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FRANCESCO GUERRA

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Stochastic variational principles and quantum mechanics

by

Francesco GUERRA
Dipartimento di Fisica, Universita di Roma « La Sapienza »,
Piazzale Aldo Moro 2, I-00185 Roma, Italy

1. INTRODUCTION

Variational principles of Lagrangian type [*1*] provide a solid foundation for the whole structure of classical mechanics and classical field theory. In a series of previous papers [*2*], [*3*], [*4*] (see also [*5*]), we have investigated a generalization of the variational principles, in the case where the smooth deterministic trial trajectories of classical mechanics are replaced by the very irregular trajectories of random diffusions in configuration space. In this approach, the main emphasis is put on the average hydrodynamic field variables, as the density and the forward and backward drifts of the diffusions. Through them one can define the action and its variations.

An interesting feature of these stochastic variational principles is that the critical processes, making stationary the action under suitable time boundary conditions, are strictly related to states of the associated quantum dynamical system, according to the general scheme of Nelson's stochastic mechanics [*5*], [*6*], [*7*]. Therefore, apart from subtleties of physical interpretation, for which we refer to [*5*], [*7*], [*8*], we can say that stochastic variational principles provide a kind of stochastic simulation of quantum mechanical behavior.

The hydrodynamic (Eulerian) approach, as introduced for example in [*2*], can be usefully complemented by a Lagrangian approach, where the main emphasis is put on trajectories and variations of trajectories, rather than on field quantities. In fact, the first pioneering attempts of Yasue, toward a stochastic calculus of variations [*9*], [*10*], [*5*], where based on this Lagrangian point of view. However, very recently, Morato [*11*] and Loffredo and Morato [12] have introduced a very simple and natural class of trajectory variations, allowing a direct treatment of the stochastic variational problem in the frame of the Lagrangian approach. In particular, they have discovered the existence of critical diffusions more general than those associated to quantum states through Nelson's stochastic mechanics, and have investigated their possible physical meaning, especially in connection with the peculiar quantum behavior of liquid Helium at very low temperatures [13].

One important feature of the Loffredo-Morato solutions is that the mean velocity field is not necessarily irrotational, as in standard stochastic mechanics. Moreover, the equations are not time reversal invariant and any solution, with generic mean velocity field, relaxes towards a solution of standard stochastic mechanics, with irrotational mean velocity field and associated to a quantum state. From this point of view, each quantum state, solution of Schroedinger equation, acts as a kind of attractor for a family of solutions of the Loffredo-Morato equations.

This feature could play a very relevant role also in the frame of the general attempts towards the understanding of quantum behavior as effect of random fluctuations of a subquantum medium, as advocated for example, from different points of view, by Bohm and Vigier [14] and by Nelson [5].

The main purpose of this paper is to analyze the connections between the Eulerian and the Lagrangian approaches to stochastic variational principles. In particular, it will be shown how different time boundary conditions can select different classes of critical diffusions. For example, solutions with irrotational mean velocity fields are selected by imposing criticality of the action under variations which keep invariant the initial and final densities of the processes. On the other hand, general solutions, not necessarily irrotational, are found by exploiting time boundary conditions where the local conditional expectations of the trajectory variations are put to zero (see for example equation (25)).

By exploiting different classes of variations we can found a very large class of critical solutions, characterized by a real parameter λ. The Loffredo-Morato equations are a special case, so as they are the equations based on the original definition of acceleration given by Nelson [15], *without* the irrotationality condition.

The organization of the paper is as follows.

In Section 2, we recall the hydrodynamic (Eulerian) form of stochastic variational principles, as explained for example in [2]. The Lagrangian frame is introduced in Section 3, where we use the forward process variations, originally exploited by Morato in [11]. In Section 4, which contains the main results of this paper, we introduce a very general class of process variations and analyze the consequences of stochastic variational principles based on them. Finally Section 5 is devoted to some conclusions and outlook for future developments.

2. EULERIAN FORM OF STOCHASTIC VARIATIONAL PRINCIPLES

Let us consider a dynamical system with configuration space R^n and Lagrangian given by

$$\mathrm{L}(q, \dot{q}) = \frac{1}{2} m\dot{q}^2 - \mathrm{V}(q). \tag{1}$$

We introduce a generic trial diffusion $q(t)$, with constant diffusion coefficient ν, and call $\rho(x, t)$ and $v_{(+)}(x, t)$, $v_{(-)}(x, t)$, $v(x, t)$ and $u(x, t)$ the density and the forward, backward, current and osmotic velocities, respectively. We have

$$v = \frac{1}{2}(v_{(+)} + v_{(-)}), \qquad u = \frac{1}{2}(v_{(+)} - v_{(-)}) = \nu\nabla \log \rho. \tag{2}$$

Then the average action is defined, as in the classical case, by

$$\mathrm{A}(t_0, t_1; q) = \int_{t_0}^{t_1} \lim \mathrm{E}\left(\frac{1}{2} m(\Delta q/\Delta t)^2 - \mathrm{V}(q(t))\right) dt, \tag{3}$$

where the limit is taken as $\Delta t \to 0^+$.

A simple calculation shows

$$\mathrm{A}(t_0, t_1; q) = \int_{t_0}^{t_1} dt \int \left(\frac{1}{2} m v_{(+)} \cdot v_{(-)} - \mathrm{V}(x)\right) \rho(x, t) dx + \ldots, \tag{4}$$

where $+ \ldots$ are infinite terms irrelevant for the variational principle, since they do not depend on the particular trial diffusion and disappear in the variation of the action [5].

We give two equivalent evaluations for the variation of A, under changes of the process. The first expression is more appropriate to an Eulerian point of view and can be introduced as follows.

Define the forward and backward transport operator

$$\mathrm{D}_{(\pm)} = \partial_t + v_{(\pm)} \cdot \nabla \pm \nu\Delta. \tag{5}$$

Introduce the generalized Hamilton-Jacobi principal function $\mathrm{S}(x, t)$, defined by the antiparabolic equation

$$\mathrm{D}_{(+)}\mathrm{S}(x, t) = \frac{1}{2} m v_{(+)}^2 + m\nu\nabla \cdot v_{(+)}, \tag{6}$$

with an arbitrary final specification $\mathrm{S}(x, t_1)$. Under an arbitrary small change of the process, with corresponding changes $\delta\rho$, $\delta v_{(\pm)}$, in Ref. [2]

it is proven that the action is changed, up to first order terms, according to

$$\delta \mathrm{A} = \int \mathrm{S}(x_1, t_1)\delta\rho(x_1, t_1)dx_1 - \int \mathrm{S}(x_0, t_0)\delta\rho(x_0, t_0)dx_0 + \\ + \int_{t_0}^{t_1} \mathrm{E}((mv - \nabla \mathrm{S}) \cdot \delta v_{(+)}(q(t), t))dt . \tag{7}$$

Then we have the following stochastic variational principle (Guerra-Morato [2]). The action is stationary under arbitrary small variations $\delta v_{(+)}$, with the time boundary conditions $\delta\rho(\cdot, t_0) = 0$, $\delta\rho(\cdot, t_1) = 0$, if and only if the current velocity field of the process can be expressed in the Hamilton-Jacobi form

$$mv = \nabla \mathrm{S} , \tag{8}$$

where S is a function satisfying the equation (6). However, (6) and (8) are equivalent to the Hamilton-Jacobi-Madelung equation [16]

$$(\partial_t \mathrm{S})(x, t) + \frac{1}{2m}(\nabla \mathrm{S})^2 + \mathrm{V}(x) - 2mv^2 \frac{\Delta\sqrt{\rho}}{\sqrt{\rho}} = 0 . \tag{9}$$

Moreover, the continuity equation must hold

$$(\partial_t \rho)(x, t) = - \nabla \cdot (\rho v) . \tag{10}$$

It is well known that the two equations (9) and (10) can be reduced to the Schroedinger equation

$$i\hbar(\partial_t \psi)(x, t) = - \frac{\hbar^2}{2m} \Delta\psi + \mathrm{V}(x)\psi , \tag{11}$$

provided one introduces the following expression of v in terms of Planck's constant [6]

$$2mv = \hbar \tag{12}$$

and defines the wave function through the following De Broglie Ansatz

$$\psi(x, t) = \sqrt{\rho(x, t)} \exp\left(\frac{i}{\hbar} \mathrm{S}(x, t)\right). \tag{13}$$

Therefore, we see that the stochastic variational principle selects critical processes associated to quantum states.

We can also introduce the Nelson acceleration [15], [6]

$$a(x, t) = \frac{1}{2}(\mathrm{D}_{(+)}v_{(-)} + \mathrm{D}_{(-)}v_{(+)}) , \tag{14}$$

and recognize that the dynamical equation (9) is in fact equivalent to the stochastic Newton equation

$$ma = - \nabla \mathrm{V} , \tag{15}$$

which originally was put by Nelson [15] at the basis of stochastic mechanics, together with the irrotationality condition (8).

Here we see that both the Hamilton-Jacobi expression (8) and the Newton equation (15) derive from the stochastic variational principle, where a crucial role has been played by the time boundary conditions $\delta\rho(\cdot, t_0) = 0$, $\delta\rho(\cdot, t_1) = 0$. Let us notice that the time boundary conditions $\delta q(t_0) = 0$, $\delta q(t_1) = 0$, usually employed in the variational principle of classical mechanics, have been replaced by the weaker boundary conditions requiring that the original process q and the varied process $q + \delta q$ have the same distributions at the initial and final times.

The second form of the action variation will be given in next Section.

3. THE LAGRANGIAN FRAME

In the Lagrangian frame the basic role is played directly by the variations δq of the process. A very simple way to build a large class of suitable variations δq has been introduced by Morato [11] and further exploited by Loffredo and Morato [12], [13].

Let us introduce a random variable $\eta(t_0)$ with values in R^n, independent of q, and define, in the probability space of q and $\eta(t_0)$, the stochastic process $\eta(t)$ as solution of the differential equation

$$\frac{d}{dt}\eta_i(t) = \eta_j(t)(\partial_j v_{(+)i})(q(t), t) + f_{(+)i}(q(t), t)\,, \tag{16}$$

with $\eta(t_0)$ as initial condition. In (16) $f_{(+)i}(x, t)$ is such that

$$\delta v_{(+)i}(x, t) = \varepsilon f_{(+)i}(x, t) + \mathrm{O}(\varepsilon^2)\,, \tag{17}$$

where ε is a small variational parameter.

Having found $\eta(t)$, we define the Morato [11] family of processes $q^\varepsilon(t)$ such that

$$q^\varepsilon(t) = q(t) + \varepsilon\eta(t) + \mathrm{O}(\varepsilon^2)\,. \tag{18}$$

Let us also define the conditional average

$$\phi(x, t) = \mathrm{E}(\eta(t) \mid q(t) = x)\,, \tag{19}$$

so that

$$\mathrm{E}(q^\varepsilon(t) \mid q(t) = x) = x + \varepsilon\phi(x, t) + \mathrm{O}(\varepsilon^2) \tag{20}$$

at each generic point x of the trajectory of the trial process $q(t)$.

For the density $\rho^\varepsilon(x, t)$ of $q^\varepsilon(t)$ we have immediately

$$\rho^\varepsilon(x, t) = \rho(x, t) + \delta\rho(x, t), \qquad \delta\rho(x, t) = -\,\varepsilon\nabla\cdot(\rho\phi)\,. \tag{21}$$

Through a very simple computation (see [11], [12] and [17]) one can easily prove the following important result.

Define the action $A(t_0, t_1; q^\varepsilon)$ as in (3) and (4) with q replaced by q^ε. Then we have

$$A(t_0, t_1; q^\varepsilon) = A(t_0, t_1; q) + \delta A, \tag{22}$$

$$\delta A = \varepsilon \Big\{ E((mv \cdot \phi)(q(t_1), t_1)) - E((mv \cdot \phi)(q(t_0), t_0)) + \\ - \int_{t_0}^{t_1} E((m(a + a') + \nabla V) \cdot \phi(q(t), t))dt \Big\} + O(\varepsilon^2),$$

where a is the Nelson acceleration (14) and a' is an additional term, discovered in [11], given by

$$a'_i = -(u_j + \nu\partial_j)(\partial_i v_j - \partial_j v_i). \tag{23}$$

Notice that, while a in (14) is time reversal invariant, a' is not. In fact, it changes sign under time reversal.

The main point of the previous result is that the expression (22) coincides with the previously found (7), provided (17) holds and $\eta(t_0)$ is adjusted so that $\delta\rho(\cdot, t_0)$ is correctly reproduced by (21) at t_0 (then it will be correctly reproduced at each later time).

Then we can exploit the expression (22) to establish a new variational principle. In fact, we have that the action is stationary, under arbitrary process variations, with the time boundary conditions $\phi(\cdot, t_0) = 0$ and $\phi(\cdot, t_1) = 0$, if and only if the following Loffredo-Morato equation holds

$$m(a + a') = -\nabla V. \tag{24}$$

Notice that there is no irrotationality condition of the type (8). Moreover, the time evolution (24) is not time reversal invariant.

Therefore, the same expression of the action (7), (22) can give very different results, if different time boundary conditions are exploited. In this case, the time boundary conditions are equivalent to require

$$E(q^\varepsilon(t) \mid q(t) = x) = x + O(\varepsilon^2) \qquad \text{for} \quad t = t_0, \qquad t = t_1. \tag{25}$$

These boundary conditions imply $\delta\rho(\cdot, t_0) = 0$, $\delta\rho(\cdot, t_1) = 0$, but they are in fact more restrictive. As a result, critical diffusions, associated to them and satisfying (24), form a larger class. In fact, in the special case where (8) holds, then (24) reduces to (9), (14).

As it is usual in variational principles, the shift from one class of time boundary conditions to another can be compensated through appropriate generalized Lagrangian multipliers. In our case, we can insert an additional term in the starting Lagrangian (3), (4) of the form

$$-E(S(q(t_1), t_1)), \tag{26}$$

for a given fixed $S(\cdot, t_1)$ function, as proposed also by Marra [18]. Then the variation (22) acquires an additional term given by

$$- \int S(x_1, t_1)\delta\rho(x_1, t_1)dx_1 = \varepsilon \int S(x_1, t_1)(\nabla \cdot (\rho\phi))(x_1, t_1)dx_1 = \\ = - \varepsilon E((\nabla S \cdot \phi)(q(t_1), t_1)). \tag{27}$$

Now the stationarity of the corrected action, with the *same* boundary conditions $\phi(\cdot, t_0) = 0$ and $\phi(\cdot, t_1) = 0$, is equivalent to (24), but in addition we have also the condition

$$mv(\cdot, t_1) = (\nabla S)(\cdot, t_1). \tag{28}$$

Therefore, the irrotationality condition is enforced at the final time and one can easily prove (see for example [17]) that it must hold at any time, as a consequence of (24). Therefore, in this case (24) reduces to the previous (8) and (15).

In conclusion, the two systems of boundary conditions can be put in agreement through the introduction of the generalized Lagrangian multiplier (26). However, without this term, the time boundary conditions with $\phi(\cdot, t_0) = 0$ and $\phi(\cdot, t_1) = 0$ give rise to critical processes satisfying the Loffredo-Morato equations (24), which are more general than those obtained through the density boundary conditions.

4. A GENERAL CLASS OF VARIATIONS

It is very simple to extend the class of process variations considered in the previous Section. In fact, independently of the variations based on (16), (17), we can introduce also backward variations based on a time inverted procedure. Let us introduce a random variable $\eta_{(-)}(t_1)$, independent of q, and define the process $\eta_{(-)}(t)$ as solution of the differential equation

$$\frac{d}{dt}\eta_{(-)i}(t) = \eta_{(-)j}(t)(\partial_j v_{(-)i})(q(t), t) + f'_{(-)i}(q(t), t), \tag{29}$$

with $\eta_{(-)}(t_1)$ as *final* condition (see also [18]). In (29) $f'_{(-)}$ is such that

$$\delta' v_{(-)i}(x, t) = \varepsilon f'_{(-)}(x, t) + O(\varepsilon^2), \tag{30}$$

where δ' is a new variation not necessarily connected with the δ variations introduced before.

By following the same method as in the previous Section, we can introduce process variations of the type

$$q'^{\varepsilon}(t) = q(t) + \delta' q(t), \qquad \delta' q(t) = \varepsilon\eta_{(-)}(t) + O(\varepsilon^2), \tag{31}$$

with

$$\phi_{(-)}(x, t) = \mathrm{E}(\eta_{(-)}(t) \mid q(t) = x). \tag{32}$$

Then the new variation of the action $\delta'\mathrm{A}$ can be expressed as in (22) with ϕ substituted by $\phi_{(-)}$ *and* a' substituted by $-a'$. Therefore, if we establish a variational principle based on $\delta'\mathrm{A} = 0$, with time boundary conditions $\phi_{(-)}(\cdot, t_0) = 0$ and $\phi_{(-)}(\cdot, t_1) = 0$, we end up with a criticality condition

$$m(a - a') = -\nabla \mathrm{V} \tag{33}$$

which is the time inverted of (24).

At this point, as it has been remarked in [*18*], we could impose criticality with respect to both sets of variations. Then we would get (24) and (33) at the same time. But in this case we have necessarily $a' = 0$ [*18*], and the system (24), (33) reduces to satisfy (8) and (15).

But there exist a more subtle procedure.

In fact, it is easy to prove the following simple result [*17*]. For any forward variation $\eta_{(+)}(t)$, as introduced in the previous Section, it is possible to find a backward variation $\eta_{(-)}(t)$ such that the following equality holds

$$\phi_{(+)}(x, t) = \phi_{(-)}(x, t). \tag{34}$$

The proof is very simple, but it involves long calculations, which can not be reported here. We refer to [*17*] for a complete proof.

For a generic real parameter λ let us consider the class of process variations given by

$$q^{\varepsilon}(t) = q(t) + \varepsilon(\lambda\eta_{(+)}(t) + (1 - \lambda)\eta_{(-)}(t)) + \mathrm{O}(\varepsilon^2). \tag{35}$$

Due to linearity, the associated action variation is given by

$$\delta \dot{\mathrm{A}} = \lambda\delta_{(+)}\mathrm{A} + (1 - \lambda)\delta_{(-)}\mathrm{A}, \tag{36}$$

where $\delta_{(+)}$, $\delta_{(-)}$ are the variations associated to $\eta_{(+)}$, $\eta_{(-)}$, respectively.

Recalling (22) for $\delta_{(+)}\mathrm{A}$ and its time inverted (with $-a'$ in place of a') for $\delta_{(-)}\mathrm{A}$, we find immediately the following general form

$$\delta \mathrm{A} = \varepsilon \left\{ \mathrm{E}((mv \cdot \phi)(q(t_1), t_1)) - \mathrm{E}((mv \cdot \phi)(q(t_0), t_0)) + \right. \\ \left. - \int_{t_0}^{t_1} \mathrm{E}((m(a_\lambda + \nabla \mathrm{V}) \cdot \phi(q(t), t))dt \right\} + \mathrm{O}(\varepsilon^2) \tag{37}$$

where ϕ is the common value of $\phi_{(+)}$, $\phi_{(-)}$ as in (34), and the new acceleration a_λ is given by

$$a_\lambda = a + (2\lambda - 1)a'. \tag{38}$$

Of course, $\lambda = 1$ gives the Loffredo-Morato expression and $\lambda = 0$ its time inverted one.

Therefore, we see that if we require stationarity of the action under process variations of the type (35), with time boundary conditions $\phi(\cdot, t_0)=0$ and $\phi(\cdot, t_1) = 0$, we obtain the criticality condition in the form of a generalized stochastic Newton equation

$$ma_\lambda = - \nabla V . \tag{39}$$

In particular, we obtain the important result that the original Nelson dynamical equation (15), *without* the irrotationality condition (8), can be obtained in the frame of a stochastic variational principle, with appropriate boundary conditions. In fact, it is sufficient to select $\lambda = 1/2$ in (35), (38).

Boundary conditions based on the density give rise to the irrotationality condition (8). Boundary conditions based on the less restrictive (25) do not enforce (8). For $\lambda > 1/2$ we have Loffredo-Morato type equations with a generic coefficient $(2\lambda - 1)$ multiplying the a' correction. For $\lambda < 1/2$ we have their time inverted counterpart. The symmetric case $\lambda = 1/2$ gives rise to the time reversal invariant Nelson equation, without the irrotationality condition.

By exploiting the same methods as in [*12*], we see also that the solutions with $\lambda > 1/2$ relax to solutions with $\lambda = 0$ *and* the irrotationality condition (i. e. Schroedinger solutions) as $t \to -\infty$. The same happens to solutions with $\lambda < 1/2$ as $t \to \infty$.

On the other hand, the solutions with $\lambda = 0$ are in general different from solutions associated to Schroedinger equation (see also Morato [*19*]).

Of course, systems of solutions associated to different values of λ can be related through generalized Lagrangian multipliers, equivalent to interactions with suitable external vector potential fields, as analyzed in [*17*].

5. CONCLUSIONS AND OUTLOOK

We have seen that stochastic variational principles have an extremely reach structure. In particular, by exploiting different classes of time boundary conditions, we can obtain a simulation of quantum mechanics, with the irrotationality condition and the Madelung equation, or a class of not necessarily irrotational solutions relaxing toward those of quantum mechanics.

Moreover, we have also seen that Nelson formulation of the second principle of dynamics, without irrotationality, can be obtained in the frame of these stochastic variational principles.

It would be very interesting to see whether the time boundary conditions employed here, and in particular the parameter λ, are connected with some physical meaning at the observational level, or are purely formal constructions.

Of course, this is strictly related to the problem of the possible physical reality of the quantum fluctuations affecting the particle motion. Surely, this problem can not be settled yet, mainly for the lack of concrete models simulating the Brownian disturbances appearing in stochastic mechanics. However, the general structure of stochastic mechanics, as explored till the present times, seems to tell us that these quantum fluctuations, if they exist, must have very peculiar features, well beyond those of thermal fluctuations or general disorder fluctuations, suitable to incorporate the main quantum mechanical properties, and in particular the full coherence of the wave function in configuration space.

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