STOCHASTIC ASPECTS OF THE QUANTUM DYNAMICS

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Abstract

Following Stratonovich, we make a general analysis of the external force manifestations in the dynamics of Markov diffusion processes. Examples of the standard Brownian motion (Zambrini's "Euclidean quantum mechanics" included) and specific Nelson diffusions are given as an illustration of the formalism.

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

$$\begin{aligned} \partial_t p &= D\triangle_x p - \nabla_x(bp) \\ \lim_{t\to s} p(y,s,x,t) &= \delta(x-y) \qquad s \leq t \end{aligned} \tag{2}$$

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

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

allows to replace (2) by the generalized diffusion equation

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

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

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

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

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

$$\begin{aligned} \lim_{\Delta t\downarrow 0}\frac{1}{\Delta t}[\int p(x,t,y,t+\Delta t)f(y,t+\Delta t)dy - f(x,t)] &= \\ &= (D_+ f)(X(t),t) \\ &= (\partial_t + b\nabla + D\triangle)f(X(t),t) \end{aligned} \tag{8}$$

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

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

This formula is a precise embodiment of the second Newton law (in the conditional mean) governing *all* Markovian diffusions consistent with (1)-(7). 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 an inevitable one, see e.g. Refs. 15,16.

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 $p(y,s,x,t), s \le t$ 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* characterization 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 $\rho(x,t)$. Indeed, in this case (see e.g. Refs.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 (Refs. 6,7) mean reads:

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

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

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

Because of (10), the drifts $b(x,t)$ and $b_*(x,t)$ are *not* mutually independent, and indeed (Refs. 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 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 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 (Refs. 10-12) demonstrate that

$$\begin{aligned}(D_+^2X)(t) &= \partial_t v + v\nabla v + \frac{1}{m}\nabla Q = (D_-^2X)(t) \\ Q(x,t) &= 2mD^2\frac{\Delta\rho^{1/2}}{\rho^{1/2}}\end{aligned} \tag{15}$$

which extends the identity (9) to $(D_-^2X)(t)$. With the density $\rho(x,t)$ in hands , 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)

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

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

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

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

$$\begin{aligned} E[X(t)] &= \int x\rho(x,t)dx \qquad \Rightarrow \\ \frac{d}{dt}E[X(t)] &= \frac{1}{2}(E[D_+X] + E[D_-X]) = E[v(X(t),t)] \end{aligned} \tag{19}$$

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.

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 to manipulate (the role attributed to the external observer). Then, we shall tell 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

$$\begin{aligned} \partial_t b + b\nabla b + D\triangle b &= \frac{1}{m}\nabla\Omega \\ b_0(x) &= b(x,0) \end{aligned} \tag{22}$$

It is a *sufficient* compatibility condition, which allows to derive the drift dynamics from this 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) 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 non-linear coupled Cauchy problem (23). It is precisely Eq. (22), which guarantees its solvability. Indeed, in virtue of the standard path integral identity:

$$\begin{aligned} p(y,s,x,t) &= \lim_{\Delta t \downarrow 0} \int dz_1 \ldots \int dz_n (4\pi D \Delta t)^{-n/2} \\ & \qquad \exp(-\frac{1}{4\pi D\Delta t}\sum_{k=0}^{n-1}[z_{k+1} - z_k - b(z_k,t_k)\Delta t]^2) \qquad (24) \\ \Delta t &= \frac{t-s}{n}, z_0 = y, z_n = x, t_0 = s, t_n = t \end{aligned}$$

it suffices to know the time developement 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

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

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

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

The semigroup composition property is here clearly seen. This in turn justifies the procedures of Refs. 10-12.

Example 1: *Free Brownian dynamics*

Let us consider the initial probability distribution of the random variable $X(0)$ of the Wiener (Brownian in the high friction regime) process in the form

$$\rho_0(x) = (\pi\alpha^2)^{-1/2} \exp[-\frac{x^2}{\alpha^2}] \qquad (27)$$

Then its statistical evolution is given by the familiar heat kernel

$$\begin{aligned} p(y,s,x,t) &= [4\pi D(t-s)]^{-1/2} \exp[-\frac{(x-y)^2}{4D(t-s)}, \qquad (28) \\ \rho(x,t) &= [\pi(\alpha^2 + 4Dt)]^{-1/2} \exp[-\frac{x^2}{\alpha^2+4Dt}], \end{aligned}$$

where $s \leq t$.

Let us notice that since the density distribution is now defined for all times $t > s$ we can introduce a convenient device allowing to reproduce a statistical past of the process (irreversible on physical grounds, but admitting this specific inversion mathematically)

$$p_*(y,s,x,t) = p(y,s,x,t)\frac{\rho(y,s)}{\rho(x,t)} \qquad (29)$$

with the properties (set $s = t - \Delta t$)

$$\begin{aligned} \int p_*(y,s,x,t)\rho(x,t)dx &= \rho(y,s) \quad s \leq t \qquad (30) \\ \int y\, p_*(y,s,x,t)\, dy &= x\frac{\alpha^2 + 4Ds}{\alpha^2+4Dt} = x - \frac{4Dx}{\alpha^2+4Dt}\Delta t = x - b_*(x,t)\Delta t, \end{aligned}$$

where $b_*(x,t) = -2D\nabla\rho(x,t)/\rho(x,t)$ and quite trivially $b(x,t) = 0$. Notice that by defining $v(x,t) = \frac{1}{2}b_*(x,t)$, because of the heat equation we have satisfied (23) with $\Omega = 0$, and

$$(\rho v)(x,t) = \int p(y,s,x,t)\rho_0(y)v_0(y)dy \tag{31}$$

Example 2: *Free quantum evolution as a diffusion process*

By defining

$$p(y,0,x,t) = (4\pi Dt)^{-1/2}\exp[-\frac{(x-y+2Dty/\alpha^2)^2}{4Dt}] \tag{32}$$

we realise that

$$\begin{aligned}\int p(y,0,x,t)(\pi\alpha^2)^{-1/2}\exp(-y^2/\alpha^2)dy &= \frac{\alpha}{[\pi(\alpha^4+4D^2t^2)]^{1/2}}\exp[-\frac{x^2\alpha^2}{\alpha^4+4D^2t^2}] \\ &= \rho(x,t) \end{aligned}\tag{33}$$

and

$$\int p(y,0,x,t)[\frac{2Dy}{\alpha^2}(\pi\alpha^2)^{-1/2}]dy = \frac{2D(\alpha^2-2Dt)x}{\alpha^4+4D^2t^2} = b(x,t)\rho(x,t), \tag{34}$$

where evidently

$$v(x,t) = b(x,t) - D\nabla\rho(x,t)/\rho(x,t) \tag{35}$$

solves equations (23) with $\Omega = 2Q$ and via the familiar Madelung transcription of the free Schrödinger dynamics $i\partial_t\psi(x,t) = -D\Delta\psi(x,t)$ with $\psi = \exp(R+iS), \rho = \exp(2R), v = 2D\nabla S$ the link between the Brownian type diffusion and the quantum mechanical evolution is established.

Example 3: *Uses of the imaginary time transformation*

The routine illustration for the imaginary time transformation is provided by considering the force-free propagation, where apparently (see.e.g. Refs. 10-12) the formal recipe gives rise to (one should be aware that to execute a mapping for concrete solutions, the proper adjustment of the time interval boundaries is indispensable):

$$\begin{aligned} i\partial_t\psi &= -D\Delta\psi \longrightarrow \partial_t\overline{\theta_*} = D\Delta\overline{\theta_*} \\ i\partial_t\overline{\psi} &= D\Delta\overline{\psi} \longrightarrow \partial_t\overline{\theta} = -D\Delta\overline{\theta}, \end{aligned}\tag{36}$$

with $it \rightarrow t$. Then

$$\begin{aligned} \psi(x,t) &= [\rho^{1/2}\exp(iS)](x,t) = \int dx' G(x-x',t)\psi(x',0), \\ G(x-x',t) &= (4\pi iDt)^{-1/2}\exp[-\frac{(x-x')^2}{4iDt}], \\ \overline{\theta_*}(x,t) &= \int dx'\, h(x-x',t)\overline{\theta_*}(x',0) \\ h(x-x',t) &= (4\pi Dt)^{1/2}\exp[-\frac{(x-x')^2}{4Dt}], \end{aligned}\tag{37}$$

where the imaginary time substitution recipe

$$h(x-x',it) = G(x-x',t)\ ,\ h(x-x',t) = G(x-x',-it) \tag{38}$$

seems to persuasively suggest the previously mentioned "evolution in imaginary time" notion, except that one *must decide in advance*, which of the two considered evolutions: the heat or Schrödinger transport, would deserve the status of the "real time diffusion".

At this point let us recall that given the initial data

$$\psi(x,0) = (\pi\alpha^2)^{-1/4} \exp\left(-\frac{x^2}{2\alpha^2}\right), \tag{39}$$

the free Schrödinger evolution $\partial_t\psi = -D\Delta\psi$ implies

$$\psi(x,t) = \left(\frac{\alpha^2}{\pi}\right)(\alpha^2 + 2iDt)^{-1/2} \exp\left[-\frac{x^2}{2(\alpha^2 + 2iDt)}\right]. \tag{40}$$

On the other hand, we have

$$\psi(x,-it) = \overline{\theta_*}(x,t) = \left(\frac{\alpha^2}{\pi}\right)^{1/4}(\alpha^2 + 2Dt)^{-1/2} \exp\left[-\frac{x^2}{2(\alpha^2 + 2Dt)}\right]. \tag{41}$$

Let us confine t to the time interval $[-T/2, T/2]$ with $DT < \alpha^2$. Then we arrive at

$$\partial_t\overline{\theta_*} = D\Delta\overline{\theta_*} \quad , \quad \partial_t\overline{\theta} = -D\Delta\overline{\theta} \quad , \quad -\frac{T}{2} \leq t \leq \frac{T}{2} \tag{42}$$

$$\overline{\theta} = \left(\frac{\alpha^2}{\pi}\right)^{1/4}(\alpha^2 - 2Dt)^{-1/2} \exp\left[-\frac{x^2}{2(\alpha^2 - 2Dt)}\right],$$

where

$$\overline{\rho}(x,t) = (\overline{\theta\theta_*})(x,t) = \left[\frac{\alpha^2}{\pi(\alpha^4 - 4D^2t^2)}\right]^{1/2} \exp\left[-\frac{\alpha^2x^2}{\alpha^4 - 4D^2t^2}\right] \tag{43}$$

with the following interesting outcome, which is certainly unpredictable if one follows the traditional Brownian intuitions: $\overline{\rho}(x,-T/2) = \overline{\rho}(x,T/2)$. However strange this probabilistic evolution would seem, it simply refers to a conditional Brownian motion (in fact the Brownian bridge with smooth ends), and clearly nothing like the "imaginary time diffusion" is here involved. We have rather executed a mapping from one real time diffusion to another, with the incompatible dynamical priciples at work.

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