $\alpha = \frac{1}{4}$; the abscissa is the dimensionless variable $u = x/(4D_0t)^{1/2}$.

For $\alpha = \frac{1}{2}$, $f(u)$ is proportional to the Bessel function K_0 and the divergence is logarithmic. In this case, one has

$$\langle p^{(1)}_{(N+1)/2}(x;t)\rangle \simeq -\frac{1}{(D_0t)^{1/2}}\sqrt{\frac{2N}{\pi^3}}\,\mathrm{e}^{-(16N/\pi^2)u^2\ln|u|}\ln|u| \tag{4.12}$$

which entails that

$$\langle p^{(1)}_{(N+1)/2}(x;t)\rangle \propto \begin{cases} -\ln|u| & \text{if} \quad |u| \ll 1 \\ \mathrm{e}^{-C'u^2} & \text{if} \quad |u| \gg 1 \end{cases} \qquad (\alpha = \tfrac{1}{2}). \tag{4.13}$$

The divergence at $x = 0$ comes from the interplay of pressure and of the frequent occurrence of a central particle with very small D. From (4.10), one finds that

$$\Delta x^2_{(N+1)/2} \simeq 8\left[\frac{\Gamma(\alpha+1)}{\Gamma(\frac{1}{2}-\alpha)}\right]^{1/\alpha}\frac{\Gamma(\frac{1}{\alpha})}{\Gamma(\frac{1}{2\alpha})}\left(\frac{2N}{\pi}\right)^{-\frac{1}{2\alpha}} D_0t. \tag{4.14}$$

Summing up, the effective diffusion constant for the central particle and for the Gamma distribution scales with N as follows:

$$\mathcal{D}_{\text{middle}} \propto N^{-\beta} \tag{4.15}$$

with

$$\beta = \begin{cases} 1 & \text{if} \quad \alpha \geqslant \frac{1}{2} \\ \dfrac{1}{2\alpha} & \text{if} \quad 0 < \alpha \leqslant \frac{1}{2}. \end{cases} \tag{4.16}$$

5. Broad distributions

The two previous examples discard the interesting case in which the diffusion constants are sampled in a broad law, possibly devoid of the usual first few moments (mean and variance). Obviously, such a case is interesting since the average front for the edge particles are expected to be strongly asymmetric and also quite diffuse, due to the pressure exerted by inner particles and the possibility of rather high diffusion constants. This fact even opens the possibility for the edge particles also to be distributed according a broad law, devoid of mean and variance. Generally speaking, I now consider the case

$$\rho(D) = \mu D_0^{\mu} Y(D - D_0) D^{-(\mu+1)} \Longleftrightarrow r(\xi) = Y(\xi - 1)\xi^{-(\mu+1)} \qquad (\mu > 0). \tag{5.1}$$

All the moments $\langle D^k \rangle$ diverge for $k \geqslant \mu$.

With the distribution (5.1), the f function (2.6) can be expressed in terms of the incomplete γ function [9]:

$$f(u) = \frac{\mu}{\pi^{1/2}} u^{-(2\mu+1)} \gamma(\mu + \tfrac{1}{2}, u^2). \tag{5.2}$$

Again, I am interested in the large-N limit, in which case the right particle density (2.11) assumes non-negligible values for u of the order of or greater than u_0 defined as

$$\left[\frac{1 + I(u_0)}{2}\right]^N = \frac{1}{2} \Longleftrightarrow u_0 \simeq \left[\frac{N}{\pi^{1/2} \ln 4} \Gamma\left(\mu + \frac{1}{2}\right)\right]^{1/(2\mu)}. \tag{5.3}$$

For genuine broad laws (μ small), u_0 is much greater than 1 even for moderately large values of N. This allows us to state again that only the large-u expansion of $I(u)$ is relevant, and to substitute everywhere the approximate expression,

$$I(u) \simeq 1 - \frac{1}{\pi^{1/2}} \Gamma(\mu + \tfrac{1}{2}) u^{-2\mu} \qquad (u \gg 1). \tag{5.4}$$

Injecting this in (2.11) yields the large-N approximation, valid for $u > 0$:

$$\langle p_N^{(1)}(x;t) \rangle \simeq N \frac{\mu}{\pi^{1/2}} \mathrm{e}^{-N\Gamma(\mu+\frac{1}{2})/(2\pi^{1/2} u^{2\mu})} u^{-(2\mu+1)} \gamma(\mu + \tfrac{1}{2}, u^2) \tag{5.5}$$

it being understood that $\langle p_N^{(1)} \rangle$ is exponentially small for $u < 0$ and can be considered as identically vanishing for $u < 0$; note that the expression (5.5) goes toward zero extremely rapidly when $u \to 0$, namely

$$\langle p_N^{(1)} \rangle \sim \mathrm{e}^{-\mathrm{Cst} N/u^{2\mu}}. \tag{5.6}$$

On the other hand, the distribution given in (5.6) is indeed a broad law in the wide sense, since (5.5) displays for any μ a power-law behaviour at (very) large u:

$$\langle p_N^{(1)}(x;t) \rangle \simeq N \frac{\mu}{\pi^{1/2}} \Gamma\left(\mu + \frac{1}{2}\right) u^{-(2\mu+1)} \qquad \left(u \equiv \frac{x}{\sqrt{4D_0 t}} \gg N^{1/(2\mu)}\right). \tag{5.7}$$

Equations (5.6) and (5.7) show that the average front for the right particle is strongly asymmetric, displaying a rather steep increase on the left (towards the inner part of the cluster) and a very slow decrease on the other side, towards the free part of space. The result (5.7) entails that the moment $\langle u^m \rangle$ exists and is finite only if the following inequality is satisfied:

$$m < 2\mu. \tag{5.8}$$

Thus, for $\mu \leqslant \frac{1}{2}$, the expectation value of x (as well as all higher moments) is infinite. The one-particle distribution (plotted in figure 3 for a few values of N) can nevertheless be characterized by the value $u_{\max}$ giving its maximum value, which turns out to coincide with u_0 (see (5.3)),

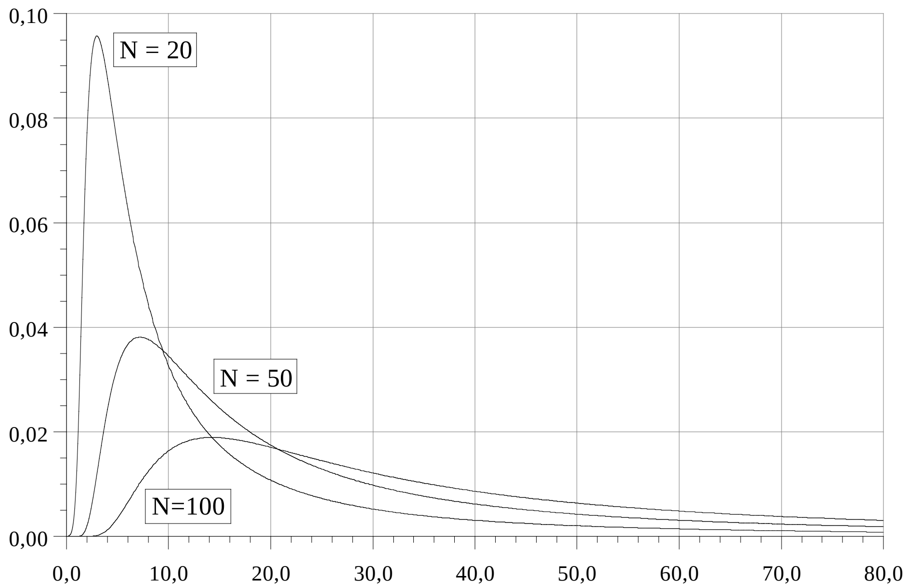

Figure 3. Exact averaged front $\langle p_N^{(1)}(x;t)\rangle$ for the right particle when the diffusion constants of the cluster are distributed according to (5.1) with $\mu = \frac{1}{2}$; the abscissa is the dimensionless variable $u = x/(4D_0t)^{1/2}$. Each curve is labelled by the number of particles in the cluster.

except for numerical factors. It is readily verified that, accordingly, the value of $\langle p_{1,N}^{(1)}\rangle$ at its maximum is $\propto N^{-1/(2\mu)}$. Overall, the maximum of $\langle p_N^{(1)}(x;t)\rangle$ moves in time as

$$x_{\max}(t) \simeq 2\left[\frac{N}{\pi^{1/2}}\Gamma\left(\mu+\frac{1}{2}\right)\frac{\mu}{2\mu+1}\right]^{1/(2\mu)}(D_0t)^{1/2}. \tag{5.9}$$

$x_{\max}$ is here the relevant rescaled coordinate; agreement is quite good with the exact results (see figure 3).

Note that for $\mu \to \infty$, (5.7) shows that $\langle p_N^{(1)}\rangle$ decreases faster than any arbitrary power of u^2, in agreement with [7]. Also note that no obvious measure of correlations here exists since for $\mu < 1$ the mean square dispersions are infinite.

6. Summary and conclusions

For the single-file diffusion problem with random diffusion constants, the asymptotic laws (large N) giving the transport coefficients and the averaged one-particle densities have been derived.

Generally speaking, the asymptotic distribution of the central particle is most often Gaussian (see (3.19)), as a result of the fact that steric effects nearly always dominate; when this is the case, the dynamical trapping of this particle is insensitive to details describing the distribution $\rho(D)$ of the diffusion constants. On the other hand, when $\rho(D)$ diverges as $D^{-1/2}$ or faster at small D ($\rho(D) \propto D^{\alpha-1}$, $\alpha \leqslant \frac{1}{2}$), the distribution of the central particle is no longer a normal one: at small x, it itself goes to infinity as $x^{-(1-2\alpha)}$ and is a stretched exponential $\mathrm{e}^{-Cx^{4\alpha}}$ at large x (see (4.10)). The effective diffusion constant scales as $N^{-1/(2\alpha)}$ for $\alpha < \frac{1}{2}$ and as N^{-1} otherwise, showing that in the N-infinite limit, as in the pure case, the motion indeed becomes subdiffusive. As observed in the pure case [7], the vanishing of the effective diffusion constant for the central particle at infinite N is in agreement with Harris's result [11], who found that a single particle (tracer) immersed in an infinite sea of other particles (*all* the particles having the same diffusion constant D) has a squared dispersion increasing as $t^{1/2}$.

By contrast, the stochastic dynamics of the edge particles is strongly dependent upon the nature (narrow or broad) of the diffusion constants probability density $\rho(D)$. When the latter is narrow and of the exponential type, the effective diffusion constant of edge particles tends toward a *finite* constant when N becomes infinite; the average coordinate increases with N as $\ln N$, faster than for the pure case. When the $\rho(D)$ is broad (i.e. behaves as a power law $D^{-(\mu+1)}$ at large D), the edge particles are themselves distributed according a broad law, devoid of mean and variance when μ is smaller than $\frac{1}{2}$. The distribution of the coordinate, strongly asymmetric (see figure 3), can nevertheless be characterized by the abscissa of its maximum (5.9); the prefactor of the latter displays a $N^{1/(2\mu)}$ scaling, i.e. rapidly increases with N when μ is small. This comes from the fact that there is a high probability to find inner particles with a large diffusion constant which, in turns, gives rise to a high 'pressure' exerted by the core of the cluster on its 'surface'.

In all cases, the averaged one-particle asymptotic density has been found; it can be written under a general form displaying the basic ingredients of the problem. For the right particle, one has

$$\langle p_N^{(1)}(x;t)\rangle \simeq N \exp\left[-\frac{N}{2}\langle 1-\Phi[x/(4Dt)^{1/2}]\rangle\right]\langle G(x,t)\rangle \tag{6.1}$$

where $\langle\cdots\rangle$ denotes averaging with the distribution $\rho(D)$ of the diffusion constants, Φ is the probability integral and G is the Gaussian distribution. For the central particle (N odd), one has

$$\langle p_{(N+1)/2}^{(1)}(x;t)\rangle \simeq \left(\frac{N}{2\pi^2 t}\right)^{1/2}\langle D^{-1/2}\rangle \exp\left[-N\langle D^{-1/2}\rangle^2\frac{x^2}{2\pi t}\right] \tag{6.2}$$

provided that the fractional moment $\langle D^{-1/2}\rangle$ exists and is finite. Otherwise, when $\rho \propto D^{\alpha-1}$ at small D with $\alpha \leqslant \frac{1}{2}$, $\langle p_{(N+1)/2}^{(1)}\rangle$ is of the form (see (4.10) for details)

$$\langle p_{(N+1)/2}^{(1)}(x;t)\rangle \simeq C|x|^{-(1-2\alpha)}\exp[-C'|x|^{4\alpha}]. \tag{6.3}$$

At large x, this gives a stretched exponential with an exponent in the range $]0,2]$, whereas the density diverges at $x=0$ as a power law ($\propto x^{-(2\alpha-1)}$); for the particular case $\alpha=\frac{1}{2}$, this singularity becomes logarithmic.

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