En vertu du Théorème 2.1, on obtient l'estimation suivante :

$$\|u^n - u^n_{kh}\| \leqslant C(h+k)\|g\|_2.$$

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A CONNECTION BETWEEN THE VARIATIONAL PRINCIPLES OF ANALYTICAL MECHANICS AND THE CONCEPTS OF PROBABILITY AND ENTROPY

BY

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To the memory of Professor Mendel Haimovici

The great efficiency of variational methods in entering upon the problems of analytical mechanics determined some scientists (among them being Louis de Broglie as well) to look for a relationship between the minimal action principle and the entropy principle. In other words, a trial was made to correlate the physical phenomenon, of selecting the real trajectory Γ from the family of virtual paths Γ^{virt}, to the reaching of a maximal probability.

On the same line, we propose a model for enlightening this connection.

a) Let us consider, in this respect, a point-like body moving in the space dimension q, during the time interval between the instants (s_1, s_2), $(s_2 > s_1)$. We divide the duration $(s_2 - s_1)$ in a great number N of identical, elementary intervals, so that

$$N = \frac{s_2 - s_1}{\delta s} \tag{1}$$

and assume that $\mathfrak{L}(q, dq/ds, s)$ is a characteristic function of the motion, in a sense which will appear clear in the forthcoming considerations.

b) We put forward the hypothesis according to which the probability of a small departure ε in the q direction, with respect to the real trajectory Γ, during the interval δs, centred around the instant s_0, is given by the expression

$$p(q, \varepsilon) = 1 - k\,[L(q+\varepsilon) - L(q)]\,\frac{\delta s}{s_2 - s_1} \tag{2}$$

where $\varepsilon = \varepsilon(s)$, and K is a constant. The probability that a derogation $\varepsilon(s)$ occurs throughout the interval $s_1 \leqslant s \leqslant s_2$ obviously will be given by the multiplication rule

$$P(s_1, s_2, \varepsilon) = \Pi\, p(q, \varepsilon) = \Pi \left\{1 - k[L(q+\varepsilon) - L(q)]\,\frac{\delta s}{s_2 - s_1}\right\} = e^{-\frac{k}{s_2 - s_1}\int_{s_1}^{s_2}[L(q+\varepsilon) - L(q)]\,ds} \tag{3}$$

c) Further on, let us estimate the value of the characteristic function L, on a curve deviated with ε from the real trajectory Γ assuming that $|\varepsilon| \ll 1$. Performing previously some partial integrations we get the following expansion

$$L(q+\varepsilon) = \mathfrak{L}(q+\varepsilon, \dot{q}+\dot{\varepsilon}, s) = \mathfrak{L}(q, \dot{q}, s) + \varepsilon\left[\mathfrak{L}'_q - \frac{d}{ds}(\mathfrak{L}'_{\dot{q}})\right] + \tag{4}$$
$$+ \frac{1}{2}\varepsilon^2\left[\mathfrak{L}''_{q^2} - \frac{d}{ds}(\mathfrak{L}''_{q\dot{q}})\right] + \frac{d}{ds}\left[\varepsilon\mathfrak{L}'_{\dot{q}} + \frac{1}{2}\varepsilon^2\mathfrak{L}''_{q\dot{q}}\right] + \frac{1}{2}\dot{\varepsilon}^2\mathfrak{L}''_{\dot{q}^2} + \ldots$$

d) But the probability P, entering the formula (3) must be a function depending on s_1, s_2, ε, accordingly, the extraterms in (4), which cannot be interpreted as coming from a power expansion, must vanish when are integrated over the range $s_1 \leqslant s \leqslant s_2$

e) As we have as an working hypothesis the limiting conditions

$$\varepsilon(s_1) = \varepsilon(s_2) = 0, \tag{4'}$$

it results that the term in (4), denoting a full derivative against s brings just no contribution to the integral in (3).

f) We have now to investigate what happens with the last term in (4). As $\varepsilon = g(s)$ and $\dot{\varepsilon} = dq(s)/ds = h(s)$ we may write

$$\dot{\varepsilon} = h\{g^{-1}(\varepsilon)\} = \chi(\varepsilon) \tag{4''}$$

and moreover

$$\frac{1}{2}\int_{s_1}^{s_2} \mathfrak{L}''_{\dot{q}^2}\dot{\varepsilon}^2 ds = \frac{1}{2}\int_{\varepsilon(s_1)}^{\varepsilon(s_2)} \mathfrak{L}''_{\dot{q}^2}\chi(\varepsilon)d\varepsilon. \tag{5}$$

We may readly ascertain that the integral in (5) is a vanishing quantity if the forthcoming condition is fulfiled

$$\mathfrak{L}''_{\dot{q}^2} = \mu \text{ (constant)} \tag{6}$$

g) Now, let us specify the stationary character of the motion, id est $\mathfrak{L}$ does not depends on s, in an explicit manner. Then, by a straightforward integration in (6) we obtain for $\mathfrak{L}$ the expression

$$\mathfrak{L} = \frac{1}{2}\mu\left(\frac{dq}{ds}\right)^2 + V(q)\frac{dq}{ds} - U(q). \tag{7}$$

We agree to impose to the Lagrange function in (7) the invariance restriction under time reversal $s \to -s$. This implies the vanishing of the function $V(q)$. Finally, we get the expression

$$\mathfrak{L} = \frac{1}{2}\mu\dot{q}^2 - U(q). \tag{8}$$

h) Concerning the structure of the unknown function $U(q)$, we put forward the hypothesis according to which $U(q)$ effectively reaches a minimum valus for $q = q_0$, and the motion elongation never surpasses some limits in the proximity of $q_0 (q_1 < q_0 < q_2)$, id est the case of small oscillations).

i) The characteristic function $\mathfrak{L}$ acquires, in this way, the final form

$$\mathfrak{L}(q, \dot{q}) = \frac{1}{2}\mu\dot{q}^2 - \frac{1}{2}U''_{q_0^2}(q-q_0)^2) + \text{Const.} \tag{9}$$

j) Proceeding from the above formula, and assuming that $\varepsilon(s)$ strongly depends on its argument s only in the neighbourhood of s_1 and s_2, we reach the formula

$$\int_{s_1}^{s_2} [L(q+\varepsilon) - L(q)]ds = \varepsilon\int_{s_1}^{s_2}\{\mathfrak{L}'_q - \frac{d}{ds}(\mathfrak{L}'_{\dot{q}})\}ds + \frac{1}{2}\varepsilon^2\tau = \Omega \tag{10}$$

$$\tau \equiv \int_{s_1}^{s_2}\left\{\mathfrak{L}''_{q^2} - \frac{d}{ds}(\mathfrak{L}''_{q\dot{q}})\right\}ds\ ;\ \Omega \equiv \varepsilon I_1 + \frac{1}{2}\varepsilon^2 I_2 + \ldots \tag{11}$$

k) Accordingly, we have

$$P(s_1, s_2; \varepsilon) = e^{-\frac{k}{s_2 - s_1}\left(\varepsilon I_1 + \frac{1}{2}\varepsilon^2 I_2 + \ldots\right)} \tag{11'}$$

l) Now, we ask the condition that the probability of performing the motion along the real trajectory should be maximal. This leads to the subsequent result

$$\left(\frac{\partial P(s_1, s_2; \varepsilon)}{\partial\varepsilon = 0}\right)^{\varepsilon=0} = 0 \to I_1 \equiv \int_{s_1}^{s_2}\left\{\mathfrak{L}'_q - \frac{d}{ds}(\mathfrak{L}'_{\dot{q}})\right\}ds = 0. \tag{12}$$

As (s_1, s_2) are arbitrary values, the condition (12) turns out be to equivalent to the Euler & Lagrange variational principle

$$\mathfrak{L}'_q - \frac{d}{ds}(\mathfrak{L}'_{\dot{q}}) = 0. \tag{13}$$

From (13) and (9) it results that the motion equation describes an harmonic oscilation around the equilibrium position q_0

$$\mu\frac{d^2q}{ds^2} + U''_{q_0^2}(q-q_0) = 0. \tag{14}$$

(In this respect, we have to remember that $U''_{q_0^2} > 0$, as far as U reaches its minimal value for q_0).

m) Now, let us come back to the expression (11) of the probability. It becomes

$$P(s_1, s_2; \varepsilon) = e^{-\frac{1}{2}k\varepsilon^2\left(\frac{I}{s_2 - s_1}\right)} \tag{15}$$

where

$$\frac{I_2}{s_2-s_1} = \frac{1}{s_2-s_1}\int_{s_1}^{s_2}\left\{\mathfrak{L}''_{q^2} - \frac{d}{ds}(\mathfrak{L}''_{q\dot{q}})\right\}ds = -\frac{1}{s_2-s_1}\int_{s_1}^{s_2} U''_{q_0^2}ds = -U''_{q_0^2} \tag{16}$$

But $0 \leqslant P(s_1, s_2; \varepsilon) \leqslant 1$, entailing for K a negative value. Consequently, we denote $K = -K_0$, $K_0 > 0$. The expected expression of the probability becomes, in this way

$$P(s_1, s_2; \varepsilon) = e^{-\frac{1}{2}k_0 U''_{q_0^2}\varepsilon^2} = f(q_0, \varepsilon). \tag{17}$$

To remark that this expression depends — as was expected — solely on the quantities q_0 (equilibrium position) and ε (derogation from the real trajectory).

n) Further on, we try to find out the statistical law for distributing the virtual trajectory nearby the real one. Let, in this respect, be $N(\varepsilon)$ the number of trajectories, whose departure lies between 0 and ε. If we assume the reasonable hypothesis, according to which $N(\varepsilon)$ is proportional to ε, then the number trajectories having a derogation ε and lying in the transgression strip $\left(\varepsilon - \frac{1}{2}\delta\varepsilon,\ \varepsilon + \frac{1}{2}\delta\varepsilon\right)$, will be $\delta N = n(q_0)\delta\varepsilon$, where $n(q_0)$ does not depend on ε. Consequently, the elementary probability $\delta\mathfrak{P}$, that a point-like body should travel at the instant s_0 (to which it corresponds, on the real trajectory, a quotation q_0) on a trajectory deviated writh ε, within the tolerance band $\delta\varepsilon$ is

$$\delta\mathfrak{P} = f(q_0, \varepsilon)n(q_0)\delta\varepsilon. \tag{18}$$

o) Obviously, this probability must be normalized, id est

$$\int d\mathfrak{P} = \int_{-\infty}^{+\infty} f(q_0, \varepsilon)n(\varepsilon)d\varepsilon = 1. \tag{19}$$

From (19) and (17) we infer the elementary probability as having the expression

$$\delta\mathfrak{P} = \sqrt{\frac{k_0}{2\pi}U''_{q_0^2}}\cdot e^{-\frac{1}{2}k_0 U''_{q_0^2}\varepsilon^2}\delta\varepsilon, \tag{20}$$

which correspond to a normal (Gauss) distribution, but whose dispersion depends, however, on the equilibrium coordinate q_0.

p) For a purely elastic motion the dispersion is constant, for any value of the coordinate and for any amplitude of the motion.

r) The free variable s is to be identified in classical mechanics with the Newtonian time, Newertheless, the results infered from this entering upon have a more general validity. For instance, s may be identified with the geodetic length from the Relativity Theory of Einstein and — in this case — μ which will be a constant quantity along the geodetic trajectory, preserves its meaning as mass of inertia.

s) If the potential energy $U(q)$ does not reach its effective minimum at q_0, then $U'_{q_0} \neq 0$ and, as a matter of fact, the formula (9) must be replaced with a more general one, namely

$$\mathfrak{L}(q, \dot{q}) = \frac{1}{2}\mu\dot{q}^2 - U'_{q_0}(q-q_0) - \frac{1}{2}U''_{q_0^2}(q-q_0)^2 + \text{Const.} \tag{21}$$

The direct consequence following from this amendment is the addition of a constant force term in the right side of the equation (14)

$$\mu\frac{d^2q}{ds^2} + U''_{q_0^2}(q-q_0) = -U'_{q_0}. \tag{22}$$

which accounts for the fact that the displacements downward and upward from the point q_0 are no longer equal. One ascertains, however, that the result (16) is not changed when the function (21) is used instead of the M restrictive version (9). Consequently, the final result, (20) keeps its meaning along trajectory, excepting the points when $U''_{q_0^2} \leqslant 0$ and $\delta\mathfrak{P}$ corresponds to the probability of deviation from the normal trajectory, in a local variational process (the fixed points for which $\delta\varepsilon_1 = 0$, $\delta\varepsilon_2 = 0$, being displaced together with the coordinate q_0).

t) In this way, the sharp determinism of Newtonian Mechanics is to a certain extent infringed, in favour of a statistical one, as is foreseen by Quantum Mechanics.

u) It is equally possible to define an entropy for our simple mechanical system by asking the proportionality between entropy and logarithm of probability. In this way, the variational process corresponds to the reaching of a maximal entropy state. This connection between variational process and probability on a side, and between probability and entropy on the other side, is to be interpreted rather as pertaining to the methodology of the theory of systems, than to the statistical Thermodynamics.

v) Some peculiar examples can be calculated using the aforementioned formulas (these situations are characterized by a parameter having the physical dimensions of $(\text{energy})^{-1}$).

z) The connections between „motion" and „probability" seems to be very sophisticated, and roughly speaking, can be presented in many „iterations" : pure non-statistical mechanics, statistical mechanics (without a global hypothesis like ergodicity), classical kinetical theories, classical statistical Thermodynamics, Quantum theories of motion.

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