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Drifts versus forces: the Ehrenfest theorem for Markovian diffusions

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Abstract

Following Stratonovich, we make a general analysis of the external force manifestations in the dynamics of Markov diffusion processes. The transformation connecting transition densities of the process with the respective (unique) Feynman–Kac kernels induces the local field of accelerations, which equals the gradient of the Feynman–Kac potential and enters the straightforward analog of the Ehrenfest theorem. The latter encompasses not only Nelson's or Zambrini's diffusions but also the familiar non-equilibrium statistical physics processes, like the standard Brownian motion in the external force field (Smoluchowski diffusions).

Let us consider [1,2] a Markovian diffusion $X(t)$ in R^1 (space dimension one is chosen for simplicity) confined to the time interval $t\in[0,T]$, with the point of origin $X(0)=x_0$. The individual (most likely, sample) particle dynamics is symbolically encoded in the Itô stochastic differential equation, which we choose in the form

$$\mathrm{d}X(t)=b(X(t),t)\,\mathrm{d}t+\sqrt{2D}\,\mathrm{d}W(t)\ , \tag{1}$$

with $X(0)=x_0$, D a diffusion coefficient, $W(t)$ a normalised Wiener noise, and where the drift field $b(x, t)$ is assumed to guarantee the existence and uniqueness of solutions $X(t)$. They are then non-explosive, i.e. the sample paths of the process cannot escape to spatial infinity in a finite time. The rules of Itô stochastic calculus imply that the transition probability density of the process (its law of random displacements) $p(y, s, x, t)$, $s\leqslant t$, solves the Fokker–Planck equation with respect to x, t,

$$\partial_t p=D\triangle_x p-\nabla_x(bp)\ ,$$
$$\lim_{t\to s} p(y,s,x,t)=\delta(x-y),\quad s\leqslant t\ . \tag{2}$$

Following Stratonovich [3] let us transform (2) by means of a substitution

$$p(y,s,x,t)=h(y,s,x,t)\,\frac{\exp\Phi(y,s)}{\exp\Phi(x,t)}\ , \tag{3}$$

which under an assumption that $b(x, t)$ is the gradient field,

$$b(x,t)=-2D\nabla\Phi(x,t)\quad\Rightarrow$$
$$\tfrac{1}{2}(b^2/2D+\nabla b)=D[(\nabla\Phi)^2-\triangle\Phi] \tag{4}$$

allows one to replace (2) by the generalised diffusion equation

$$\partial_t h=D\triangle_x h-\{-\partial_t\Phi+D[-\triangle\Phi+(\nabla\Phi)^2]\}h\ ,$$
$$\lim_{t\to s} h(y,s,x,t)=\delta(x-y)\ . \tag{5}$$

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Its solution (to be strictly positive) can be represented in terms of the Feynman–Kac (Cameron–Martin) formula, which integrates contributions $\exp[-\int_s^t \Omega(x,u)\,\mathrm{d}u/2mD]$ from the *auxiliary* potential $\Omega(x,t)$,

$$\Omega/m = 2D\{-\partial_t\Phi + D[-\triangle\Phi + (\nabla\Phi)^2]\}$$
$$= -2D\partial_t\Phi + D\nabla b + \tfrac{1}{2}b^2\,, \qquad (6)$$

with respect to the conditional [4] Wiener measure

$$h(y,s,x,t) = \int \exp\left(-\frac{1}{2mD}\int_s^t \Omega(x,u)\,\mathrm{d}u\right)\mathrm{d}W[y|x]\,. \qquad (7)$$

Since, as a consequence of (1), (2), $h(y,s,x,t)$ must be strictly positive, we recognize it as the integral kernel of the dynamical semigroup operator

$$\exp\left(-\frac{1}{2mD}\int_s^t (2mD^2\triangle - \Omega)\,\mathrm{d}u\right),$$

with the appropriate restrictions (continuity, boundedness from below) on $\Omega(x,t)$, and hence Φ implicitly. All that is valid under an assumption that the process respects the natural [16] boundary data where the density of the diffusion (hitherto not explicitly introduced) vanishes, with boundary points at infinity.

Given $p(y,s,x,t)$, we can utilise the Itô formula [1,2,5,8] which for any smooth function of the random variable states that its forward time derivative in the conditional mean reads

$$\lim_{\Delta t\downarrow 0}\frac{1}{\Delta t}\left(\int p(x,t,y,t+\Delta t) f(y,t+\Delta t)\,\mathrm{d}y - f(x,t)\right)$$
$$= (D_+ f)(X(t),t) = (\partial_t + b\nabla + D\triangle) f(X(t),t)\,, \qquad (8)$$

with $X(t)=x$. Then, for the second forward derivative (in the conditional mean) of the diffusion process $X(t)$, in virtue of (4), (6) we have

$$(D_+^2 X)(t) = (D_+ b)(X(t),t)$$
$$= (\partial_t b + b\nabla b + D\triangle b)(X(t),t)$$
$$= \frac{1}{m}\nabla\Omega(X(t),t)\,. \qquad (9)$$

This formula is a precise embodiment of the second Newton law (in the conditional mean) governing *all* Markovian diffusions consistent with (1)–(7), albeit it is "Euclidean looking". The *auxiliary potential $\Omega(x,t)$ plays here the role of the corresponding force field potential*: a somewhat surprising outcome for anyone familiar with the large friction (Smoluchowski) limit of the phase space Brownian motion, however definitely [15] an inevitable one.

Our previous discussion refers to the individual (sample) features of a particle propagation in contact with the randomly perturbing environment: the Wiener noise is superimposed on the systematic field $b(x,t)$ of local drifts. By attributing an initial probability distribution $\rho_0(x)=\rho(x,0)$ to the random variable $X(t)$, we pass to the *statistical ensemble* (hence collective) analysis. Because of (1), (2) the forward dynamics of the density $\rho(x,t)=\int\rho_0(y)p(y,0,x,t)\,\mathrm{d}y$ is uniquely defined. The microscopic law of random displacements $p(y,s,x,t)$, $s\leqslant t$, generates all possible random propagation scenarios (sample paths) from each chosen point of origin $X(0)=x_0$, for the flight duration times $t>0$. The statistical outcome (prediction about the most likely future of an individual particle) is casually considered as independent of the assumed probability distribution $\rho(x_0)$. However, once introduced, this density sets a statistical correlation between individual members of the ensemble, even if there are no mutual interactions to be accounted for. An interesting *ensemble* characterisation of the random motion is here possible by introducing (for Markov processes only) the transition density $p_*(y,s,x,t)$,

$$\rho(x,t)p_*(y,s,x,t) = p(y,s,x,t)\rho(y,s)\,, \qquad (10)$$

which allows one to trace back the most likely statistical past of particles *conditioned to comprise the evolving statistical ensemble* with the distribution $\rho(x,t)$. One should consult Refs. [6,7] to realize that any realistic diffusion (the free Brownian motion included!) admits (10): it has nothing to do with a physically realizable reversal of the generally irreversible process. In this case [5,8] we can define the *backward* time derivative of the process $X(t)$ (now supplemented by the distribution $\rho(x,t)$), which in the jointly conditional and ensemble [6,7] mean reads

$$\lim_{\Delta t \downarrow 0} \frac{1}{\Delta t}\left(x - \int p_*(y, t-\Delta t, x, t) y \, dy\right)$$
$$= (D_- X)(t) = b_*(X(t), t) , \quad (11)$$

with the corresponding Itô formula for $f(x, t)$,

$$(D_- f)(X(t), t)$$
$$= (\partial_t + b_* \nabla - D\triangle) f(X(t), t) . \quad (12)$$

Because of (10) the drifts $b(x, t)$ and $b_*(x, t)$ are *not* mutually independent, and indeed [5,8,9] on domains free of nodes (ρ vanishing at the boundaries) we have

$$b_*(x, t) = b(x, t) - 2D\nabla \ln \rho(x, t) . \quad (13)$$

Consequently, the current velocity [5] field

$$v(x, t) = \tfrac{1}{2}(b + b_*)(x, t) \quad (14)$$

can be viewed as the one supplementary to $\rho(x, t)$ (it induces the osmotic velocity [5] notion $u(x, t) = D\nabla \ln \rho(x, t) = \frac{1}{2}(b - b_*)$ in turn) characteristic of the stochastic flows. This time elevated to the macroscopic (statistical ensemble) level. In terms of the local velocity fields $u(x, t)$, $v(x, t)$, both of which are gradient fields, one can explicitly [10–12] demonstrate that

$$(D_+^2 X)(t) = \partial_t v + v\nabla v + \frac{1}{m}\nabla Q = (D_-^2 X)(t) ,$$

$$Q(x, t) = 2mD^2 \frac{\Delta \rho^{1/2}}{\rho^{1/2}} , \quad (15)$$

which extends the identity (9) to $(D_-^2 X)(t)$. With the density $\rho(x, t)$ in hands we can evaluate the mean (ensemble expectation) values of (15) and (9),

$$E[(D_+^2 X)(t)] = E[(D_-^2 X)(t)]$$
$$= \frac{1}{m} E[\nabla \Omega(X(t), t)] , \quad (16)$$

where because of (cf. the original version of the Ehrenfest theorem [13,14] in quantum mechanics, which exploits the previously mentioned property that the probability density vanishes at the boundaries of the integration volume)

$$E[\nabla Q(X(t), t)] = 0 \quad (17)$$

a classical Liouville equation in the mean holds, with the "Euclidean looking" potential (in view of the absence of a minus sign)

$$E[(\partial_t v + v\nabla v)(X(t), t)]$$
$$= \frac{1}{m} E[(\nabla \Omega)(X(t), t)] . \quad (18)$$

On the other hand, in virtue of the continuity equation, we have

$$E[X(t)] = \int x\rho(x, t) \, dx \quad \Rightarrow$$
$$\frac{d}{dt} E[X(t)] = \tfrac{1}{2}(E[D_+ X] + E[D_- X])$$
$$= E[v(X(t), t)] , \quad (19)$$

and furthermore (see also Ref. [15])

$$\frac{d^2}{dt^2} E[X(t)] = \frac{d}{dt} E[v(X(t), t)]$$
$$= E[(\partial_t v + v\nabla v)(X(t), t)]$$
$$= \frac{1}{m} E[\nabla \Omega(X(t), t)] . \quad (20)$$

Hence the "Euclidean looking" second Newton law is found to be respected by the diffusion process (1) both in the conditional ((9)) and the ensemble ((15), (20)) mean.

Notice that the auxiliary potential in the form $\Omega = 2Q - V$ where V is any Rellich class (to allow for the Feynman–Kac formula for the semigroup kernel) representative, defines drifts of Nelson's diffusions, for which $E[\nabla Q] = 0 \Rightarrow E[\nabla \Omega] = -E[\nabla V]$, i.e. the "standard looking" form of the second Newton law in the mean arises.

Our previous discussion associates an a priori given drift (control) field $b(x, t)$, $t \in [0, T]$, with a potential $\Omega(x, t)$. Clearly, we encounter here a fundamental problem of what is to be interpreted by a physicist (external observer) as the external force field manifestation in the diffusion process. Let us invert our previous reasoning and take not $b(x, t)$ but $\Omega(x, t)$, $t \in [0, T]$, to be given a priori as a *primary dynamical control* for the Markovian diffusion (1), (2), which in principle we are capable to manipulate (the role attributed to the external observer). Then we shall say that the diffusion respects the second Newton law in the conditional mean, if

$$(D_+^2 X)(t) = \frac{1}{m} \nabla \Omega(X(t), t) \tag{21}$$

holds true.

The evolution in time of the gradient drift field $b(x, t)$ and that (given a priori) of $\Omega(x, t)$ are *compatible* if

$$\partial_t b + b\nabla b + D\triangle b = \frac{1}{m}\nabla\Omega\,,$$

$$b_0(x) = b(x, 0)\,. \tag{22}$$

It is a *sufficient* compatability condition, which allows one to derive the drift dynamics from that of $\Omega(x, t)$. In the time-independent case there is no real freedom in the choice of the initial Cauchy data for Eq. (22), and an identity $\Omega_0(x) = m(D\nabla b_0 + \frac{1}{2} b_0^2)(x) = \Omega(x, 0)$ must be satisfied.

Eq. (22) sets a well defined Cauchy problem for $b(x, t)$ in terms of $\Omega(x, t)$. If we associate an initial probability distribution $\rho_0(x)$ with $X(0)$, then our (sufficient) compatability condition (22) can be *equivalently* (!) written as the coupled Cauchy problem

$$\partial_t \rho = -\nabla(\rho v), \quad \partial_t v + v\nabla v = \frac{1}{m}\nabla(\Omega - Q)\,,$$

$$\rho_0(x) = \rho(x, 0), \quad v_0(x) = v(x, 0)\,, \tag{23}$$

where $b_0(x) = v_0(x) + D\nabla \ln \rho_0(x)$, with the initial data essentially unrestricted, except for the time-independent case.

Remark 1. One should not be misled by the seemingly complicated form of the nonlinear coupled Cauchy problem (23). It is precisely Eq. (22) which guarantees its solvability. Indeed, in virtue of the standard path integral identity [1]

$$p(y, s, x, t) = \lim_{\Delta t \downarrow 0} \int \mathrm{d}z_1 \ldots \int \mathrm{d}z_n \, (4\pi D\Delta t)^{-n/2}\,,$$

$$\exp\left(-\frac{1}{4\pi D\Delta t} \sum_{k=0}^{n-1} [z_{k+1} - z_k - b(z_k, t_k)\Delta t]^2 \right),$$

$$\Delta t = \frac{t-s}{n}, \quad z_0 = y, \quad z_n = x, \quad t_0 = s, \quad t_n = t\,, \tag{24}$$

it suffices to know the time development of the drift $b(x, t)$ to have uniquely specified the time evolution of $\rho(x, t) = \int p(y, s, x, t)\rho(y, s)\,\mathrm{d}y$, once $\rho_0(x)$ is given.

Remark 2. Since

$$p(y, s, x, t) = \lim_{\Delta t \downarrow 0} \int \mathrm{d}z_1 \ldots \int \mathrm{d}z_n \prod_{k=0}^{n-1} p(z_k, t_k, z_{k+1}, t_{k+1})\,, \tag{25}$$

we can perform the Stratonovich substitution (3) for each entry separately, and observe [3] that

$$p(y, s, x, t) = \exp[\Phi(y, s) - \Phi(x, t)] \times \lim_{\Delta t \downarrow 0} \int \mathrm{d}z_1 \ldots \int \mathrm{d}z_n \prod_{k=0}^{n-1} h(z_k, t_k, z_{k+1}, t_{k+1})\,. \tag{26}$$

The semigroup composition property is here clearly seen. It in turn justifies the procedures of Refs. [10–12].

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Appendix. Hydrodynamic representation of Markov diffusions

At this point it seems instructive to comment on the essentially hydrodynamical features (compressible fluid/gas case) of problem (23), where the "pressure" term ∇Q is quite annoying from the traditional kinetic theory perspective. Although (23) has a conspicuous Euler form, one should notice that if the starting point of our discussion would be a typical Smolochowski diffusion, whose drift is given by the Stokes formula (i.e. is proportional to the external force $F = -\nabla V$ acting on diffusing molecules), then its external force factor is precisely the one retained from the original Kramers phase-space formulation of the high friction affected random motion. In the Euler description of fluids and gases the very same force which is present in the Kramers (or Boltzmann in the traditional discussion) equation should reappear on the right-hand side of the local conservation law (momentum balance formula) (23). Except for the harmonic oscillator example in view of (4) this is generally *not* the case in application to diffusion processes.

Following the hydrodynamic tradition let us analyze the issue in more detail. We consider a reference volume (control interval) $[\alpha, \beta]$ in R^1 (or $\Lambda \subset R^1$), which at time $t \in [0, T]$ comprises a certain fraction of particles (fluid constituents), for an instant of course. Since we might deal with a flow (proportional to the current velocity $v(x, t)$) the time rate of particle loss by the volume $[\alpha, \beta]$ at time t is equal to the flow outgoing through the boundaries, i.e.

$$-\partial_t \int_\alpha^\beta \rho(x, t)\, dx = \rho(\beta, t) v(\beta, t) - \rho(\alpha, t) v(\alpha, t) , \tag{27}$$

which is a consequence of the continuity equation. To analyze the momentum balance, let us allow for an infinitesimal deformation of the boundaries of $[\alpha, \beta]$ to have entirely compensated the mass (particle) loss (27),

$$[\alpha, \beta] \to [\alpha + v(\alpha, t)\Delta t, \beta + v(\beta, t)\Delta t] .$$

Effectively, we then pass then to the locally co-moving frame. This implies

$$\lim_{\Delta t \downarrow 0} \frac{1}{\Delta t}\left(\int_{\alpha + v_\alpha \Delta t}^{\beta + v_\beta \Delta t} \rho(x, t+\Delta t)\, dx - \int_\alpha^\beta \rho(x, t)\, dx \right)$$
$$= \lim_{\Delta t \downarrow 0} \frac{1}{\Delta t}\left(\int_{\alpha + v_\alpha \Delta t}^{\alpha} \rho(x, t)\, dx + \Delta t \int_\alpha^\beta \partial_t \rho\, dx + \int_\beta^{\beta + v_\beta \Delta t} \rho(x, t)\, dx \right) = 0 . \tag{28}$$

Let us investigate what happens to the local flows $(\rho v)(x, t)$ if we proceed in the same way (leading terms only are retained),

$$\int_{\alpha + v_\alpha \Delta t}^{\beta + v_\beta \Delta t} (\rho v)(x, t+\Delta t)\, dx - \int_\alpha^\beta (\rho v)(x, t)\, dt$$
$$\sim -(\rho v^2)(\alpha, t)\Delta t + (\rho v^2)(\beta, t)\Delta t + \Delta t \int_\alpha^\beta \partial_t(\rho v)\, dx . \tag{29}$$

Because of (23) we have

$$\partial_t(\rho v) = -\nabla(\rho v^2) + \rho \nabla(\Omega - Q) \tag{30}$$

and the rate of momentum change associated with the control volume $[\alpha, \beta]$ is

$$\lim_{\Delta t \downarrow 0} \frac{1}{\Delta t}\left(\int_{\alpha + v_\alpha \Delta t}^{\beta + v_\beta \Delta t} (\rho v)(x, t+\Delta t) - \int_\alpha^\beta (\rho v)(x, t) \right)$$
$$= \int_\alpha^\beta \rho \nabla(\Omega - Q)\, dx . \tag{31}$$

However

$$\nabla Q = \nabla P/\rho, \quad P = D^2 \rho \Delta \ln \rho , \tag{32}$$

and consequently

$$\int_\alpha^\beta \rho \nabla(\Omega - Q)\, dx = \int_\alpha^\beta \rho \nabla \Omega\, dx - \int_\alpha^\beta \nabla P\, dx$$
$$= E[\nabla \Omega]_\alpha^\beta + P(\alpha, t) - P(\beta, t) . \tag{33}$$

Clearly, $\nabla \Omega$ refers to the Euler-type volume force, while ∇Q (or more correctly P) refers to the "pressure" effects entirely due to the particle transfer rate through the boundaries of the considered volume. The latter property can be consistently attributed to the Wiener noise proper: it sends particles away from the areas of larger concentration. See, e.g., also Ref. [7] for a discussion of the Brownian recoil principle, which reverses the original Wiener flows.

As it appears, the validity of the stochastic differential representation of the diffusion implies the validity of the hydrodynamical representation (23) of the process. This in turn gives a distinguished status to the auxiliary potential $\Omega(x, t)$. We encounter here a fundamental problem of what is to be interpreted by a physicist (observer) as the *external force field manifestation* in the diffusion process. Should it be dictated by the drift form following Smoluchowski and Kramers, or rather by $\nabla \Omega$ entering the evident (albeit "Euclidean looking") second Newton law, respected by the diffusion? In the standard derivations of the Smoluchowski equation the deterministic part (force and friction terms) of the Langevin equation is postulated. What, however, if the experimental data pertain to the local conservation laws like (23) and there is no direct (experimental) access to the microscopic dynamics?

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