# Noise and determinism in diffusion

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It is well known that the study of stochastic process started from the Einstein [1] and Langevin [2] works on Brownian motion. Brownian motion (i.e. the erratic movement of a grains suspended in liquid) was observed by the botanist Robert Brown as early as in 1827. Being a botanist, Brown was interested in the motion as a possible manifestation of life. To this aim, he made a series of careful experiments which excluded the biological origin of the motion.

The Langevin mechanical model for Brownian motion is based on two key ingredients: a *deterministic* viscous drag and a *stochastic* force due to the impacts of the molecules. The drag can be written, assuming a spherical grain, as $6\pi\mu a\mathbf{v}$ (where $\mu$ is the dynamical viscosity of the fluid, $a$ the grain radius and $\mathbf{v}$ the grain velocity). The stochastic term will be denoted by $\eta$, which is assumed with zero mean and short correlated in time, and which represents the collisions of molecules on the grain.

The Langevin equation for Brownian motion is nothing but the Newton equation for the grain:

$$m\frac{d\mathbf{v}}{dt} = -6\pi a\mu\mathbf{v} + \eta \tag{1}$$

which, introducing the viscous relaxation time $\tau = m/(6\pi a\mu)$, can be written as

$$\frac{d\mathbf{v}}{dt} = -\frac{1}{\tau}\mathbf{v} + \frac{1}{m}\eta \tag{2}$$

By taking the scalar product of (2) with the grain position $\mathbf{r}$, averaging over many grains and assuming $\eta$ not correlated with position, one obtains

$$\frac{d^2}{dt^2}\langle r^2\rangle + \frac{1}{\tau}\frac{d}{dt}\langle r^2\rangle = 2\langle v^2\rangle \tag{3}$$

If the Brownian particle is in thermal equilibrium with fluid at temperature $T$ we have

$$\langle v^2\rangle = \frac{3kT}{m} \tag{4}$$

($k$ is the Boltzmann constant). Integrating twice in time with the appropriate initial conditions (at $t = 0$ we can suppose $r = 0$ without loosing generality) one finally get

$$\langle r^2(t) \rangle = \frac{6kT}{m} \tau^2 \left[ \frac{t}{\tau} - (1 - e^{-t/\tau}) \right] \tag{5}$$

The solution (5) contains two asymptotic regimes:

- $t \ll \tau$ the expansion of the exponential gives, at leading order,

$$\langle r^2(t) \rangle \simeq \frac{3kT}{m} t^2 \tag{6}$$

which is the ballistic regime, i.e. (6) is nothing but a complicate way to write $\mathbf{r} = \mathbf{v}t$;

- $t \gg \tau$ in this case one obtains the well known diffusive regime

$$\langle r^2(t) \rangle \simeq 6Dt \tag{7}$$

where $D = kT\tau/m = kT/(6\pi a \mu)$ is the diffusion coefficient.

The diffusion coefficient depends on the grain size, but it is usually very small also for microscopic grains. Considering, as an example, $a = 10^{-6}\, m$ in water at room temperature one gets $D \simeq 10^{-13}\, m^2/s$.

The reason for reporting the above very classic exercise, is only to stress the fact that diffusion (i.e. $\langle r^2 \rangle \sim t$) is obtained only asymptotically ($t \gg \tau$). This is a consequence of central limit theorem which assures Gaussian distributions and diffusive behavior in the limit of many independent collisions. The necessary, and sufficient, condition for observing diffusive regime is the existence of a finite correlation time (here represented by $\tau$) for the microscopic dynamics. Let us stress that this is the important ingredient for diffusion, and *not* a stochastic microscopic dynamics. We will see below that diffusion can arise even in completely deterministic systems.

In order to study more in detail the properties of diffusion, let us introduce the simplest model of Brownian motion, i.e. the one-dimensional random walk. The walker moves on a line making discrete jumps $v_i = \pm 1$ at discrete times. The position of the walker, started at the origin at $t = 0$, will be

$$R(t) = \sum_{i=1}^{t} v_i \tag{8}$$

Assuming equiprobability for left and right jumps (no mean motion), the probability that at time $t$ the walker is in position $x$ will be

$$p_t(R=x) = prob\left[\begin{array}{c}\frac{t-x}{2} steps - 1 \\ \frac{t+x}{2} steps + 1\end{array}\right] = \frac{1}{2^t}\left(\begin{array}{c} t \\ \frac{t+x}{2}\end{array}\right) \tag{9}$$

For large $t$ and $x$ (i.e. after many microscopic steps) we can use Stirling approximation and get

$$p_t(x) = \sqrt{\frac{t}{2\pi(t^2-x^2)}}\exp\left[-\frac{t+x}{2}\ln\frac{t+x}{2} - \frac{t-x}{2}\ln\frac{t-x}{2}\right] \tag{10}$$

The well known Gaussian distribution is recovered only in the core, i.e. for $x \ll t$. In this case from (10) we get

$$p_t(x) = \sqrt{\frac{1}{2\pi t}}\exp\left(-\frac{x^2}{2t}\right) \tag{11}$$

An important remark is that Gaussian distribution (11) is intrinsic of diffusion process, independent on the distribution of microscopic jumps: indeed only the first two moments of $v_i$ enter into expression (11). This is, of course, the essence of the central limit theorem. Following the above derivation, it is clear that this is true only in the core of the distribution. The far tails keep memory of the microscopic process and are, in general, not Gaussian. As an example, in Figure 1 we plot the pdf $p_t(x)$ at step $t = 100$ compared with the Gaussian approximation. Deviations are evident in the tails.

The Gaussian distribution (11) can be obtained as the solution of the diffusion equation which governs the evolution of the probability in time. This is the Fokker-Planck equation for the particular stochastic process. A direct way to relate the one-dimensional random walk to the diffusion equation is obtained by introducing the master equation, i.e. the time evolution of the probability [3]:

$$p_{t+1}(x) = \frac{1}{2}p_t(x-1) + \frac{1}{2}p_t(x+1)\,. \tag{12}$$

In order to get a continuous limit, we introduce explicitly the steps $\Delta x$ and $\Delta t$ and write

$$\frac{p_{t+1}(x) - p_t(x)}{\Delta t} = \frac{(\Delta x)^2}{2\Delta t}\frac{p_t(x+1) + p_t(x-1) - 2p_t(x)}{(\Delta x)^2}\,. \tag{13}$$

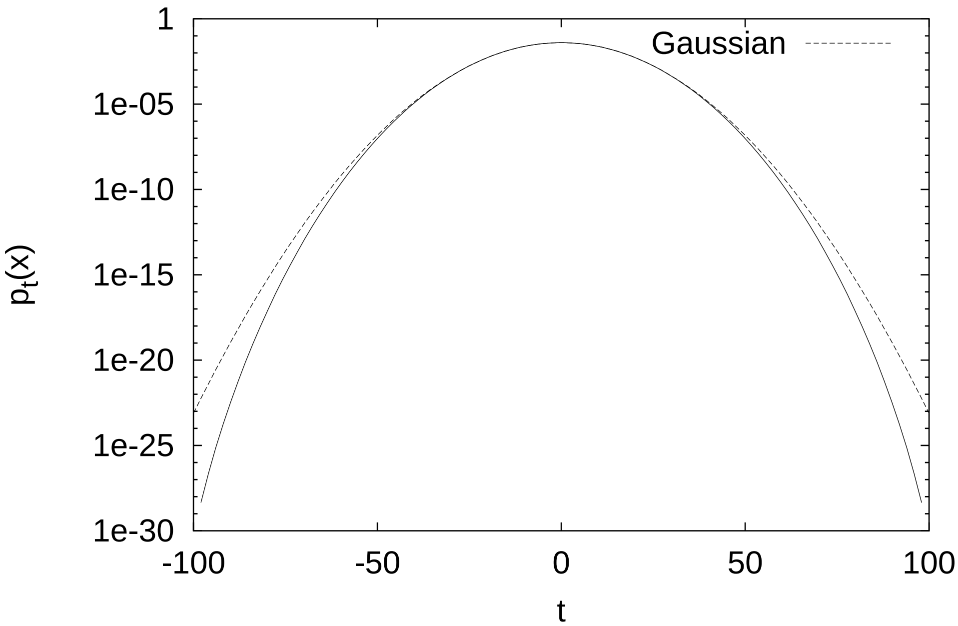


Figure 1: Probability distribution function of the one-dimensional random walk after $t = 100$ steps. The dashed line is the Gaussian distribution

Now, taking the limit $\Delta x, \Delta t \to 0$ in such a way that $(\Delta x)^2/\Delta t \to 2D$ (the factor 2 is purely conventional) we obtain the diffusion equation

$$\frac{\partial p(x,t)}{\partial t} = D \frac{\partial^2 p(x,t)}{\partial x^2} \, . \tag{14}$$

The way the limit $\Delta x, \Delta t \to 0$ is taken reflects the scaling invariance property of diffusion equation. The solution to (14) is readily obtained as

$$p(x,t) = \frac{1}{\sqrt{4\pi D t}} \exp\left(-\frac{x^2}{4Dt}\right) \, . \tag{15}$$

Diffusion equation (14) is here written for the probability $p(x,t)$ of observing a marked particle (a tracer) in position $x$ at time $t$. The same equation can have another interpretation, in which $p(x,t) = \theta(x,t)$ represents the concentration of a scalar quantity (marked fluid, temperature, pollutant) as function of time. The only difference is, of course, in the normalization.

As already stated time decorrelation is the key ingredient for diffusion. In the random walker model it is a consequence of randomness: the steps $v_i$ are random uncorrelated variables and this assures the applicability of central limit theorem. But we can have a finite time correlation and thus diffusion also without randomness. To be more specific, let us consider the following deterministic model (standard map [4]):

$$\begin{cases} \theta(t+1) = \theta(t) + J(t+1) \\ J(t+1) = J(t) + K \sin\theta(t) \end{cases} \tag{16}$$

The map is known to display chaotic behavior for $K > K_c \simeq 0.9716$. For

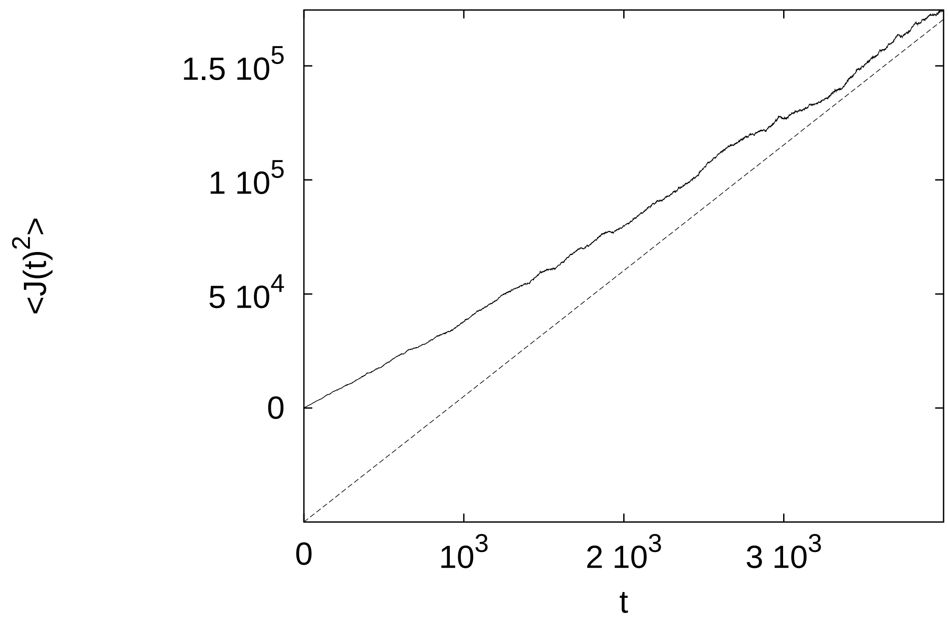


Figure 2: Square dispersion $\langle J(t)^2 \rangle$ for the standard map at $K = 10.5$. The dashed line is the RPA prediction.

large times, $J(t)$ is large and thus the angle $\theta(t)$ rotates rapidly. In this limit, we can assume that at each step $\theta(t)$ decorrelates and thus write

$$J(t)^2 = K^2 \left( \sum_{t'=1}^{t} \sin\theta(t') \right)^2 \simeq K^2 \langle \sin^2\theta \rangle t = 2Dt \tag{17}$$

The diffusion coefficient $D$, in the random phase approximation, is obtained by the above expression as $D_{RPA} = K^2/4$. In Figure 2 we plot a numerical simulation obtained with the standard map. Diffusive behavior is clearly visible at long time.

The two examples discussed above are in completely different classes: stochastic for the random walk (8) and deterministic for the standard map (16). Despite this difference in the microscopic dynamics, both lead to a macroscopic diffusion equation and Gaussian distribution. This demonstrates how diffusion equation is of general applicability.

The random walk model (8) can be extended to higher dimensions. It is clear that the macroscopic properties described above, i.e. diffusive behavior and Gaussian distribution, are independent on dimensionality. There are other macroscopic properties which, on the contrary, depend on the dimension of the space. One particularly important property is the ability of the walker to come back at the starting point (recurrence). It is clear that, increasing the space dimensionality, the walker has more opportunity to wander in the space without never return at the origin. Indeed, the following theorem holds [5, 6]

*one- and two-dimensional random walks are persistent, i.e. return with probability one to the origin; d-dimensional random walks with* $d \geq 3$ *are transient, i.e. there is a finite probability that the walker never return to the origin.*

The demonstration of the theorem is rather simple. Let us introduce the probability $u(t)$ that the walker is at the origin at time $t$ and $f(t)$ the probability that it is at the origin at $t$ for the first time (after $t = 0$). Persistence means

$$f \equiv \sum_{t=0}^{\infty} f(t) = 1 \tag{18}$$

while transient means $f < 1$ (we have defined $f(0) = 0$). It is not difficult to understand that

$$u(t) = f(t) + f(t-1)u(1) + f(t-2)u(2) + ... + f(1)u(t-1) \tag{19}$$

Defining $u(0) = 1$ and introducing the characteristic functions $F(s) = \sum_{t=0}^{\infty} s^t f(t)$ and $U(s) = \sum_{t=0}^{\infty} s^t u(t)$, multiplying (19) by $s^t$ and summing over $t$ we get

$$U(s) = 1 + U(s)F(s) \tag{20}$$

In this way persistence, i.e. $\lim_{s\to 1} F(s) = 1$ is equivalent to the condition

$$\lim_{s\to 1} U(s) = \sum_{t=0}^{\infty} u(t) = \lim_{T\to\infty} \sum_{t=0}^{T} u(t) = \infty \tag{21}$$

The latter equality express the obvious fact that if the process is persistent the walker passes infinitely often at the origin (and at any other point).

For large $t$ we can approximate $u(t)$ in (21) with the Gaussian distribution $u(t) \simeq p_t(0)$. In one-dimension from (11) we have

$$p_t(0) = \frac{1}{\sqrt{2\pi t}} \tag{22}$$

In generic dimension $d$, the pdf is still a Gaussian, product of $d$ Gaussian, and thus $p_t(0) \simeq 1/t^{d/2}$. From (21) we have, for $T \to \infty$,

$$\sum_{t=0}^{T} u(t) \sim \int_0^T \frac{dt}{t^{d/2}} \sim \begin{cases} t^{1/2} & \text{for} \quad d=1 \\ \ln T & \text{for} \quad d=2 \\ T^{-d/2+1} & \text{for} \quad d \geq 3 \end{cases} \tag{23}$$

and thus $U(s)$ diverges for $d \leq 2$. As an example, for $d = 3$ one gets [5] $U(1) \simeq 1.51$ which means by (20) that $f = 0.34$, i.e. there is about 66% probability that the walker never came back to the origin.

Now let us consider the more complex situation of dispersion in a non-steady fluid with velocity field $\mathbf{v}(\mathbf{x}, t)$. For simplicity will we consider incompressible flow (i.e. for which $\nabla \cdot \mathbf{v} = 0$) which can be laminar or turbulent, solution of Navier-Stokes equation or syntetically generated according to a given algorithm. In presence of $\mathbf{v}(\mathbf{x}, t)$, the diffusion equation (14) becomes the *advection-diffusion* equation for the concentration $\theta(\mathbf{x}, t)$

$$\frac{\partial \theta}{\partial t} + \mathbf{v} \cdot \nabla \theta = D \triangle \theta \,. \tag{24}$$

Equation (24) is linear in $\theta$ but nevertheless it can display very interesting and non trivial properties even in presence of simple velocity fields. In the following we will consider a very simple example of diffusion in presence of an array of vortices. The example will illustrate in a nice way the basic mechanisms and effects of interaction between deterministic ($\mathbf{v}$) and stochastic ($D$) components.

Let us remark that we will not consider here the problem of transport in turbulent velocity field. This is a very classical problem, with obvious and important applications, which has recently attracted a renewal theoretical interest as a model for understanding the basic properties of turbulence [7].

Before going into the example, let us make some general consideration. We have seen that in physical systems the molecular diffusivity is typically very small. Thus in (24) the advection term dominates over diffusion. This is quantified by the Peclet number, which is the ratio of the typical value of the advection term to the diffusive term

$$Pe = \frac{v_0 l_0}{D} \tag{25}$$

where $v_0$ is the typical velocity at the typical scale of the flow $l_0$. With $\tau_0 \simeq l_0/v_0$ we will denote the typical correlation time of the velocity.

The central point in the following discussion is the concept of *eddy diffusivity.* The idea is rather simple and dates back to the classical work of Taylor [8]. To illustrate this concept, let us consider a Lagrangian description of dispersion in which the trajectory of a tracer $\mathbf{x}(t)$ is given by

$$\frac{d\mathbf{x}(t)}{dt} = \mathbf{v}(\mathbf{x}(t), t) + \eta(t) \tag{26}$$

where each component of the molecular noise $\eta$ is a Gaussian white noise with zero mean and correlation

$$\langle \eta(t)\eta(t')\rangle = 2D\delta(t-t')\,. \tag{27}$$

Being interested in the limit $Pe \to \infty$, in the following we will assume $D = 0$.

Starting from the origin, $\mathbf{x}(0) = 0$, and assuming $\langle \mathbf{v}\rangle = 0$ we have $\langle \mathbf{x}(t)\rangle = 0$ for ever. The square displacement, on the other hand, grows according to

$$\frac{d}{dt}\langle \frac{1}{2}\mathbf{x}(t)^2\rangle = \langle \mathbf{x}(t)\cdot \mathbf{v}_L(t)\rangle = \int_0^t \langle \mathbf{v}_L(s)\cdot \mathbf{v}_L(t)\rangle ds \tag{28}$$

where we have introduced, for simplicity of notation, the Lagrangian velocity $\mathbf{v}_L(t) = \mathbf{v}(\mathbf{x}(t), t)$. Define the Lagrangian correlation time $\tau_L$ from

$$\int_0^\infty \langle \mathbf{v}_L(s)\cdot \mathbf{v}_L(0)\rangle ds = \langle \mathbf{v}_L(0)^2\rangle \tau_L \tag{29}$$

and assume that the integral converge so that $\tau_L$ is finite. From (28), for $t \gg \tau_L$ we get

$$\langle \mathbf{x}(t)^2\rangle = 2\tau_L \langle \mathbf{v}_L^2\rangle t \tag{30}$$

i.e. diffusive behavior with diffusion coefficient (eddy diffusivity) $D^E = \tau_L \langle \mathbf{v}_L^2 \rangle$.

This simple derivation shows, once more, that diffusion has to be expected in general in presence of a finite correlation time $\tau_L$. Coming back to the advection-diffusion equation (24), the above argument means that for $t \gg \tau_L$ we expect that the evolution of the concentration, for scales larger than $l_0$, can be described by an effective diffusion equation, i.e.

$$\frac{\partial \langle \theta \rangle}{\partial t} = D_{ij}^E \frac{\partial^2 \langle \theta \rangle}{\partial x_i \partial x_j} \tag{31}$$

The computation of the eddy diffusivity for a given Eulerian flow is not an easy task. It can be done explicitly only in the case of simple flows, for example by means of homogenization theory [9, 10]. In the general case it is relatively simple to give some bounds, the simplest one being $D^E \geq D$, i.e. the presence of a (incompressible) velocity field enhances large-scale transport. To be more specific, let us now consider the example of transport in a one-dimensional array of vortices (cellular flow) sketched in Figure 3. This simple two-dimensional flow is useful for illustrating the transport across barrier. Moreover, it naturally arises in several fluid dynamics contexts, such as, for example, convective patterns [11].

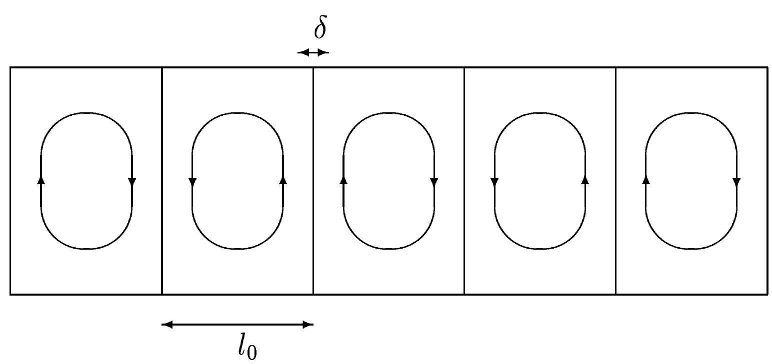


Figure 3: Cellular flow model. $l_0$ is the size of vortices, $\delta$ is the thickness of the boundary layer.

Let us denote by $v_0$ the typical velocity inside the cell of size $l_0$ and let $D$ the molecular diffusivity. Because of the cellular structure, particles inside a vortex can exit only as a consequence of molecular diffusion. In a characteristic vortex time $\tau_0 \simeq l_0/v_0$, only the particles in the boundary layer of thickness $\delta$ can cross the separatrix where

$$\delta^2 \simeq D\tau_0 \simeq D\frac{l_0}{v_0}\,. \tag{32}$$

These particles are ballistically advected by the velocity field across the vortex so they see a "diffusion coefficient" $l_0^2/\tau_0$. Taking into account that this fraction of particles is $\delta/l_0$ we obtain an estimation for the effective diffusion coefficient as

$$D^E \simeq \frac{\delta}{l_0}\frac{l_0^2}{\tau_0} \simeq \sqrt{Dl_0v_0} \simeq DPe^{1/2} \tag{33}$$

The above result, which can be made more rigorous, was confirmed by nice experiments made by Solomon and Gollub [11]. Because, as already stressed above, typically $Pe \gg 1$, one has from (33) that $D^E \gg D$. On the other hand, this result do not mean that molecular diffusion $D$ plays no role in the dispersion process. Indeed, if $D = 0$ there is not mechanism for the particles to exit from vortices.

Diffusion equation (31) is the typical long-time behavior in generic flow. There exist also the possibility of the so-called anomalous diffusion, i.e. when the spreading of particle do not grow linearly in time, but with a power law

$$\langle x^2(t)\rangle \simeq t^\nu \tag{34}$$

with $\nu \neq 1$. The case $\nu < 1$ corresponds to the so-called subdiffusive behavior (where formally $D^E = 0$) while $\nu > 1$ is called superdiffusion.

Superdiffusion arises when the Taylor argument for deriving (30) fails and formally $D^E \to \infty$. This can be due to two mechanisms: the divergence of $\langle \mathbf{v}_L^2\rangle$ (which is the case of *Lévy flights*), or the lack of decorrelation and thus $T_L \to \infty$ (*Lévy walks*). The second case is more physical and it is related to the existence of strong correlations in the dynamics, even at large times and scales.

One of the simplest examples of Lévy walks is the dispersion in a quenched random shear flow [12, 13]. The flow, sketched in Figure 4, is a superposition of strips of size $\delta$ of constant velocity $v_0$ with random directions.

Let us now consider a particle which moves according to (26). Because the velocity field is in the $x$ direction only, in a time $t$ the typical displacement in the $y$ direction is due to molecular diffusion only

$$\delta y \simeq \sqrt{Dt} \tag{35}$$

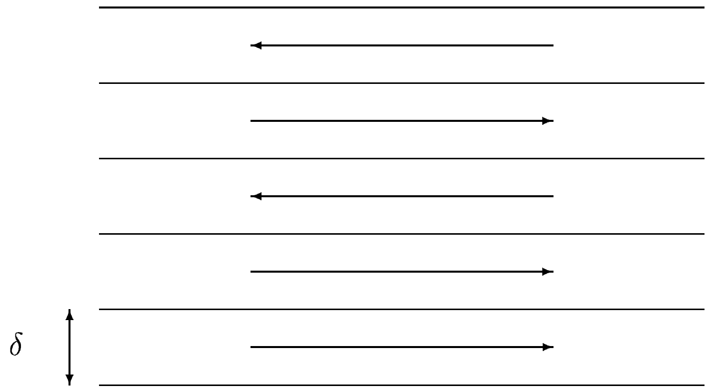


Figure 4: Random shear of $\pm v_0$ velocity in strips of size $\delta$

and thus in this time the walker visits $N = \delta y/\delta$ strips. Because of the random distribution of the velocity in the strips, the mean velocity in the $N$ strips is zero, but we may expect about $\sqrt{N}$ unbalanced strips (say in the right direction). The fraction of time $t$ spent in the unbalanced strips is $t\sqrt{N}/N$ and thus we expect a displacement

$$\delta x \simeq v_0 \frac{t}{\sqrt{N}} \,. \tag{36}$$

From (35) we have $N \simeq \sqrt{Dt}/\delta$ and finally

$$\langle \delta x^2 \rangle \simeq \frac{v_0^2 \delta}{\sqrt{D}} t^{3/2} \tag{37}$$

i.e. a superdiffusive behavior with exponent $\nu = 3/2$.

The origin of the anomalous behavior in the above example is in the quenched nature of the shear. This leads to an infinite decorrelation time for Lagrangian tracers and thus to a singularity in (30). We conclude this example by observing that for $D \to 0$ (37) gives $\langle \delta x^2 \rangle \to \infty$. This is not a surprise because in this case the motion is ballistic and the correct exponent becomes $\nu = 2$.

As it was in the case of standard diffusion, also in the case of anomalous diffusion the key ingredient is not randomness. Again, the standard map model (16) is known to show anomalous behavior for particular values of $K$. An example is plotted in Figure 5 for $K = 6.9115$ in which one find $\langle J(t)^2 \rangle \simeq t^{1.33}$.

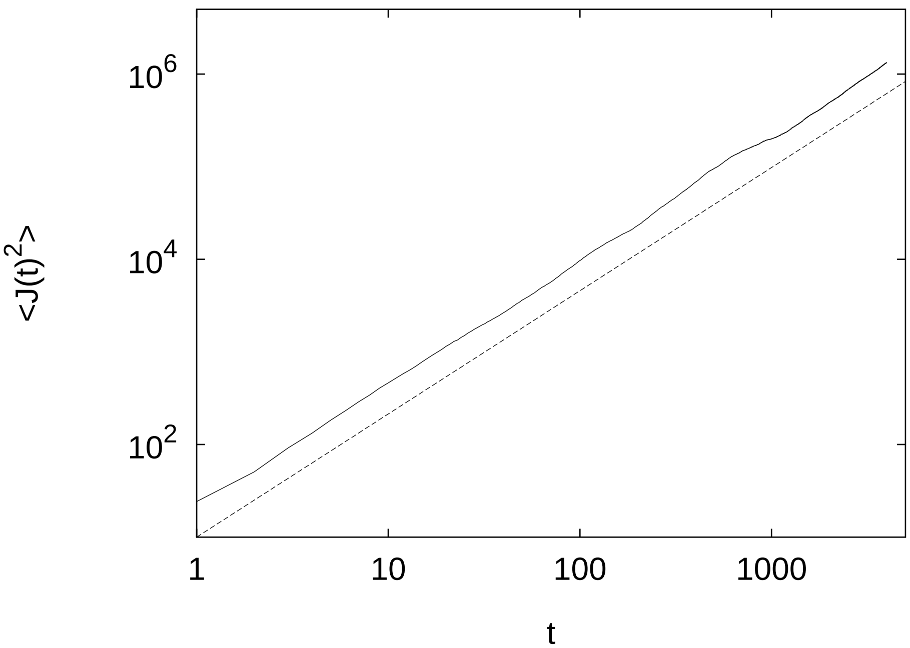


Figure 5: Square dispersion $\langle J(t)^2 \rangle$ for the standard map at $K = 6.9155$. The dashed line is $t^{1.33}$.

The qualitative mechanism for anomalous dispersion in the standard map can be easily understood: a trajectory of (16) for which $K \sin \theta^* = 2\pi m$ with $m$ integer, corresponds to a fixed point for $\theta$ (because the angle is defined modulo $2\pi$) and linear growth for $J(t)$ (ballistic behavior). It can be shown that the stability region of these trajectories in phase space decreases as $1/K$ [14, 6] and, for intermediate value of $K$, they play a important role in transport: particles close to these trajectories feel very long correlation times and perform very long jumps. The contribution of these trajectory, as a whole, gives the observed anomalous behavior.

Now, let us consider the cellular flow of Figure 3 as an example of subdiffusive transport. We have seen that asymptotically (i.e. for $t \gg l_0^2/D$) the transport is diffusive with effective diffusion coefficient which scales according to (33). For intermediate times $l_0/v_0 \ll t \ll l_0^2/D$, when the boundary layer structure has set in, one expects anomalous subdiffusive behavior as a consequence of fraction of particles which are trapped inside vortices [15]. A simple model for this problem is the comb model [13, 16]: a random walk on a lattice with comb-like geometry. The base of the comb represents the boundary layer of size $\delta$ around vortices and the teeth, of length $l_0$, represent the inner area of the convective cells. For the analogy with the flow of Figure 3 the teeth are placed at the distance $\delta = \sqrt{Dl_0/v_0}$ (32).

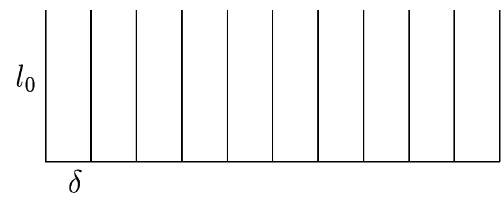

Figure 6: The comb model geometry

A spot of random walker (dye) is placed, at time $t = 0$, at the base of the comb. In their walk on the $x$ direction, the walkers can be trapped into the teeth (vortices) of dimension $l_0$. For times $l_0/v_0 \ll t \ll l_0^2/D$, the dye invades a distance of order $(Dt)^{1/2}$ along the teeth. The fraction $F(t)$ of active dye on the base (i.e. on the separatrix) decreases with time as

$$F(t) \simeq \frac{\delta}{(Dt)^{1/2}} \tag{38}$$

and thus the effective dispersion along the base coordinate $b$ is

$$\langle b^2(t) \rangle \simeq F(t)Dt \simeq \delta (Dt)^{1/2} \tag{39}$$

In the physical space the corresponding displacement will be

$$\langle x^2(t) \rangle \simeq \langle b^2(t) \rangle \frac{l_0}{\delta} \simeq l_0 (PeDt)^{1/2} \tag{40}$$

i.e. we obtain a subdiffusive behavior with $\nu = 1/2$.

The above argument is correct only for the case of free-slip boundary conditions. In the physical case of no-slip boundaries, one obtains a different exponent $\nu = 2/3$ [15]. The latter behavior has been indeed observed in experiments [17].

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