THE EHRENFEST THEOREM FOR MARKOV DIFFUSIONS

P. GARBACZEWSKI
Institute of Theoretical Physics
University of Wrocław, pl. M. Borna 9
PL-50 205 Wrocław, Poland

Abstract. The transformation connecting transition densities of the diffusion process with the respective Feynman-Kac kernels, induces the local field of accelerations which equals the gradient of the Feynman-Kac potential and becomes the straightforward analog of the Ehrenfest theorem.

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:

$$dX(t) = b(X(t),t)dt + \sqrt{2D}\,dW(t) \tag{1}$$

with $X(0) = x_0, D$ a diffusion coefficient, $W(t)$ a normalised Wiener noise, and 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) $p(y,s,x,t), s \leq t$ solves the Fokker-Planck equation with respect to x,t

$$\partial_t p = D\triangle_x p - \nabla_x(bp) \tag{2}$$

$$lim_{t\rightarrow s} p(y,s,x,t) = \delta(x-y) \qquad s \leq t$$

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

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

This allows us to replace (2) by the generalised diffusion equation

$$\partial_t h = D\triangle_x h - (-\partial_t\Phi + D[-\triangle\Phi + (\nabla\Phi)^2])h\ . \tag{5}$$

$$lim_{t\rightarrow s} h(y,s,x,t) = \delta(x-y)$$

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

$$\frac{\Omega}{m} = 2D(-\partial_t\Phi + D[-\Delta\Phi + (\nabla\Phi)^2]) = -2D\partial_t\Phi + D\nabla b + \frac{1}{2}b^2 \tag{6}$$

with respect to the conditional[4] Wiener measure

$$h(y,s,x,t) = \int exp[-\frac{1}{2mD}\int_s^t \Omega(x,u)du]dW[y|x] \ . \tag{7}$$

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 $exp[-\frac{1}{2mD}\int_s^t(2mD^2\Delta - \Omega)du]$ with the appropriate restrictions (continuity, boundedness from below) on $\Omega(x,t)$, and hence Φ implicit. All this is valid under the 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

$$lim_{\Delta t\downarrow 0}\frac{1}{\Delta t}[\int p(x,t,y,t+\Delta t)f(y,t+\Delta t)dy - f(x,t)] = \ . \tag{8}$$

$$(D_+f)(X(t),t) = (\partial_t + b\nabla + D\Delta)f(X(t),t)$$

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

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

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 bit 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 $\rho(x,t) = \int \rho_0(y)p(y,0,x,t)dy$ is uniquely defined. The microscopic law of random displacements $p(y,s,x,t), s \leq t$ 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 $p_*(y,s,x,t)$

$$\rho(x,t)p_*(y,s,x,t) = p(y,s,x,t)\rho(y,s) \tag{10}$$

which allows 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 (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:

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

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

$$(D_-f)(X(t),t) = (\partial_t + b_*\nabla - D\Delta)f(X(t),t) \tag{12}$$

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

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

Consequently, the current velocity[5] field

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

can be viewed as the 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

$$(D_+^2X)(t) = \partial_t v + v\nabla v + \frac{1}{m}\nabla Q = (D_-^2X)(t) \tag{15}$$

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

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

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

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

$$E[\nabla Q(X(t),t)] = 0 \tag{17}$$

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

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

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

$$E[X(t)] = \int x\rho(x,t)dx \qquad \Rightarrow$$

$$\frac{d}{dt}E[X(t)] = \frac{1}{2}(E[D_+X] + E[D_-X]) = E[v(X(t),t)] \tag{19}$$

and furthermore (see also Ref. 15)

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

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 we are in principle capable of manipulating (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 this (given a priori) of $\Omega(x,t)$ are *compatible* if

$$\partial_t b + b\nabla b + D\Delta b = \frac{1}{m}\nabla\Omega \tag{22}$$

$$b_0(x) = b(x,0) \ .$$

It is a *sufficient* compatibility condition, which allows us to derive the drift dynamics from this $\Omega(x,t)$. 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) compatibility condition (22) can be *equivalently (!)* written as the coupled Cauchy problem

$$\begin{aligned} \partial_t \rho &= -\nabla(\rho v) \\ \partial_t v + v\nabla v &= \frac{1}{m}\nabla(\Omega - Q) \\ \rho_0(x) = \rho(x,0), & \; v_0(x) = v(x,0) \end{aligned} \tag{23}$$

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, by virtue of the standard path integral identity[1]:

$$p(y,s,x,t) = lim_{\Delta t\downarrow 0}\int dz_1 \ldots \int dz_n (4\pi D\Delta t)^{-n/2} \tag{24}$$

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

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

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

Remark 2: Since

$$p(y,s,x,t) = lim_{\Delta t\downarrow 0}\int dz_1 \ldots \int dz_n \prod_{k=o}^{n-1} p(z_k,t_k,z_{k+1},t_{k+1}) \tag{25}$$

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

$$p(y,s,x,t) = exp[\Phi(y,s) - \Phi(x,t)]lim_{\Delta t\downarrow 0}\int dz_1 \ldots \int dz_n \prod_{k=0}^{n-1} h(z_k,t_k,z_{k+1},t_{k+1}) \; . \tag{26}$$

The semigroup composition property is here clearly seen. It in turn justifies the procedures of Refs. 10–12, see also Refs. 15–17.

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