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Diffusion process in a flow

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We analyze circumstances under which the microscopic dynamics of particles which are driven by a forced, gradient-type flow can be consistently interpreted as a Markovian diffusion process. In the case of conservative forces (we adopt a smooth, deterministic version of ''stirring'' without any circular motion), the repulsive case only, $\vec{F}=\vec{\nabla}V$ with $V(\vec{x},t)$, bounded from below, is unquestionably admitted by the compatibility conditions. To allow for an attractive force, the process must induce a nonstandard compensating pressure term in the local (momentum) conservation law. In particular, that applies to a probabilistic interpretation of a compressible Euler flow with an arbitrary external (Newtonian) forcing. [S1063-651X(98)08701-7]

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Whenever one tries to analyze random perturbations that are either superimposed upon or intrinsic to a driving deterministic motion, quite typically a configuration space equation $\dot{\vec{x}}=\vec{v}(\vec{x},t)$ is invoked, which is next replaced by a formal infinitesimal representation of an Itô diffusion process $d\vec{X}(t)=\vec{b}(\vec{X}(t),t)dt+\sqrt{2D}d\vec{W}(t)$. Here $\vec{W}(t)$ stands for the normalized Wiener noise, and D for a diffusion constant. The dynamical meaning of $\vec{b}(\vec{x},t)$ relies on a specific diffusion input and its possible phase-space (e.g., Langevin) implementation, that entail a detailed functional relationship of $\vec{v}(\vec{x},t)$ and $\vec{b}(\vec{x},t)$, and justify such notions as: diffusion in an external force field, diffusion under various strains, diffusion along, against, or across the driving deterministic flow [1], and diffusion with shear effects [2]. The pertinent mathematical formalism corroborates both the Brownian motion of a single particle in flows of various origin and the diffusive transport of neutrally buoyant components in flows of the hydrodynamic type.

Our major issue is a probabilistic interpretation of various linear and nonlinear partial differential equations of physical relevance. Expressing this in more physical terms, we address an old-fashioned problem of ''how nonlinear'' and ''how time dependent'' the driving velocity field can be to yield a consistent stochastic diffusion process (or the Langevin-type dynamics). Another issue is to obtain hints about a possible non-deterministic origin of such fields [3].

Clearly, in random media that are statistically at rest, diffusion of single tracers or dispersion of pollutants are well described by the Fickian outcome of the molecular agitation, and also in the presence of external force fields (then in terms of Smoluchowski diffusions). On the other hand, it is of fundamental importance to understand how flows in a random medium (fluid, as example) affect dispersion. Such velocity fields are normally postulated as *a priori* given agents in the formalism, and their (molecular or else) origin is disregarded. Moreover, the force exerted upon tracers is usually viewed independently from the forcing (''stirring'') that might possibly perturb the random medium itself.

Except for suitable continuity and growth restrictions, necessary to guarantee the existence of the process $\vec{X}(t)$ governed by the Itô stochastic differential equation, the choice of the driving velocity field $\vec{v}(\vec{x},t)$ and hence of the related drift $\vec{b}(\vec{x},t)$ is normally (in typical physical problems) regarded as arbitrary (except for being ''not too nonlinear'').

The situation looks deceivingly simple [2], if we are (for example) interested in a diffusion process interpretation of passive tracers dynamics in the *a priori* given flow whose velocity field is a solution of the nonlinear partial differential equation, be it Euler, Navier-Stokes, Burgers or the like. An implicit assumption, that passively buoyant tracers in a fluid have a negligible effect on the flow, looks acceptable (basically in the case when the concentration of a passive component in a flow is small). Then one is tempted to view directly the fluid velocity field $\vec{v}(\vec{x},t)$ as the forward drift $\vec{b}(\vec{x},t)$ of the process, with the contaminant being diffusively dispersed along the streamlines.

Here apparent problems arise: irrespectively of a specific physical context and the phenomenology (as, e.g., the Boltzmann equation with its, as yet, not well understood Brownian motion approximation) standing behind the involved partial differential equations, some stringent mathematical criteria must be met to justify the diffusion process scenario, be it merely a crude approximation of reality.

That is, in general, the assumed nonlinear evolution rule for $\vec{v}(\vec{x},t)$ must be checked against the dynamics that is allowed to govern the space-time dependence of the forward drift field $\vec{b}(\vec{x},t)$ of the pertinent process [4], which is *not* at all arbitrary. The latter is ruled by standard consistency conditions that are respected by any Markovian diffusion process, and additionally by the rules of the forward and backward Itô calculus, [1,4], the mathematical input that is frequently ignored in the physical literature.

We have analyzed this issue before [5], where, as a by-product of the discussion, the forced Burgers dynamics

$$\partial_t \vec{v}_B + (\vec{v}_B \cdot \vec{\nabla})\vec{v}_B = D\triangle \vec{v}_B + \vec{\nabla}\Omega \tag{1}$$

and the diffusion-convection equation

$$\partial_t c + (\vec{v}_B \cdot \vec{\nabla}) c = D\triangle c \tag{2}$$

[originally, for the concentration $c(\vec{x},t)$ of a passive component in a flow], in the case of gradient velocity fields, were found to be generic to a Markovian diffusion process input. In that case the dynamics of the concentration (in general this notion *does not* coincide with the probability density) results from the stochastic process whose density $\rho(\vec{x},t)$ evolves according to the standard Fokker-Planck equation

$$\partial_t \rho = D \triangle \rho - \vec{\nabla} \cdot (\vec{b}\rho), \tag{3}$$

the forward drift solves an evolution equation

$$\partial_t \vec{b} + (\vec{b} \cdot \vec{\nabla})\vec{b} = -D \triangle \vec{b} + \vec{\nabla}\Omega, \tag{4}$$

and there holds

$$\vec{b} \doteq \vec{v}_B + 2D\vec{\nabla} \ \ln\rho. \tag{5}$$

The previous reasoning can be easily exemplified by considering the standard (neglecting external forces) Brownian motion with the initial (arbitrary, but sufficiently regular) density $\rho_0(\vec{x})$. Its evolution $\rho_0(\vec{x}) \to \rho(\vec{x},t)$ is implemented by the conventional heat kernel $p(\vec{y},s,\vec{x},t) = [4\pi D(t-s)]^{-1/2}\exp[-(\vec{x}-\vec{y})^2/4D(t-s)]$, where $\vec{x}$ and $\vec{y}$ stand for space variables, while t and s, $0 \leqslant s < t$, refer to respective time instants. The backward drift of the process (a solution of the unforced Burgers equation), is defined as follows: $\vec{v}_B(\vec{x},t) = -2D\vec{\nabla} \ \ln\rho$. The pertinent concentration dynamics is given by

$$c(\vec{x},t) = \int p_*(\vec{y},0,\vec{x},t)c_0(\vec{y})d^3y, \tag{6}$$

where $p_*(\vec{y},0,\vec{x},t) \doteq p(\vec{y},0,\vec{x},t)[\rho_0(\vec{y})/\rho(\vec{x},t)]$, and clearly refers to a tagged population of Brownian particles which belong to an overall diffusing Brownian ensemble. Indeed, if we arbitrarily decompose the density of the process into $\rho = \rho_1 + \rho_2$, and regard $\rho_1(\vec{x},t)$ as the density of a tagged Brownian population, then an appropriate definition of the concentration (effectively, we deal with the percentage of tagged particles in the generic flow) is

$$c(\vec{x},t) = \frac{\rho_1(\vec{x},t)}{\rho(\vec{x},t)}. \tag{7}$$

By inspection, one can check the validity of the diffusion-convection equation.

By combining intuitions which underly the self-diffusion description [6] with those appropriate for probabilistic solutions of the so-called Schrödinger boundary-data and next-interpolation problems [5,7,8], the above argument can be generalized to arbitrary conservatively forced diffusion processes, quite irrespectively of a physical context in which their usage can be justified.

Let us consider a density $\rho(\vec{x},t), t \geqslant 0$ of a stochastic diffusion process, solving the Fokker-Planck equation (3). For drifts that are gradient fields, the potential Ω in Eqs. (1) and (4) (*whatever* its functional form is), *must* allow for a representation formula, reminiscent of the probabilistic Cameron-Martin-Girsanov transformation

$$\Omega(\vec{x},t) = 2D\left[\partial_t \Phi + \frac{1}{2}\left(\frac{\vec{b}^2}{2D} + \vec{\nabla} \cdot \vec{b}\right)\right], \tag{8}$$

where $\vec{b}(\vec{x},t) = 2D\vec{\nabla}\Phi(\vec{x},t)$.

For the existence of the Markovian diffusion process with the forward drift $\vec{b}(\vec{x},t)$, we must resort to potentials $\Omega(\vec{x},t)$ that are *not* completely arbitrary functions. Technically [7], the minimal requirement is that the admissible potential is bounded from below. This restriction will have profound consequences for our further discussion of diffusion in a flow.

If we set $\rho = \rho_1 + \rho_2$ again, and demand that $\rho_1 \neq \rho$ solves the Fokker-Planck equation with the very same drift $\vec{b}(\vec{x},t)$, as ρ does, then as a necessary consequence of the general formalism [5,7], the concentration $c(\vec{x},t) = \rho_1(\vec{x},t)/\rho(\vec{x},t)$, solves an associated diffusion-convection equation $\partial_t c + (\vec{v}_B \cdot \vec{\nabla})c = D \triangle c$. Here, the flow velocity $\vec{v}_B(\vec{x},t)$ coincides with the backward drift of the generic diffusion process with the density $\rho(\vec{x},t)$.

We should clearly discriminate between forces whose effect is a ''stirring'' of the random medium and those acting selectively on diffusing particles, with a negligible effect on the medium itself. For example, the traditional Smoluchowski diffusion processes in conservative force fields are considered in random media that are statistically at rest. Following the standard (phase-space, Langevin) methodology, let us set $\vec{b}(\vec{x}) = (1/\beta)\vec{K}(\vec{x})$, where β is a (large) friction coefficient and $\vec{K}$ represents an external Newtonian force per unit of mass (e.g., an acceleration) that is of gradient from $\vec{K} = -\vec{\nabla}U$. Then the effective potential Ω reads

$$\Omega = \frac{\vec{K}^2}{2\beta^2} + \frac{D}{\beta}\vec{\nabla} \cdot \vec{K}, \tag{9}$$

and the only distinction between the attractive or repulsive cases can be read out from the term $\vec{\nabla} \cdot \vec{K}$. For example, the harmonic attraction or repulsion $\vec{K} = \mp \alpha \vec{x}$, $\alpha > 0$ would give rise to a harmonic repulsion, if interpreted in terms of $\vec{\nabla}\Omega$, in view of $\Omega = (\alpha^2/2\beta^2)\vec{x}^2 \mp 3D\alpha/\beta$. The innocent looking $\mp 3D(\alpha/\beta)$ renormalization of the quadratic function gives rise to entirely different diffusion processes, with an equilibrium measure arising in case of $U(\vec{x}) = +(\alpha/2)\vec{x}^2$ only.

The situation would not change under the incompressibility condition (cf. also the probabilistic approaches to the Euler, Navier-Stokes, and Boltzmann equations [9]). Following Townsend's [2] early investigation of the diffusion of heat spots in isotropic turbulence, we may choose $U(\vec{x}) = (\alpha/2)x^2 - (\alpha/4)(y^2 + z^2)$, which implies $\vec{\nabla} \cdot \vec{K} = 0$. Then, $\Omega(\vec{x}) = (\alpha^2/2\beta^2)[x^2 + \frac{1}{4}(y^2 + z^2)]$; hence the repulsive Ω is produced again in the equation of motion characterizing a stationary diffusion in an incompressible fluid: div $\vec{v} = 0$, $\vec{b} = \vec{b}_* = \vec{v} \to (\vec{v} \cdot \nabla)\vec{v} = \vec{\nabla}\Omega$. By formally changing the sign of Ω, we would arrive at the attractive variant of the problem; that is, however, *incompatible* with the diffusion process scenario in view of the unboundedness of $-\Omega$ from below.

We have thus arrived at the major point of our discussion: *a priori*, there is no way to incorporate the attractive forces which affect (drive) the flow and nonetheless generate a consistent diffusion-in-a-flow transport. Clearly, there is no reason to exclude the attractive variants of the potential Ω from considerations, since the deterministic motion is consistent with them. However, if the diffusion is to be involved, we can save the situation only by incorporating (hitherto unconsidered) ''pressure'' term effects as suggested by the general form of the compressible Euler ($\vec{F}=-\vec{\nabla}V$ stands for external volume forces, and ρ for the fluid density that *itself* undergoes a stochastic diffusion process) equation

$$\partial_t \vec{v}_E+(\vec{v}_E\cdot\vec{\nabla})\vec{v}_E=\vec{F}-\frac{1}{\rho}\vec{\nabla}P, \tag{10}$$

or the incompressible [9] Navier-Stokes equation

$$\partial_t \vec{v}_{\rm NS}+(\vec{v}_{\rm NS}\cdot\vec{\nabla})\vec{v}_{\rm NS}=\frac{\nu}{\rho}\triangle\vec{v}_{\rm NS}+\vec{F}-\frac{1}{\rho}\vec{\nabla}P, \tag{11}$$

both to be compared with Eqs. (1) and (4), that set dynamical constraints for respectively backward and forward drifts of a Markovian diffusion process.

Notice that the acceleration term $\vec{F}$ in Eqs. (10) and (11) is normally regarded as arbitrary, while the corresponding term $\vec{\nabla}\Omega$ in Eqs. (1) and (3) involves a bounded from below function $\Omega(\vec{x},t)$. Since, in the case of gradient velocity fields, the dissipation term in the incompressible Navier-Stokes equation (11) identically vanishes, we should concentrate on analyzing the possible ''forward drift of the Markovian process'' meaning of the Euler flow with the velocity field $\vec{v}_E$ [Eq. (10)].

At this point it is useful, at least on formal grounds, to invoke the standard phase-space argument that is valid for a Markovian diffusion process taking place in a given flow $\vec{v}(\vec{x},t)$ with as yet unspecified dynamics or physical origin. We account for an explicit force exerted upon diffusing particles, while not necessarily directly affecting the driving flow itself. That is [2,4], for infinitesimal increments of phase-space random variables, we set

$$d\vec{X}(t)=\vec{V}(t)dt,$$
$$d\vec{V}(t)=\beta[\vec{v}(\vec{x},t)-\vec{V}(t)]dt+\vec{K}(\vec{x})dt+\beta\sqrt{2D}d\vec{W}(t). \tag{12}$$

Following the leading idea of the Smoluchowski approximation, we assume that β is large, and consider the process for times significantly exceeding β^{-1}. Then an appropriate choice of the velocity field $\vec{v}(\vec{x},t)$ (boundedness and growth restrictions are involved) may in principle guarantee [4] the convergence of the spatial part $\vec{X}(t)$ of process (12) to the Itô diffusion process with infinitesimal increments (where the force $\vec{K}$ effects can be safely ignored if we are interested mostly in the driving motion)

$$d\vec{X}(t)=\vec{v}(\vec{x},t)dt+\sqrt{2D}d\vec{W}(t). \tag{13}$$

However, one cannot blindly insert in the place of the forward drift $\vec{v}(\vec{x},t)$ any of the previously considered bulk velocity fields, without going into apparent contradictions. Specifically, Eq. (4) with $\vec{v}(\vec{x},t)\leftrightarrow\vec{b}(\vec{x},t)$ must be valid.

By resorting to velocity fields $\vec{v}(\vec{x},t)$ which obey $\triangle\vec{v}(\vec{x},t)=0$, we may pass from Eq. (4) to an equation of the Euler form, Eq. (10), provided Eq. (8) holds true, and then the right-hand-side of Eq. (4) involves a bounded from below effective potential Ω.

An additional requirement is that

$$\vec{F}-\frac{1}{\rho}\vec{\nabla}P\doteq\vec{\nabla}\Omega. \tag{14}$$

Clearly, in the case of a constant pressure, we are left with the dynamical constraint ($\vec{b}\leftrightarrow\vec{v}_E$),

$$\partial_t\vec{b}+(\vec{b}\cdot\vec{\nabla})\vec{b}=\vec{F}=\vec{\nabla}\Omega, \tag{15}$$

combining simultaneously the Eulerian fluid and the Markov diffusion process inputs, *if and only if* $\vec{F}$ is repulsive, e.g. $-V(\vec{x},t)$ is bounded from below. Quite analogously, by setting $\vec{F}=\vec{0}$, we would obtain a constraint on the admissible pressure term, in view of

$$\partial_t\vec{b}+(\vec{b}\cdot\vec{\nabla})\vec{b}=-\frac{1}{\rho}\vec{\nabla}P=\vec{\nabla}\Omega. \tag{16}$$

In both cases of Eqs. (15) and (16), the effective potential Ω must respect the functional dependence (on a forward drift and its potential) prescription (8). In addition, the Fokker-Planck equation (3) with the forward drift $\vec{v}_E(\vec{x},t)\doteq\vec{b}(\vec{x},t)$ must be valid for the density $\rho(\vec{x},t)$.

To our knowledge, in the literature there is only one known specific class of Markovian diffusion processes that would render the right-hand side of Eq. (10) repulsive but nevertheless account for the troublesome Newtonian accelerations; e.g., those of the form $-\vec{\nabla}V$, with $+V$ bounded from below. Such processes have forward drifts that, for each suitable, bounded from below function $V(\vec{x})$, solve the nonlinear partial differential equation

$$\partial_t\vec{b}+(\vec{b}\cdot\vec{\nabla})\vec{b}=-D\triangle\vec{b}+\vec{\nabla}(2Q-V), \tag{17}$$

with the compensating pressure term

$$Q\doteq 2D^2\frac{\triangle\rho^{1/2}}{\rho^{1/2}}\doteq\frac{1}{2}\vec{u}^2+D\vec{\nabla}\cdot\vec{u}, \tag{18}$$

$$\vec{u}(\vec{x},t)=D\vec{\nabla}\ \ln\rho(\vec{x},t).$$

A discussion can be found in Refs. [4,5,7,8].

Clearly, we have

$$\vec{F}=-\vec{\nabla}V,\quad \vec{\nabla}2Q=-\frac{1}{\rho}\vec{\nabla}P, \tag{19}$$

where

$$P(\vec{x},t)=-2D^2\rho(\vec{x},t)\triangle\ \ln\rho(\vec{x},t). \tag{20}$$

Effectively, P is here defined up to a time-dependent constant. Another admissible form of the pressure term reads (summation convention is implicit)

$$\frac{1}{\rho}\vec{\nabla}_k[\rho(2D^2\partial_j\partial_k)\ln\rho]=\vec{\nabla}_j(2Q). \qquad (21)$$

If we consider a subclass of processes for which the dissipation term identically vanishes (a number of examples can be found in Refs. [7]),

$$\triangle\vec{b}(\vec{x},t)=0, \qquad (22)$$

Eq. (17) takes a conspicuous Euler form (10), $\vec{v}_E\leftrightarrow\vec{b}$.

Let us notice that Eqs. (20) and (21) provide for a generalization of the more familiar, equation of state $P\sim\rho$, thermodynamically motivated and suited for ideal gases and fluids. In the case of density fields for which $-\triangle\ln\rho\sim$const, the standard relationship between the pressure and the density is reproduced. In the case of density fields obeying $-\triangle\ \ln\rho=0$, we are left with at most a purely time-dependent or constant pressure. Pressure profiles may be highly complex for arbitrarily chosen initial density and/or the flow velocity fields.

To conclude the present discussion, let us invoke Refs. [9,6,7]. The problem of a diffusion process interpretation of various partial differential equations is known to extend beyond the original parabolic equations setting, to general nonlinear velocity field equations. On the other hand, the nonlinear Markov jump processes associated with the Boltzmann equation, in the hydrodynamic limit, are believed to imply either an ordinary deterministic dynamics with the velocity field solving the Euler equation, or a diffusion process whose drift is a solution of the incompressible Navier-Stokes equation (in general, without our curl$\vec{v}=0$ restriction), [6,9]. The case of *arbitrary* external forcing has never been satisfactorily solved.

Our reasoning went otherwise. We asked for the admissible space-time dependence of general velocity fields that are to play the role of forward drifts of Markovian diffusion processes, and at the same time can be met in physically signicant contexts. Therefore various forms of the Fokker-Planck equation for tracers driven by familiar compressible velocity fields were discussed.

Our finding is that solutions of the compressible Euler equation are appropriate for the description of the general nondeterministic (e.g., random and Markovian) dynamics running under the influence of both attractive and repulsive stirring forces, and refer to a class of Markovian diffusion processes orginally introduced in Refs. [4,7,3]. That involves only the gradient velocity fields (a couple of issues concerning the curl$\vec{b}\neq0$ velocity fields and their nonconservative forcing were raised in Ref. [5]).

Remark: Let us stress that a standard justification of the hydrodynamic limit for a tracer particle invokes a Brownian particle in an equilibrium fluid. An issue of how much the tracer particle disturbs the fluid (random medium) locally, and how far away from the tracer particle the thermal equlibrium conditions regain their validity [6], is normally disregarded. Moreover, in the standard derivation of local conservation laws from the Boltzmann equation, the forcing term on the right-hand side of the Euler or Navier-Stokes equation up to scalings does coincide with the force acting on each single particle comprising the system. Thus, in this framework, there is no room for any discrimination between forces acting upon tagged particles and those perturbing the spatial flows (once on the level of local averages).

Quite on the contrary, the force term in the Kramers equation and that appearing in the related local conservation law for the forward drift or for the current velocity of the diffusion process are known *not* to coincide in general. Typically, the action of an external force is confined to diffusing (tagged) particles with *no* global or local effect on the surrounding random medium, cf. standard derivations of the Smoluchowski equation. This feature underlies problems with the diffusion process interpretation of general partial differential equations governing physically relevant velocity fields. Specifically, any external intervention (forcing) upon a stochastically evolving (in the diffusion process approximation) system gives rise to a perturbation of local flows, which seldom can be analyzed as forcing any definite type on the molecular level. The Smoluchowski theory is a notable exception here, but in this one has no room for genuine flows and velocity field profiles which are generated in the random medium.

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