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FEYNMAN INTEGRALS, DIFFUSION PROCESSES AND QUANTUM SYMPLECTIC TWO-FORMS

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ABSTRACT. This is an introduction to a stochastic version of E. Cartan's symplectic mechanics. A class of time-symmetric ("Bernstein") diffusion processes is used to deform stochastically the exterior derivative of the Poincaré–Cartan one-form on the extended phase space. The resulting symplectic two-form is shown to contain the (a.e.) dynamical laws of the diffusions. This can be regarded as a geometrization of Feynman's path integral approach to quantum theory; when Planck's constant reduce to zero, we recover Cartan's mechanics. The underlying strategy is the one of "Euclidean Quantum Mechanics".

1. Introduction

Fifty one years after the publication by R. Feynman of his work on the space-time approach to non-relativistic quantum mechanics [1] the evidence is still growing that, one day, such an approach could surpass the original theory of self-adjoint operators in Hilbert space built by the founders of quantum theory.

Feynman's approach has proved to be a powerful heuristic tool in so many theoretical instances beyond the imagination of its creator in 1948 that little doubt is possible in this respect.

However it is still true, so many years after [1], that a global picture, mathematically consistent, of Feynman's space-time approach, is not available.

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This certainly does not mean that our understanding of the mathematical content of Feynman's ideas is not better than in 1948! Considerable progress have been done in various directions, especially along the functional analytic line that constitutes the "voie royale" between regular quantum theory in Hilbert space and the theory of path integrals. The works [2] and [3] ought to establish this beyond doubt.

Consider a quantum Hamiltonian observable of the simple form

$$H = -\frac{\hbar^2}{2}\Delta + V(q,t) \ . \tag{1}$$

Here H is a self adjoint operator in $L^2(M)$, where M is a Riemannian manifold. For most of this article, M will be $\mathbf{R}^n$. $L^2(M)$ denotes the space of square integrable complex valued quantum states of the system driven by H. The potential $V : M \to \mathbf{R}$ is Borel measurable with, possibly, a smooth time dependence and $\hbar$ denotes Planck's constant. Such systems have been under particular investigation, because heuristic arguments suggest that the *classical* limit is obtained as $\hbar \to 0$ and this classical knowledge has been used as the starting point for studying the quantum system. The classical action functional associated with equation (1),

$$S_L : \ \Omega^q := \Big\{ q(\cdot) \in C^2\Big([t_0,t), M\Big), \ \ q(t) = q \ \ \text{fixed} \Big\} \to \mathbf{R} \ ,$$

$$q(\cdot) \longrightarrow \int_{t_0}^{t} L\Big(\dot q(\tau), q(\tau), \tau\Big)\, d\tau \ , \tag{2}$$

where the Lagrangian $L : TM \times \mathbf{R} \to \mathbf{R}$ reduces here to

$$L(\dot q, q, t) = \frac{1}{2}|\dot q|^2 - V(q,t) \ , \tag{3}$$

is of fundamental importance: if $\psi_\chi(q,t)$ denotes the state of the corresponding quantum system (given that $\psi_\chi(q,t_0) = \chi(q)$), Feynman's most influential contribution is the following heuristic integral representation

$$\psi_\chi(q,t) = \int_{\Omega^q} \chi(\omega(0))\, e^{\frac{i}{\hbar}S_L[q(\cdot)]}\, \mathcal{D}\omega \ , \tag{4}$$

where $\mathcal{D}\omega = \prod_{t_0 \le \tau \le t} d\omega(\tau)$ is used as a measure on the path space Ω^q.

The expression (4) has been interpreted through time discretisation of the trajectories ω, with

$$q_j = \omega(j\epsilon) \qquad \text{for} \qquad \epsilon = \frac{t - t_0}{n}, \quad j = 0, 1, \ldots, n \; .$$

In [4] page 34, the authors note the difficulty that the discretized acceleration

$$\ddot{q} = \frac{q_{j+1} - 2\,q_j + q_{j-1}}{\epsilon^2} \tag{5}$$

diverges as $\epsilon \to 0$. In Nelson [5], a Lie–Trotter product formula is introduced to show convergence as a strong limit in L^2 of the time discretisations, to give rigorous definition to formula (4), but the method does not lead to a well defined integration over path space.

Considering the problem in imaginary time and replacing τ by $-i\tau$ for $\tau > 0$, the underlying measure in the resulting counterpart to formula (4) is the Wiener measure, which is well defined. Of course, the Wiener measure has support on continuous, but not continuously differentiable paths; the acceleration (5) and the Lagrangian (3), for example, are divergent along such paths.

Taking the ϵ length discretisation scheme, one may compute in one space dimension

$$\left\langle q_j \left(\frac{q_j - q_{j-1}}{\epsilon} \right) \right\rangle_{S_L} - \left\langle \left(\frac{q_{j+1} - q_j}{\epsilon} \right) q_j \right\rangle_{S_L} = i\,\hbar \; , \tag{6}$$

where $\langle \cdot \rangle_{S_L}$ denotes the (formal) expectation with respect to the complex weight in formula (4). This leads Feynman in [4] page 177 towards a heuristic trajectorial description of the quantum picture in which formula (6) may be regarded as a reinterpretation of Heisenberg's uncertainty principle and where the quantum trajectories have the same regularity as the typical Brownian paths. Many authors, following considerations by N. Bohr, believe that a trajectorial description cannot be made rigorous and is incompatible with several basic concepts in quantum theory. In the article [33], a rigorous trajectorial description is given in the very restrictive case of stationary states, where V is a time independent potential and ψ_χ is an eigenvector for the operator H. In that description, the interpretation of the uncertainty principle simply as analogous to the quadratic variation of a Brownian motion is not enough; it is more connected with the concentration of the nodes, which are of order $O(\hbar)$ apart as $\hbar \to 0$.

In the Euclidean version of the problem, the Laplacian term may be interpreted in terms of a Wiener process. When the potential V is taken into consideration, a Girsanov theorem argument may be used to construct a Bernstein diffusion. Using the drifts of these diffusions, one may construct the Euclidean counterparts of the quantities in formulae (5) and (6). In the Euclidean framework, the underlying measure is well defined and the problems encountered in real time, associated with lack of a well defined probability measure, are no longer present.

Our aim here is to describe the starting point of the stochastic symplectic geometry underlying this Euclidean mechanics and to extend it, wherever it is possible to do so rigorously, to the real time setting. More precisely, the aim is to generalise Cartan's theory of integral invariants [6], developing the "Euclidean Quantum Mechanics" programme initiated in the mid eighties (cf. [9]).

2. Cartan's classical energy – impulsion tensor and its bilinear covariant

This section starts with some basic material from classical Hamiltonian mechanics according to E. Cartan [6]. Cf. also [32].

By the 'least action principle', the extremal points of the action functional S_L satisfy the Euler Lagrange equations

$$\frac{d}{dt}\left(\frac{\partial L}{\partial \dot{q}^i}\right)(\dot{q}, q, t) - \frac{\partial L}{\partial q^i}(\dot{q}, q, t) = 0, \quad i = 1, \dots, n \ , \tag{7}$$

where n is the dimension of M. The momentum (conjugate to q^i) is defined by

$$p_i = \frac{\partial L}{\partial \dot{q}^i}(\dot{q}, q, t) \ . \tag{8}$$

Provided these n equations can be solved in $\dot{q}$,

$$\dot{q}^i = \dot{q}^i(q, p, t) \ ,$$

one defines the Hamiltonian H as the Legendre transform of the Lagrangian L,

$$H(q,p,t) = p_i\,\dot{q}^i - L(\dot{q},q,t)\ , \tag{9}$$

and it can be seen that the n differential equations of the second order equation (7) become the $2n$ first order equations

$$\dot{q}^i = \frac{\partial H}{\partial p_i}, \quad \dot{p}_i = -\frac{\partial H}{\partial q^i}\ . \tag{10}$$

The (q^i, p_i) are the canonical conjugate coordinates of the $2n$ dimensional phase space of the classical dynamical system. When H is time dependent, it is useful to introduce an extended phase space with coordinates (q^i, p_i, τ, E). Then the Hamilton equations with Hamiltonian

$$\tilde{H}(q,p,\tau,E) = H(q,p,\tau) - E \tag{11}$$

coincides on the manifold $\tilde{H} = 0$ with equation (10) to which are added

$$\dot{\tau} = -\frac{\partial \tilde{H}}{\partial E} = 1, \quad \dot{E} = \frac{\partial \tilde{H}}{\partial \tau} = \frac{\partial H}{\partial \tau}\ . \tag{12}$$

The dot now denotes the derivative with respect to another time parameter which may be identified with the old one on $\tilde{H} = 0$. If H is time independent, the time coordinate is cyclical and its conjugate coordinate E is a first integral of the dynamical system.

Consider an arbitrary point $(q,p,\tau,E) = A$ in the extended phase space, parameterised by two parameters α and β. In Cartan's discussion of the problem, a 'differential' δ is used to denote differentiation with respect to an underlying parameter. Let δ_1 denote $\frac{\partial}{\partial\alpha}$ and let δ_2 denote $\frac{\partial}{\partial\beta}$ and consider $(\delta_1 q, \delta_1 p, \delta_1\tau, \delta_1 E)$ and $(\delta_2 q, \delta_2 p, \delta_2\tau, \delta_2 E)$. Considering the 'area element' of the parallelogram spanned by these two 'displacement' vectors, one obtains the symplectic or canonical two form

$$\Omega(\delta_1,\delta_2) = \sum_{i=1}^{n}(\delta_1 p_i\,\delta_2 q^i - \delta_1 q^i\,\delta_2 p_i) + (\delta_1\tau\,\delta_2 E - \delta_1 E\,\delta_2\tau)\ . \tag{13}$$

Now consider the starting point A as well as the two varied ones as initial conditions of three solutions of the extended Hamiltonian system (10)–(12), it is easy to compute that, for any initial data q,p,τ,E, $\delta_i q^j$,$\delta_i p_j$,$\delta_i\tau$,$\delta_i E$,

$$\frac{d}{dt}\Omega(\delta_1,\delta_2) = 0\ . \tag{14}$$

This was first observed by Lagrange. In other words, for any Hamiltonian H, $\Omega(\delta_1, \delta_2)$ is an integral invariant of the motion. The right hand side of equation (13) is termed a *bilinear covariant* by E. Cartan in [6]. By integration over the two underlying parameters α and β, it follows that any simply connected surface in extended phase space, bounded by a curve and such that each point is the initial condition of a Hamiltonian trajectory has a constant area under the evolution. The introduction of (13) is motivated by the study of

$$\omega_\delta := p\,\delta q - H\,\delta t \;, \tag{15}$$

which is called the *energy – impulsion tensor* in [6].

A certain amount of care has to be taken with the notation when the differential with respect to time is considered. This will be especially the case in our stochastic generalization.

When the space and time variables are regarded as functions of a parameter, Cartan shows that

$$\delta S_L = [\omega_\delta]_{t_0}^{t} + \int_{t_0}^{t} \left(\frac{d^2 q}{d\tau^2} + \frac{\partial V}{\partial q} \right) \delta q \; d\tau \;. \tag{16}$$

In particular, the integration of ω_δ along solutions of the Euler Lagrange equations, shows that $\int \omega_\delta$ is time invariant; it is an integral invariant of the equations of motion. Conversely, Cartan shows that the *only* system of O.D.E.s admitting $\int \omega_\delta$ as an integral invariant is precisely (10)–(12). This amounts to showing that $\Omega(d, \delta) = 0$ for any δq, δp, δt, where d denotes the differential along the trajectory, δ being an arbitrary variation.

As equation (16) shows, ω_δ is closely related to Hamilton's action functional (2). Cartan observes that if the following identity holds along trajectories for the displacement in the state space

$$\delta q^i = \dot{q}^i \,\delta\tau \;, \tag{17}$$

then the energy – impulsion tensor ω_δ may be identified with the integrand of the action functional since

$$\int_{t_0}^{t} p_i\, dq^i - H\, d\tau = \int_{t_0}^{t} L\, d\tau \;. \tag{18}$$

(comparing with (9)). Notice that in (17) Cartan does not really treat δq, $\delta\tau$ as differentials.

3. A class of time symmetric diffusion processes

Let $(\Omega, (\mathcal{P}_t)_{t\geq t_0}; (\mathbf{P}_x)_{x\in M})$ denote the probability space of the canonical realization of the Wiener process $w_t : t \geq t_0$ with values in $M = \mathbf{R}^n$. Here Ω denotes $C(\mathbf{R}_+, M)$, $\mathcal{P}_t$ the increasing filtration representing the past of the process and $\mathbf{P}_x$ its law when it starts from $x \in M$ at time t_0. Assuming for simplicity the (Borel measurable) potential $V : M \to \mathbf{R}$ of equation (1) is time independent, one can decompose it into its positive and negative parts $V^+ = \max(V, 0)$ and $V^- = \max(-V, 0)$ and assume that

(19)
$$E_x\left[\exp\left\{\int_{t_0}^{t_1} V^-(w_\tau)\,d\tau\right\}\right]<\infty \text{ and } \mathbf{P}_x\left[\int_{t_0}^{t_1} V^+(w_\tau)\,d\tau < +\infty\right]=1 \text{ a.e.},$$

where E_x denotes the expectation with respect to $\mathbf{P}_x$. Under these conditions, it is known that the integral kernel h of the heat equation on $L^2(M)$ associated with the Hamiltonian H, namely

$$h(x,\, t - t_0,\, y) = \text{kernel}\left(\exp\left\{-\frac{(t-t_0)}{\hbar}\,H\right\}\right)(x, y), \qquad x, y \in M\ , \tag{20}$$

is jointly continuous in all its variables and strictly positive. Using this and a given pair of positive measurable functions on M, denoted by $\eta^*_{t_0}$ and η_{t_1}, which are analytic vectors for H in the interval $[t_0, t_1]$ (this can be seen in [9]), one shows the existence of an M valued diffusion $z_t : t_0 \leq t \leq t_1$, whose finite dimensional distributions are of the form

(21)
$$\begin{aligned}&\mathbf{P}(d\xi_1, \tau_1, ..., d\xi_n, \tau_n)\\ &= \int \eta^*_{t_0}(x)\, h(x, \tau_1 - t_0, \xi_1) \cdots h(\xi_n, t_1 - \tau_n, y)\, \eta_{t_1}(y)\ dx\, d\xi_1 \cdots d\xi_n\, dy\end{aligned}$$

for $t_0 \leq \tau_1 \leq \ldots \leq \tau_n \leq t_1$. This process is a *Bernstein* diffusion z_t, $t \in [t_0, t_1]$, which is now entirely determined from the data of a pair of probability densities p_0 and p_1 at the extremities of the time interval. Indeed, these data allow us to determine the pair $\{\eta^*_{t_0}, \eta_{t_1}\}$ needed for equation (21) via the system

$$\begin{cases} \eta^*_{t_0}(x) \displaystyle\int_{\mathbf{M}} h(x, t_1 - t_0, y)\, \eta_{t_1}(y)\ dy \ = \ p_0(x) \\ \eta_{t_1}(y) \displaystyle\int_{\mathbf{M}} \eta^*_{t_0}(x)\, h(x, t_1 - t_0, y)\ dx \ = \ p_1(y) \end{cases} \tag{22}$$

which is known (under our hypothesis on h) to have a unique positive, but not necessarily integrable, solution $\{\eta^*_{t_0}, \eta_{t_1}\}$ if p_0 and p_1 are strictly positive probability densities [10]. This is the sketch of the original construction of those diffusions, their history is outlined in [9]. Others, more general and inspired by Csiszär and Föllmer have been developed since then. See [11] for a very recent survey.

What makes Bernstein diffusions special is that, although they are generally (i.e. for an arbitrary choice of boundary probabilities, p_0 and p_1 in equation (22)) inhomogeneous Markov processes, they are nevertheless perfectly time symmetric on $[t_0, t_1]$ by construction, in a sense which is now made clear. It follows clearly from the form of the Hamiltonian (1) that z_t should solve some $\mathcal{P}_t$ - Itô stochastic differential equation [12]

$$dz_t = B(t, z_t)\, dt + \hbar^{1/2}\, dw_t \ . \tag{23}$$

In the construction, one interprets the drift vector field B on M as the mean velocity

$$B(t, z_t) = Dz_t \equiv \lim_{\epsilon \to 0} E\left[\frac{z_{t+\epsilon} - z_t}{\epsilon} \,|\, \mathcal{P}_t\right] , \tag{24}$$

where $E[\cdot\,|\,\mathcal{P}_t]$ denotes the conditional expectation given $\mathcal{P}_t$. Now, using (21), one verifies easily that, when the densities are smooth,

$$B(q,t) = -\nabla S(q,t) \tag{25}$$

where the scalar field S is defined by

$$S(q,t) = -\hbar \log \eta(q,t) \tag{26}$$

and η solves the heat equation for (1) with (positive) final condition

$$\begin{cases} \hbar \dfrac{\partial \eta}{\partial t} &= H\eta \qquad t \in [t_0, t_1] \\ \eta(q, t_1) &= \eta_{t_1}(q) \ . \end{cases} \tag{27}$$

It is shown in [11] that such a construction requires naturally the following finite kinetic energy condition

$$E\left[\int_{t_0}^{t_1} |Dz_t|^2 \, dt\right] < \infty \ . \tag{28}$$

The time reversed process is defined by $\hat{z}_t = z_{t_0+(t_1-t)}$ and corresponds to exchanging the probability densities p_0 and p_1 at the extremities of $[t_0, t_1]$. The drift associated by equation (24), which is given by

$$D\hat{z}_t \equiv -D_*\, z_{t_0+(t_1-t)}, \qquad t_0 \le t \le t_1 \ , \tag{29}$$

is measurable with respect to the *decreasing* filtration $\hat{\mathcal{F}}_t = \mathcal{P}_{(t_0+(t_1-t))}$ representing the future of z_t. Here D_* is defined as

$$D_* \, z_\tau = \lim_{\epsilon \downarrow 0} E\left[\frac{z_\tau - z_{\tau-\epsilon}}{\epsilon} \,|\, \mathcal{F}_\tau\right] . \tag{30}$$

This method was used by Nelson [13] in another context and permits one to attribute two different drifts to the same time symmetric diffusion process z_t, $t \in [t_0, t_1]$. By analogy with equation (24) and (27), one may verify that this backward drift is given by

$$B_*(q,t) = \nabla S_*(q,t) \ , \tag{31}$$

where S_* is defined by $S_*(q,t) = -\hbar \log \eta^*(q,t)$ and η^* solves the heat equation adjoint to (27) with positive initial condition $\eta^*_{t_0}$,

$$\begin{cases} -\hbar \dfrac{\partial \eta^*}{\partial t} = H\eta^* \qquad t_0 \le t \le t_1 \\ \eta^*(q,t_0) = \eta^*_{t_0} \ . \end{cases} \tag{32}$$

The pair of heat equations (32) and (27) may be regarded as the 'imaginary time' counterparts of Schrödinger's equation and its complex conjugate [9].

The class of Bernstein processes arises naturally in the context of a probabilistic treatment of the imaginary time analogue of Feynman's approach. From equations (24), (25) and (27), one verifies that, when H is of the form (1),

$$DDz_t = DB = \nabla V(z_t,t) \quad \text{a.e. .} \tag{33}$$

Unfortunately, as pointed out earlier, the 'acceleration' along the path in equation (5) is divergent, even in imaginary time and one has to consider instead the 'smoothed' quantity given in equation (33). It is important to note the sign in front of the ∇V. Unlike classical mechanics, there is no negative sign (this results from $\tau \to -i\tau$ mentioned in the introduction), showing that the set up is not exactly analogous to classical mechanics. For a way to recover the correct sign cf. a modification to the Bernstein process developed in [33].

Starting from equations (24) and (25), as well as (31), one computes using $\Pr\{z_t \in dq\} = \eta^*\eta(q,t)\, dq$ (as in [9]) that

$$E\Big[z_t \, D_* z_t - z_t \, Dz_t\Big] = \hbar \ , \tag{34}$$

which is the imaginary time analogue of equation (6). Inspection of equation (6) will show the role played by the reversibility of the Bernstein diffusion.

There are serious differences between the limit as $\hbar \to 0$ of the Bernstein diffusion and classical mechanics, even after making the necessary allowances for the change of sign noted in equation (34). This is connected with the onset of downward jumps in the associated Burgers' equation (i.e. the equation solved by the drift B defined in (25)–(26)) as $\hbar \to 0$ and, in general, where these downward jumps occur, it is not true that $z^{(0)} := \lim_{\hbar\to 0} z^{(\hbar)}$ satisfies $\frac{d^2 z}{dt^2} = \nabla V(z_t, t)$. The quantity $\hbar$ does not, as one might naïvely expect, measure the deviation from classical mechanics in the benign way that equation (34) might suggest. Some striking examples, showing the impact on the dynamics of the onset of downward jumps in the Burgers' equation are given in the first section of [33].

A rigorous counterpart has been developed in imaginary time for most of the non rigorous considerations made by Feynman in real time. Cf. [14].

4. Stochastic exterior derivative of one forms and stochastic calculus of variation

The classical calculus of variations finds critical points of functionals associated with the classical Lagrangian mechanics; for example, the derivation of equation (7) from equation (2), for classical trajectories. The basis of a variational approach to deal with Euclidean Quantum Mechanics was introduced in [14] and [16].

Let us show that the classical connection (cf. for ex. [15]) between the critical point of action functionals linear in the velocity, i.e. one form ω on M, and the exterior derivative of ω is preserved in this framework.

DEFINITION 1 ([16]). *For F a "regular" functional defined on $(\Omega, \rho\mu^{\hbar})$, where $\mu^{\hbar}$ is the Wiener measure with parameter $\hbar$ and ρ any positive Radon–Nikodym density s.t. $\rho\mu^{\hbar}$ is the law of a process z_t of the form (23) in the domain of F, one says that z_t is critical point of F when $(\nabla F, \phi)_1 = 0$ a.s., $\forall\, \phi : \Omega \to \mathcal{H}$. Here $\mathcal{H}$ is the Cameron–Martin subspace of the path space Ω, ∇ the gradient defined in Malliavin calculus [17] and $(\cdot,\cdot)_1$ the scalar product in $\mathcal{H}$.*

PROPOSITION 1. *Let* $A \in C^3(\mathbf{R}^n \to \mathbf{R}^n)$. *A* $\mathbf{R}^n$*-valued process of the form (23) with* $z_{t_0} = x$ *and s.t.* $E[\sup_{t_0<t<T} |z_t|^2] < \infty$ *is* critical point *of the functional*

$$E_{x,t_0} \int_{t_0}^{T} A_i(z_t) \circ dz_t^i \ , \tag{35}$$

where $\circ$ *denotes Stratonovich symmetric integral* [12] *if and only if*

$$(\nabla_j A_i - \nabla_i A_j)\, B^i + \frac{\hbar}{2}(\nabla_j \nabla_k A_k - \Delta A_j) = 0 \quad \text{(a.s.)} \tag{36}$$

along z_t, $t_0 \le t \le T$ *(where Einstein summation convention has been used).*

Proof. Using the relation between Stratonovich and forward Itô's integral and the definition (24), the functional (35) can be expressed as

$$E_{x,t_0}\left[\int_{t_0}^{T} \left(A_i(z_t)\, Dz_t^i + \frac{\hbar}{2}\nabla^k A_k\right) dt\right] \equiv E_x\left[\int_{t_0}^{T} L(Dz_t, z_t)\, dt\right] . \tag{37}$$

If F denotes this functional, Itô's calculus and an integratio by parts with respect to the time parameter gives

$$\begin{aligned} (\nabla F, \phi)_1 &= E_{x,t_0}\left[\int_{t_0}^{T} \left(\frac{\partial L}{\partial z}\phi + \frac{\partial L}{\partial Dz} D\phi\right) dt\right] \\ &= E_{x,t_0}\left[\int_{t_0}^{T} \phi\left(\frac{\partial L}{\partial z} - D\frac{\partial L}{\partial Dz}\right) dt\right] = 0, \quad \forall \phi : \Omega \to \mathcal{H} \ , \end{aligned} \tag{38}$$

where we have assumed $\frac{\partial L}{\partial Dz}(Dz_T, z_T) = 0$ for simplicity (this can always be implemented with an additional transversality condition). It follows that

$$\frac{\partial L}{\partial z} - D\frac{\partial L}{\partial Dz} = 0 \quad \text{a.s.} \ . \tag{39}$$

The operator D introduced in (24) may be extended to any smooth vector field depending on t and z_t. Itô's formula for a smooth test function $f : \mathbf{R}_+ \times \mathbf{R}^n \to \mathbf{R}^n$ gives

$$D = \frac{\partial}{\partial t} + B^i \nabla_i + \frac{\hbar}{2}\Delta \ . \tag{40}$$

Using this, (39) coincides with (36) for the Lagrangian of (37). □

The first term of (36) arises in classical mechanics. It is known (cf. for example [8]), that the inclusion of a magnetic field with potential vector A in a Lagrangian system such as (3), defined by $\tilde{L} = L + (A, \dot{q})$, transforms the original Euler Lagrange equation (7) into

$$\dot{p}_i = -\nabla_i V + (\nabla_j A_i - \nabla_i A_j)\, \dot{q}^j \ . \tag{41}$$

The second term of (36) is not a classical term and arises from the 'quadratic variation' of the noise in the stochastic calculus. Denoting ϕ by δz (for "variation of z"), one can introduce the concept of a stochastic "exterior derivative" d of the 1-form $A_i \circ dz^i$ through

$$\begin{aligned} 0 &= E_{x,t_0}\Big[\int_{t_0}^{T} d(A_i \circ dz_t^i)\,(B, \delta z)\Big] \\ &= \sum_{i,j} E_{x,t_0}\Big[\int_{t_0}^{T} (\nabla_j A_i - \nabla_i A_j)\, \delta z_j\, B_i\ dt \\ &\qquad + \tfrac{\hbar}{2}\,(\nabla_j \nabla_k A_k - \Delta A_j)\, \delta z_j\ dt\Big] \end{aligned} \tag{42}$$

for any variation δz along z. This expression can be written in a way which relates it more closely to the classical setting; Cartan's bilinear covariant of the classical 1- form (A, dq) given in [6]:

$$E_{x,t_0}\Big[\int_{t_0}^{T} (\nabla_j A_i - \nabla_i A_j)\, \delta z_j\, dz_i + \frac{\hbar}{2}\,(\nabla_j \nabla_k A_k - \Delta A_j)\, \delta z_j\ dt\Big] \ . \tag{43}$$

The exterior derivative of an exact form $\omega = dS(z_t)$, where S is a regular scalar field, must be zero. It follows from the definition that this is the case only if

$$\nabla_j \nabla^k \nabla_k S - \Delta \nabla_j S = 0 \ . \tag{44}$$

This is clearly the case when $M = \mathbf{R}^n$. For a Riemannian manifold, some care should be taken, because the Laplace–Beltrami operator does not commute anymore with the gradient. The Laplace–de Rham operator Δ_{DR} does commute and therefore the Laplacian of (40) ought to be understood as Δ_{DR} when defining stochastic parallel displacement of vectors along Brownian paths in problems related to Euclidean Quantum Mechanics [18] and [19].

PROPOSITION 2. *Under the same hypotheses as for Proposition 1, a critical point of the functional (35) solves, almost everywhere,*

$$(\nabla_j A_i - \nabla_i A_j)\, B_*^i - \frac{\hbar}{2}\,(\nabla_j \nabla^k A_k - \Delta A_j) = 0 \ . \tag{45}$$

where B_* is the backward drift (30).

Proof. The proof is similar to that of proposition 1, except that a backward formulation of the problem is used (cf. [20]). The associated Lagrangian becomes

$$L_*(D_* z_t, z_t) = A_i\, D_* z_t^i - \frac{\hbar}{2} \nabla^k A_k \ .$$

The difference is the change of sign in the correction term. An 'Euler Lagrange' equation may be computed in much the same way as before;

$$D_* \frac{\partial L_*}{\partial D_* z} - \frac{\partial L_*}{\partial z} = 0 \ ,$$

resulting in equation (44). □

To provide a formulation as close to the classical as possible, the average drift is introduced

$$v^i = \frac{1}{2} (B_*^i + B^i) \ . \tag{46}$$

Its behaviour under time reversal is the same as the one of a classical velocity, in contrast with the one of the drifts B and B_* taken separarely.

DEFINITION 2. *The* symmetric stochastic exterior derivative *of the one form* $(A(z_t) \circ dz_t)$ *on the vector fields* v *and* X *is given by*

$$d(A_i \circ dz^i)(v, X) = (\nabla_j A_i - \nabla_i A_j)\, v^i\, X^j \ . \tag{47}$$

As a matter of fact, it is easier to understand the appearance of the average drift v by observing that we could reinterpret the first term of the r.h.s. of (43) as involving a Stratonovich differential $\circ dz^i$ instead of the (forward) Itô's one $\cdot dz^i$. Then using again the general relation $y \circ dz = y \cdot dz + \frac{1}{2}\, dy \cdot dz$ (cf. [12, p.100]) one verifies that

$$\begin{aligned} &\int (\nabla_j A_i - \nabla_i A_j)\, \delta z^j \circ dz_\tau^i \\ &= \int (\nabla_j A_i - \nabla_i A_j)\, \delta z^j\, dz_\tau^i + \tfrac{\hbar}{2} (\nabla_j \nabla^i A_i - \Delta A_j)\, \delta z^j\, d\tau \end{aligned} \tag{48}$$

so that the quantum deformation term in our initial definition (42) of the exterior derivative of $A_i \circ dz^i$ is precisely due to the difference between the Itô (forward) and Stratonovich integrals. Of course, the same would be true for the backward Itô's definition underlying (45). Taking the expectation of the l.h.s of (48), using the symmetric time discretization of Stratonovich (cf. [20, 13]) and the continuity of the paths, we get

$$E_{x,t_0} \int (\nabla_j A_i - \nabla_i A_j)\, \delta z^j \, \frac{1}{2}\, (D z^i_\tau + D_* z^i_\tau)\, d\tau$$
$$= E_{x,t_0} \int (\nabla_j A_i - \nabla_i A_j)\, \delta z^j \, v^i \, d\tau$$

whose integrand coincides with our definition (47).

We mention without proof the following elementary extension of Proposition 1.

PROPOSITION 3. *Let $A \in C^{3,2}(\mathbf{R}^n \times \mathbf{R} \to \mathbf{R}^n)$ and $h \in C^{2,2}(\mathbf{R}^n \times \mathbf{R} \to \mathbf{R})$. A $\mathbf{R}^n$-valued process z_τ of the form (23), with $z_{t_0} = x$ is a critical point of the functional*

$$E_{x,t_0} \int_{t_0}^{T} A_i(z_\tau, \tau) \circ d z^i_\tau + h(z_\tau, \tau)\; d\tau \tag{49}$$

in the same sense as in Proposition 1 if and only if

$$(\nabla_j A_i - \nabla_i A_j)\, B^i + \frac{\hbar}{2}\, (\nabla_j \nabla^k A_k - \Delta A_j) + \left(\nabla_j h - \frac{\partial A_j}{\partial \tau} \right) = 0 \quad \text{a.s.} \tag{50}$$

along z_τ. The quantum deformation term can be eliminated from (50) by the same symmetrization procedure as before.

Let us apply this to the class of diffusion processes introduced in §3. If B denotes, as before, the drift of Bernstein diffusion, we say that

$$\Sigma = \left\{ (t, q, B(q,t)) \mid (t,q) \text{ in a simply connected domain of } \mathbf{R} \times \mathbf{R}^n \right\}$$

is a stochastic Lagrange set when the following stochastic version of the Poincaré–cartan one-form

$$\omega = B(z_t, t) \circ d z_t + \epsilon(z_t, t)\, dt \tag{51}$$

is exact. Notice that only the (q,t) variables are involved here in contrast with the usual classical definition in the phase space. So (51) should be interpreted as the stochastic counterpart of $p(q,t)\, dq - H(q, p(q,t), t)\, dt$, i.e. the integrand of the action functional (18) after substitution to the momentum p as a function of q and t. The scalar function ϵ in (51) is defined by such property.

PROPOSITION 4. *Σ is a stochastic Lagrange set when*

a) *In case B is continuous, iff there is a scalar field $S(q,t)$ of $C^{2,1}$ class s.t.*

(52) $$B(q,t) = -\nabla S(q,t) \ ,$$

(53) $$\frac{\partial S}{\partial t} + \frac{1}{2}|\nabla S|^2 + \frac{\hbar}{2}\Delta S + V \equiv \frac{\partial S}{\partial t}(q,t) + \epsilon(q,t) = 0 \ .$$

The scalar field S is given explicitly by (26), and ϵ is called the energy random variable of the system.

b) *In case B is of $C^{1,1}$ class, iff in a simply connected domain*

(54) $$\nabla_k B^i - \nabla_i B^k = 0 \ ,$$

(55) $$\frac{\partial}{\partial t} B^i = \nabla_i \epsilon \ .$$

Notice that at the classical limit $\hbar = 0$ of smooth trajectories, and except for a few changes of signs of Euclidean origin, this is a classical result (cf. [22]), justifying our terminology.

Proof.

a) ω of (51) is exact so there is a scalar S s.t. $\omega = -dS$. ¿From this follow (52) and (53). The first relation was already known (25). The second follows from (25) and the fact that η solves the heat equation (27).

b) When B is of $C^{1,1}$ class, $d\omega = -ddS = 0$ which is, by (50), equivalent (in a simply connected domain and for $A = B$, $h = \epsilon$) to (54) and (55). □

The equation (53) is called the Hamilton–Jacobi–Bellman equation [23] and became increasingly important, in recent years, both under the effects of its relevance to stochastic control theory and as a motivation for the development of the method of viscosity in nonlinear PDE [24]. In our perspective, it is the proper quantum deformation of the classical Hamilton–Jacobi equation.

Let us conclude this section by a basic property of the energy random variable, needed afterwards

COROLLARY 1. *Along any Bernstein diffusion z_t*

$$D\epsilon(z_t,t) = \frac{\partial V}{\partial t}(z_t,t) \quad \text{a.e.} \tag{56}$$

In particular, if the system is conservative (i.e. the scalar potential V is not explicitly time dependent) then the energy random variable is a $\mathcal{P}_t$-martingale.

Proof. By Proposition 4, $S(q,t) = -\hbar \log \eta(q,t)$ and $\epsilon(q,t) = -\frac{\partial S}{\partial t}(q,t)$. The conclusion follows from the definition (40) of D and the form of the Hamiltonian (1).

When V is time independent we have $D\epsilon(z_t,t) = 0$ i.e. (cf. (24))

$$E\Big[\epsilon(z_{t+\Delta t}, t+\Delta t) \,|\, \mathcal{P}_t\Big] = \epsilon(z_t,t) \quad \forall\, \Delta t > 0 \;, \tag{57}$$

which (besides the obvious integrability requirement $\epsilon(z_t,t) \in L^1$) is precisely the definition of a martingale. Cf. [25]. □

5. Stochastic canonical two-form

It is clear from §4 that our probabilistic generalization of a point in the classical extended phase space (cf. §2) is now

$$A = \Big(z_t,\; B(z_t,t),\; t,\; \epsilon(z_t,t)\Big) \tag{58}$$

for the class of Bernstein diffusions defined in §3, where B and ϵ denote, respectively, the drift and energy random variables. At time t_0 these data provide, in particular, the initial conditions of the equations of motion, in our regularized Hamiltonian form, i.e. by (24), (33), and (56),

$$Dz_t = B\,, \quad DB = \nabla V\,, \quad D\epsilon = \frac{\partial V}{\partial t} \quad \text{a.e.} \tag{59}$$

To build two variations $A_1 + \delta_1 A$ and $A + \delta_2 A$ such that these two neighbouring random variables could define the initial conditions of two new solutions of the same equations (59) requires some care. This can be interpreted as the result of some change of space-time variables close to the identity

$$\begin{cases} Q = q + \alpha\, X(q,t) + o(\alpha) \\ \tau = t + \alpha\, T(q,t) + o(\alpha) \end{cases} \tag{60}$$

where $\alpha \in \mathbf{R}$, $X \in C^{2,1}(\mathbf{R}^n \times \mathbf{R} \to \mathbf{R}^n)$, $T \in C^{2,1}(\mathbf{R}^n \times \mathbf{R} \to \mathbf{R})$ together with the effect of (60) on the drift and energy variables B, ϵ. But, in terms of Itô calculus, the change of time parameter evaluated on a diffusion like (23) is, in itself, alarming: it result into a new diffusion whose law is not absolutely continuous with respect to the one of z_t. Notice that this is true even if T depends only on t and not on the space variable q. As a matter of fact, if $T = T(q = z_t, t)$ such transformation is meaningless in probability theory. The right perspective is to interpret (60) as acting on a space-time process (z_t, t) (i.e. the counterpart of the classical extended configuration space) and to impose that after the transformation (60), the same heat equation (27) is solved in the new variables (Q, τ). Then one shows

PROPOSITION 5 ([26, 27]). *Those conditions are satisfied by each solution (X, T) of the system of PDE:*

(61)

$$\frac{\partial T}{\partial t} = 2\frac{\partial X^i}{\partial q^i} \text{ (no summation)}, \qquad \frac{\partial T}{\partial q^i} = 0, \qquad \frac{\partial X^i}{\partial t} = 0 \ ,$$

$$\frac{\partial T}{\partial t} V + X^i \frac{\partial V}{\partial q^i} + T\frac{\partial V}{\partial t} = 0, \qquad \frac{\partial X^i}{\partial q^j} + \frac{\partial X^j}{\partial q^i} = 0, \quad i,j = 1,...,n \ , i \neq j$$

where V is assumed to be at least of $C^{1,1}$ class.

Those linear equations are a special case of the defining equations of the (Lie) symmetry group of the heat equation (27). They form an over-determined system and, therefore, have solutions.

Now we want to study the stochastic counterpart of the classical symplectic two-form (13). What plays the roles of $(\delta_j q, \delta_j \tau)$, $j = 1, 2$, there is clearly $(X_j, T_j) = (\frac{\partial Q}{\partial \alpha}_{|\alpha=0}, \frac{\partial \tau}{\partial \alpha}_{|\alpha=0})$, given our definition (60). We need to make sense of the associated $(\delta_j B, \delta_j \epsilon)$, $j = 1, 2$.

LEMMA 1. *When the equations (61) hold, the variations of the drift and energy random variables are given by*

$$(\delta_j B)^i = B_k \frac{\partial X_j^i}{\partial q^k}, \quad \delta_j \epsilon = -\epsilon \frac{dT_j}{dt}, \quad j = 1, 2, \quad i, k = 1, ..., n \ .$$

Proof. Consider the effect of the change of space-time variables (60) in the SDE (23). Up to the first order in the parameter α it is, using

Itô's theorem,

(62)

$$dQ_\tau = \Big(B + \alpha(DX - B\dot{T})\Big)(Q_\tau, \tau)\, d\tau + \left(\mathbf{1} + \alpha\left(X_q - \frac{\dot{T}}{2}\mathbf{1}\right)\right)\sqrt{\hbar}\, d\widetilde{W}_\tau$$

where $\mathbf{1}$ is a $n \times n$ identity matrix, X_q denotes the matrix $(\frac{\partial X^i}{\partial q^k})$, $i, k = 1, ..., n$, and $\widetilde{W}_\tau$ is a $\mathbf{R}^n$-valued $\mathcal{P}_\tau$ Wiener process. By the first and the last equations (61) these diffusions are absolutely continuous with respect to the onè solving (23). Together with the third defining equation, this allows to compute that the variation of the drift $DX - B\dot{T} = -BX_q$ as claimed.

The second claim follows in the same way. □

Definition 3. *Let $(X_j, T_j) = (\delta_j z, \delta_j t)$, $j = 1, 2$, be a couple of solutions of the defining equations (61) and $(\delta_j B, \delta_j \epsilon)$ the associated variations of drift and energy defined in Lemma 1. We call stochastic canonical or symplectic two-form the expression*

(63)

$$E\Big[(\delta_1 B_i\, \delta_2 z^i - \delta_1 z^i\, \delta_2 B_i) - (\delta_1 t\, \delta_2 \epsilon - \delta_1 \epsilon\, \delta_2 t)\Big] \equiv E[M_t(z_t)] \equiv \Omega_\eta(\delta_1, \delta_2)$$

where the suffix η in Ω_η is a reminder that the left hand side is computed in term of a (positive) solution η of the heat equation (27).

Theorem 1. *The stochastic canonical two-form (63) of the system driven by the heat equation (27) is an invariant of the motion in the sense that $DM_t(z_t) = 0$ a.s..*

Proof. Using Lemma 1, the integrand of (63) can be written

$$M_t = \left[-B_k\left(X_1^i\, \frac{\partial X_2^i}{\partial q^k} - \frac{\partial X_1^i}{\partial q^k}\, X_2^i\right) + \varepsilon(T_1\, \dot{T}_2 - \dot{T}_1\, T_2)\right], \quad i, k = 1, ..., n\ .$$

By Itô's calculus, some laborious calculations using the fact that (X_j, T_j), $j = 1, 2$, both solve the defining equations (61), and the properties of the basic Bernstein diffusion z_t, show that $M_t(z_t)$ is a $\mathcal{P}_t$-martingale. □

The first application by E. Cartan of his concept of symplectic two-form is the case where the variation δ_1 in (13) is arbitrary and δ_2 is the ordinary differential (denoted by d) along the trajectories. The fact that $\Omega(\delta, d) = 0$ for any variation δq, δp and δt provides a new derivation of the Hamiltonian equations of motion (10) and (12) (cf. [6]).

The same is true in our probabilistic generalization, with a necessary proviso: if we need to interpret one of the variations in (63) as a stochastic differential along the continuous paths $t \mapsto z_t$ of the diffusion, we have to specify which differential. The remark after (48) suggests the following:

PROPOSITION 6. *Consider the stochastic symplectic two-form*

$$E\int_{t_0}^{t_1}(\delta z^i \circ dB_i - \delta B_i \circ dz^i) + (\delta t\, d\epsilon - \delta\epsilon\, dt) \equiv \Omega_\eta(d,\delta) \tag{64}$$

where $\circ$ and d refer to the Stratonovich integral. This integral vanishes $\forall\, \delta z$, δB, δt admissible (i.e. $\forall\, X$, δB and T as defined before) if the regularized Hamiltonian equations (59) holds a.e..

REMARK. Since $\delta t = T$ is of bounded variation process by construction (cf. (61)) it is not necessary to specify the kind of stochastic differentials used in the second term of the l.h.s. of (64).

Proof. Let us do this computation in $\mathbf{R}^3$ for simplicity. By Lemma 1 and (52)–(53)

$$\delta\epsilon = -\epsilon\dot T = \left(\frac{1}{2}|B|^2 + \frac{\hbar}{2}\nabla B\right)\dot T - \dot T\, V\ .$$

Using the defining equations (61) this reduces to

$$\delta\epsilon = B\,\delta B + \frac{\hbar}{3}\nabla B\ \nabla X + X\,\nabla V + T\,\dot V\ .$$

According to Itô's rule $F\circ dG = F\,dG + \frac{1}{2}\,dF\,dG$

$$\delta z\circ dB = X\,dB + \frac{\hbar}{6}\nabla B\ \nabla X\ dt$$

and

$$\delta B\circ dz = \delta B\,dz - \frac{\hbar}{6}\nabla B\ \nabla X\ dt\ .$$

The left hand side of (64) can, therefore, be written as

$$E\int_{t_0}^{t_1} X(dB - \nabla V\,dt) + \delta B\,(-dz + B\,dt) + T\left(d\epsilon - \frac{\partial V}{\partial t}\,dt\right) \tag{65}$$

which is zero $\forall\, X$, T and δB admissible only if the Hamiltonian equations (59) hold a.e.. □

6. Further directions of investigation and prospects

Let us come back on Cartan's observation (17) on the relation between the energy-impulsion tensor ω_δ and the integrand of the action functional S_L.

Given (61), a probabilistic counterpart for us is to impose that, at any time,

$$X^i = B^i T, \quad i = 1, ..., n \ , \tag{66}$$

where B denotes, as before, the drift vector field of a Bernstein diffusion.

Using Proposition 5, one verifies easily that (66) is possible only if $B(q,t)$ is of the form

$$B^i(q,t) = \frac{1}{2}\frac{\dot{T}}{T}(t)\, q^i + \frac{\alpha}{T(t)} \tag{67}$$

where α is a constant vector in $\mathbf{R}^n$ and T solves $\ddot{T}(t) = 0$.

Going further with (40), we see that

$$DB^i = 0 \ . \tag{68}$$

In other words, by (33), we are dealing exclusively with solutions of the free ($V = 0$) equations of motion.

(67) is the typical drift of a Gaussian Bernstein diffusion. Such processes, for Hamiltonian H of the form (1) have been studied of their own (cf. [28, 29, 30]). They are known to carry a symplectic structure. Notice, however, that the stochastic symplectic geometry sketched here is much more general: it is not limited a priori to Gaussian probability measures.

Regarding the concept of dynamical laws, in this framework, let us point out that, in spite of the $\mathcal{P}_t$-stochastic differential equation (or of its counterpart with respect to the decreasing filtration $\mathcal{F}_t$) it is the second order equation (33) which capture their essence. In consequence, we define the local flow of (canonical) transformations associated with (33), for example, by

$$\begin{gathered} \phi_i : \mathbf{R}^{2n} \to \mathbf{R}^{2n} \\ \begin{pmatrix} M_t^1 \\ M_t^2 \end{pmatrix} \mapsto \begin{pmatrix} z_t \\ Dz_t \end{pmatrix} \end{gathered} \tag{69}$$

where $\phi = \phi(M_t^1, M_t^2, t)$, with M_t^1, M_t^2 two $\mathcal{P}_t$-martingales playing the role of initial conditions of (33).

For example, consider $n = 1$ and $V(q) = \frac{\omega^2}{2} q^2$, $\omega =$ cste. Then

(70)
$$\begin{pmatrix} z_t \\ Dz_t \end{pmatrix} = \begin{pmatrix} \phi_1(M_t^1, M_t^2, t) \\ \phi_2(M_t^1, M_t^2, t) \end{pmatrix} = \begin{pmatrix} \cosh \omega t & \sinh \omega t \\ \sinh \omega t & \cosh \omega t \end{pmatrix} \begin{pmatrix} M_t^1 \\ M_t^2 \end{pmatrix}.$$

Notice that here the solutions are analytic $\forall\, t$, an exceptional situation. The existence of the martingales M_t^1, M_t^2 for simple systems with linear flows like this one is assured by the Theorem of Noether proved in [27].

The analytical and geometrical properties of such flows (with general scalar potentials V) should be studied carefully.

The defining relations (61) of the symmetry group allow us to characterize the transformations taking positive solutions of the heat equations (27) (with their associated Bernstein diffusion) into other positive solutions of the same equation. This is the probabilistic counterpart of a very special class of canonical transformation in Hamiltonian mechanics: those whose scalar potential V is not changed. Another special canonical transformation is, of course, the time evolution. The proper geometrical definition of a canonical transformation is one, from the (extended) phase space into itself, preserving the symplectic two-form [8].

By Theorem 1 we know that the stochastic canonical two-form Ω_η is preserved under the dynamics. This should be extended to the largest possible class of canonical transformations between Bernstein diffusions.

The main missing Theorem in such a stochastic symplectic geometry is the relevant Stokes Theorem [32]. It is needed to turn the local statement of Theorem 1, involving only canonical transformations close to the identity, to a global one. The right hand side of (63) should define the exterior derivative of the stochastic one-form

(71)
$$\omega_{\delta_1} = B\,\delta_1 z + \epsilon\,\delta_1 t$$

generalizing Cartan's energy-impulsion tensor (15). In the classical case, the integral of ω_δ over a closed loop in the extended phase space coincides with a double integral of $d\omega_\delta$ [6]. This one is a relative integral invariant in Cartan's sense and we should understand its probabilistic generalization. This involves clearly integration over the whole symmetry group, not only over the Lie algebra used implicitly here.

What are, finally, the relations between the indirect interpretation of Feynman's ideas advocated here, this "Euclidean Quantum Mechanics", and regular quantum theory in Hilbert space?

They are very close. In fact, our probabilistic analogy is close enough to allow to guess new Theorems in quantum theory. In [31] it is shown that our approach of symmetries in §5 (in a slightly more general version) translates into a new Theorem of regular quantum theory in Hilbert space, always richer in its predictions than the familiar Theorems in $L^2(M)$.

The general aim of Euclidean Quantum Mechanics is therefore the same as Feynman's one, but using the advances of stochastic analysis since the fifties: to draw systematically the advantages of an approach to quantum theory where the concept of trajectories in space-time is preserved.

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