

## Onsager principle for nonlinear mechanical systems modeled by stochastic dissipative equations

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A CLASSICAL MECHANICAL SYSTEM subjected to frictional forces is considered in the limit of large frictional coefficient. Random white noise is also introduced in conformity to the fluctuation-dissipation theorem. The velocity is split into a deterministic component plus a random stochastic component consequently, the evolution operator (generator) for the probability density in configuration space is evaluated recalling previous work by the same author, by stochastically averaging the flux of particles. The averages depend upon the history of the system, but memory may be eliminated by suitably defining the drift, in the limit of large time.

The fundamental solution of the diffusion equation is recast into the form of a Feynman path integral, and subsequently transformed into an Onsager–Machlup path integral, whose regressive stationary solutions satisfy the minimum entropy production principle. It is focused upon the role played by the appropriate definition of drift velocity adopted in this approach, allowing for interpretation of the Onsager–Machlup potential.

**Key words:** stochastic dynamics, minimum entropy production principle, functional integration.

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### 1. Introduction

IN PREVIOUS PAPERS it was investigated upon a stationary action principle for dissipative mechanical systems, where various forms of the dissipative force were considered as dependent upon the phase space variables [1, 2].

The equations of the motion considered, governing the evolution in time of those systems, were Langevin equations, which were assumed to satisfy the fluctuation-dissipation relations [3–5], while the corresponding configurational transition probability densities were shown to evolve according to the Smoluchowski equation, which is the Fokker–Planck equation restricted to configuration space [6–11]. This work, which is intended to follow this line of investigation, is restricted to consider the case of very large frictional coefficient, so that the resulting motion is in the overdamped regime.

The aim of the present work is the derivation of path-integral expressions for the fundamental solutions of the Smoluchowski equations, describing the evolution in time of the transition probability densities [12–14]. The main scope is to prove that, if the appropriate equation for the drift is established, which is the gradient of a velocity potential, then not only a great simplification in the diffusion operator occurs, yielding a memoryless Markovian evolution equation, but also the path integral solution transforms into the expression given by Onsager and Machlup for linear systems, thus providing a natural generalization of that theory. At the same time, a clear connection is established between the Onsager–Machlup function and the basic physical variables characterizing the system.

The definition of path-integrals for the solutions of these equations is rather controversial in the nonlinear case [15–21]. This leads to uncertainty upon the weight to be assigned to different points of each segment into which the trajectory is subdivided [15], and consequently, to somewhat artificial adjustments over the normalization factors, so that the required differential equations should be satisfied.

In this work it is shown that by defining properly the weight, equivalence between the Feynman and Onsager–Machlup path-integral results, by using an algebraic identity due to M. RONCADELLI [22]. In the present case, the action is not simply the solution of a Hamilton–Jacobi equation for the given potential like in [22], but rather the singular solution of a Hamilton–Jacobi–Riccati (HJR) equation, whose potential energy function is created by the equilibrium solution of the Smoluchowski equation (4.1') (see Eq. (4.10)), through the drift velocity and diffusion coefficient.

This HJR equation is identified, with leading orders of the expansion in inverse powers of the frictional coefficient, to that one which was proved (Eqs. (2.4), (2.6)) to model the drift velocity of a system driven by a random force, described by a Langevin equation. This allows to interpret and to give a correspondence between the terms appearing in the Onsager–Machlup formulation of path-integral, as well as in the Feynman path average, with the external potential acting in the Langevin equation (Eq. (4.13)).

It is not a trivial fact that the two procedures are exactly consistent with each other, which is a confirmation of the exactness of the whole scheme, leading from Langevin to the Smoluchowski equation (see Sec. 4).

## 2. Dynamical model for a coupled system

A non-isolated dynamical system is considered, for simplicity one-dimensional, which is strongly coupled to a larger system called the bath, thereby continuously exchanging energy with the environment. Therefore the complete

Hamiltonian, representing the energy of the system in interaction, is written as:

$$(2.1) \quad H(p, q, t) = \frac{p^2}{2m} + U(q) - q\Xi(t),$$

where the phase coordinates of the system are  $q$  and  $p$  as usual, and  $m$  is its mass.  $U(q)$  is the potential energy which is assumed to be a smooth function of the arguments,  $\Xi(t)$  is a real physical force which is the result of the complete interaction of the small system with the environment (see, for instance [23]). By its nature it is very irregular and unpredictable, since it is the result of many uncorrelated and independent phenomena. Consequently, it is computationally convenient to model it as a mathematically defined random quantity (i.e. not endowed with a definite value as a function of time, but with a distribution of admissible values with well defined statistical properties). It is therefore *assumed* that  $\Xi(t)$ ,  $t \in (-\infty, +\infty)$  is a stationary Gaussian stochastic process with zero mean, whose realizations will be denoted by  $\xi(t)$ . Depending upon the nature of the physical system under consideration, the random force  $\xi(t)$  will in general have a finite correlation time [24], which is assumed here to be so small as to be considered vanishing on the time-scale of interest [25]. Therefore it is assumed to be the white noise property [7]

$$(2.2) \quad \langle \xi(t)\xi(s) \rangle = 2m\beta T\delta(t-s),$$

where the brackets denote stochastic averages of the realizations  $\xi(t)$  of the Wiener process,  $t$  and  $s$  are time coordinates,  $\beta$  is the frictional coefficient,  $T$  the absolute temperature in energy units (or natural [3] units),  $\delta(\alpha)$  being the Dirac  $\delta$ -function whose argument is  $\alpha$ . Since the stochastic process  $\Xi(t)$ ,  $t \in (-\infty, +\infty)$  is the limit of processes with nonvanishing correlation times, the Stratonovich rules, which are the ordinary rules of calculus, may be used (see [24, 25] and references therein). From the theorem of CALLEN and WELTON [4], or the second fluctuation dissipation theorem, follows that the small system experiences a frictional force proportional to velocity

$$(2.3) \quad f_v = -\beta p.$$

The equations of motion for the system coupled to the environment can be deduced from the Hamilton–Jacobi–Yasue (HJY) partial differential equation in two independent variables  $q$  and  $t$  [1, 2, 26]:

$$(2.4) \quad \frac{1}{2m} \left( \frac{\partial f}{\partial q} \right)^2 + U(q) - q\xi(t) + \beta f(q, Q, t) + \frac{\partial f}{\partial t} = 0,$$

where  $f(q, Q, t)$  is the generating function of a canonical transformation of variables from  $(p, q)$  to  $(P, Q)$ , where  $Q$  is a constant of the motion. In order to take

into account the stochastic nature of the system motion, it is convenient to split the function  $f$  into two components:

$$(2.5) \quad f(q, Q, t) = \varphi(q, Q) + \tilde{f}(q, Q, t).$$

Upon substitution of Eq. (2.5) into (2.4), the following pair of equations is obtained by introduction of a separating function  $G(q, Q)$ :

$$(2.6) \quad \frac{1}{2m} \left( \frac{\partial \varphi}{\partial q} \right)^2 + U(q) + \beta \varphi(q, Q) = G(q, Q),$$

$$(2.6') \quad \frac{1}{2m} \left( \frac{\partial \tilde{f}}{\partial q} \right)^2 + \frac{1}{m} \frac{\partial \varphi}{\partial q} \frac{\partial \tilde{f}}{\partial q} - q \xi(t) + \beta \tilde{f}(q, Q, t) + \frac{\partial \tilde{f}}{\partial t} = -G(q, Q).$$

Accordingly, as it was proven in [8–11], the equations of motion for the variable  $q(t)$  follow in the form:

$$(2.7) \quad \frac{dq}{dt} = \frac{1}{m} p(q, Q) + \frac{1}{m} \tilde{p}(q(t), Q, t),$$

$$(2.7') \quad \frac{d\tilde{p}}{dt} + \left( \frac{1}{m} \frac{\partial^2 \varphi}{\partial q^2} + \beta \right) \tilde{p}(q, Q, t) = \xi(t) - \frac{\partial G}{\partial q},$$

with

$$(2.8) \quad p(q, Q) = \frac{\partial \varphi}{\partial q}, \quad \tilde{p}(q, Q, t) = \frac{\partial \tilde{f}}{\partial q}.$$

$G(q, Q)$  being an arbitrary smooth function of the arguments to be appropriately defined later. It will be shown (see Eqs. (3.2'), (3.8)), that through an appropriate definition of  $G(q, Q)$ ,  $(1/m)p(q, Q)$  and  $(1/m)\tilde{p}(q, Q, t)$  acquire a clear physical significance, which is the drift velocity and the diffusive velocity respectively, while the diffusion equation for the two-time probability density is considerably simplified into a memoryless Markovian equation.

Equations (2.7), (2.7') are the characteristic curves of Eq. (2.6').  $\tilde{p}(q, Q, t)$  is given by the formal solution

$$(2.9) \quad \tilde{p}(q(t), Q, t) = \int_{-\infty}^t ds \mathcal{G}(t, s) \left\{ \xi(s) - \frac{\partial G}{\partial q(s)} \right\}$$

with

$$(2.9') \quad \mathcal{G}(t, s) = \exp \left\{ -\frac{1}{m} \int_s^t \frac{\partial p}{\partial q(\alpha)} d\alpha - \beta(t-s) \right\}.$$

Eqs. (2.7) and (2.7') may be solved with the boundary conditions prescribed in the quoted references, assuming that the system should be equilibrated with the environment in temperature  $T$ , at time  $t_0$ , and moreover:

$$(2.10) \quad q(t_0) = q_0.$$

Eq. (2.7) bears some similarity to a Langevin equation, because the second term on the rhs is mainly a function of time alone in the limiting case of high frictional coefficient  $\beta$ ; but in fact, it is not strictly a Gaussian random variable, because it is the weighted sum of a collection of Gaussian random variables, plus a trajectory-dependent term, which becomes a term dependent upon the final point of the trajectory in that limiting case. Through the imposed boundary conditions,  $\tilde{p}(t)$  may be regarded as a Gaussian–Markov random variable with vanishing small correlation time, zero average and constant variance, only in the limit of large  $\beta$  and by means of the appropriate definition of  $G(q, Q)$  [8–11], explained in the next paragraph. Actually, the correlation function

$$(2.11) \quad \frac{1}{m^2} \langle \tilde{p}(t) \tilde{p}(s) \rangle \xrightarrow{\beta \rightarrow +\infty} \frac{T}{m} \exp\{-\beta |t - s|\} \xrightarrow{\beta \rightarrow +\infty} 2 \frac{T}{m\beta} \delta(t - s),$$

what is proved in Appendix A. Most of the following developments, however, do not rely upon these limiting properties, which are however generally assumed in most treatments of the Brownian noise [12, 13, 15, 19, 20].

### 3. The diffusion equation in configuration space

The diffusion equation in configuration space may be obtained through the equation of continuity, and using (2.7)

$$(3.1) \quad \frac{\partial}{\partial t} \langle \delta(q(t) - q) \rangle = -\frac{\partial}{\partial q} \frac{1}{m} p(q) \langle \delta(q(t) - q) \rangle - \frac{\partial}{\partial q} \frac{1}{m} \langle \tilde{p}(q(t), Q, t) \delta(q(t) - q) \rangle$$

where, using the prime to denote differentiation with respect to  $q$  [8–11]:

$$(3.2) \quad \frac{1}{m} \langle \tilde{p}(q(t), Q, t) \delta(q(t) - q) \rangle = \langle \mathcal{D}(t, t_0) \delta'(q(t) - q) \rangle - \frac{1}{m} \int_{-\infty}^t d\alpha \int_{-\infty}^{+\infty} d\eta \langle \delta(q(t) - q) \mathcal{G}(t, \alpha) \delta(q(\alpha) - \eta) \times [\mathcal{D}(\alpha, t_0) p''(\eta) + g(\eta)] \rangle,$$

$$(3.2') \quad g(\eta) = \frac{\partial G}{\partial \eta},$$

with

$$(3.3) \quad \mathcal{D}(\alpha, t_0) = \int_{-\infty}^{\alpha} ds \int_{-\infty}^{\max(\alpha, t_0)} d\sigma \frac{\delta q(\alpha)}{\delta k(\sigma)} \mathcal{G}(\alpha, s) \langle \xi(s) \xi(\sigma) \rangle.$$

This expression holds also for  $\alpha < t_0$ , although the response functions are, in the latter case, more involved (see [11]).

In Eq. (3.2) the first term on the rhs may easily be integrated over  $dq$ , and the result is zero under the appropriate boundary conditions at infinity.

Upon expansion of the first term in the rhs of (3.2) into powers of the autocorrelation function  $\langle \xi(s) \xi(\sigma) \rangle$ , this term may be recast into the form of a differential operator acting upon the variable  $q$ , say:

$$(3.4) \quad \langle \mathcal{D}(t, t_0) \delta'(q(t) - q) \rangle = -\frac{\partial}{\partial q} \hat{D}_q(t, t_0) \langle \delta(q(t) - q) \rangle.$$

Then, Eq. (3.2) is rearranged in the following manner:

$$(3.5) \quad \begin{aligned} \frac{1}{m} \langle \tilde{p}(q(t), Q, t) \delta(q(t) - q) \rangle &= -\frac{\partial}{\partial q} \hat{D}_q(t, t_0) \langle \delta(q(t) - q) \rangle \\ &- \frac{1}{m} \int_{-\infty}^{+\infty} d\eta \int_{t_0}^t d\alpha \langle \delta(q(t) - q) \mathcal{G}(t, \alpha) \hat{D}_\eta(\alpha, t_0) \delta(q(\alpha) - \eta) \rangle p''(\eta) \\ &- \frac{1}{m} \int_{-\infty}^{+\infty} d\eta \int_{t_0}^t d\alpha \langle \delta(q(t) - q) \mathcal{G}(t, \alpha) \delta(q(\alpha) - \eta) \rangle g(\eta) \\ &- \frac{1}{m} \int_{-\infty}^{+\infty} d\eta \int_{-\infty}^{t_0} d\alpha \langle \delta(q(t) - q) \mathcal{G}(t, \alpha) \delta(q(\alpha) - \eta) [\mathcal{D}(\alpha, t_0) p''(\eta) + g(\eta)] \rangle. \end{aligned}$$

There results further

$$(3.6) \quad \begin{aligned} &\langle \tilde{p}(q(t_0), Q, t_0) \delta(q(t_0) - q_0) \rangle \\ &= \langle \tilde{p}(q(t_0), Q, t_0) \delta(q(t_0) - q_0) \\ &\quad - \delta(q(t_0) - q_0) \int_{-\infty}^{+\infty} d\eta \int_{-\infty}^{t_0} d\alpha \langle \mathcal{G}(t_0, \alpha) \delta(q(\alpha) - \eta) [\mathcal{D}(\alpha, t_0) p''(\eta) + g(\eta)] \rangle \\ &= \delta(q(t_0) - q_0) \int_{-\infty}^{t_0} \langle \mathcal{G}(t_0, s) [\xi(s) - g(q(s))] \rangle ds. \end{aligned}$$

Bounds on the rhs may be evaluated using (3.3) if the response functions are conveniently bounded. A rough estimate may be obtained by putting

$$\begin{aligned}
 (3.7) \quad & \int_{-\infty}^{t_0} ds \left\langle \exp \left\{ -\beta(t_0 - s) - \frac{1}{m} \int_s^{t_0} p'(q(\alpha)) d\alpha \right\} (\xi(s) - g(q(s))) \right\rangle \\
 & \cong_{\beta \rightarrow +\infty} \int_{-\infty}^{t_0} ds \exp \left\{ - \left( \beta + \frac{1}{m} p'(q_0) \right) (t_0 - s) \right\} \langle (\xi(s) - g(q(s))) \rangle \\
 & \cong \frac{-g(q_0)}{\beta + \frac{1}{m} p'(q_0)}.
 \end{aligned}$$

Consequently, in Eq. (3.5) it is possible to disregard the last term, on the ground that the function  $\mathcal{G}(t, \alpha) = \mathcal{G}(t, t_0)\mathcal{G}(t_0, \alpha)$  is a rapidly decreasing function of the time difference  $t - t_0$ .

Another approximation has been introduced in the rhs of Eq. (3.5), namely the neglect of correlations between  $\mathcal{D}(\alpha, t_0)$  and coordinate values at times subsequent to  $\alpha$ , which makes the operator  $\hat{D}_\eta(\alpha, t_0)$  acting upon the variable  $\eta$  only. The Markov assumption that the subsequent evolution of the system is determined only by the coordinate distribution at time  $\alpha$  for  $\alpha \geq t_0$ , is justified by considering that, for large  $\beta$ , the fluctuating part of velocity decays so fast to equilibrium<sup>1)</sup>, that the subsequent evolution of the system is determined by the sole coordinate value and the subsequent values of the force, being largely independent of the past history. This however does not exclude the correlations between coordinate values anterior and posterior to the time labelled  $\alpha$  to persist. However, for  $\beta$  tending to infinity, these correlations are assumed to decay in a very short time interval, consequently as far as this assumption is valid<sup>2)</sup>, the second and third terms in the rhs of this equation cancel identically in both  $\alpha$  and  $\eta$ , for  $\alpha \gg t_0$ , upon defining<sup>3)</sup>:

$$(3.8) \quad g(\eta) = - \lim_{\alpha \rightarrow +\infty} \hat{D}_\eta^{\text{tr}}(\alpha, t_0) p''(\eta).$$

By this tool, the memory term is also eliminated from the rhs of Eq. (3.2) in

<sup>1)</sup>From (3.4) it follows that the velocity probability distribution is dependent upon the coordinate probability density and its derivatives.

<sup>2)</sup>This can be done only up to  $O(1/\beta^4)$ . For higher orders in  $1/\beta$ , correlations with subsequent values of time must be taken into account, and the memory term yields also corrections to the diffusion coefficient [10].

<sup>3)</sup>This requires some sort of uniformity in the convergence of the diffusion coefficient to the limit value with respect to the assumed initial conditions.

that limit, so that Eq. (3.1) results in the simple Markovian form:

$$(3.9) \quad \frac{\partial}{\partial t} \langle \delta(q(t) - q) \rangle = -\frac{\partial}{\partial q} \frac{1}{m} p(q, Q) \langle \delta(q(t) - q) \rangle \\ + \frac{\partial^2}{\partial q^2} \left[ \lim_{t-t_0 \rightarrow +\infty} \hat{D}_q(t, t_0) \right] \langle \delta(q(t) - q) \rangle,$$

with

$$(3.10) \quad \langle \delta(q(t) - q) \rangle = P_2(q, t/q_0, t_0),$$

where  $P_2(q, t/q_0, t_0)$  is the two-time transition probability density from  $q_0, t_0$  to  $q, t$ . The main interest here is the limiting form of Eq. (3.9) as  $t - t_0 \rightarrow +\infty$ . Then the equation governing the two-time transition probability density is

$$(3.9') \quad \frac{\partial}{\partial t} P_2(q, t/q_0, t_0) = \left[ -\frac{\partial}{\partial q} \frac{1}{m} p(q, Q) + \frac{\partial^2}{\partial q^2} \hat{D}_q^\infty \right] P_2(q, t/q_0, t_0).$$

The propagator for this equation  $K(q, t/q_1, t_1)$  with  $t_1 \gg t_0$ , does not represent the true transition probability density, but a transition probability for a substitutive pseudo-Markov process, under suitable assumptions, in order to reproduce the temporal evolution of fluctuations over a stationary state [29, 30].

Therefore, we have succeeded in describing the evolution of probability density of the system through a Markovian equation, by taking the whole probability distribution at a single time as a set of variables, the memory term in the evolution equation having been made vanishing identically. As a result, in the limit  $t - t_0 \rightarrow +\infty$  the drift velocity is constrained to obey a HJY equation supplemented by an additional term, the Riccati term, given by Eqs. (3.2'), (3.8). If  $\hat{D}_q^\infty$  is a constant number, then Eq. (2.6) becomes a true HJYR equation in a strict sense.

#### 4. The propagator of the diffusion equation

In the following we shall be concerned with the limit for  $\beta \rightarrow +\infty$  of Eq. (3.9'), and therefore take the leading terms of the asymptotic [2, 10] expansion in powers of  $1/\beta$  of each coefficient of that equation. The following singular solution of Eq. (2.6) is used (see [2, 8–10]), which does not contain arbitrary parameters or constants of the motion:

$$(4.1) \quad p(q, Q) = -\frac{U'(q)}{\beta} + O\left(\frac{1}{\beta^3}\right).$$

There results

$$(4.1') \quad \frac{\partial P_2}{\partial t} = \left[ \frac{\partial}{\partial q} \frac{1}{m\beta} U' + \frac{\partial^2}{\partial q^2} \frac{T}{m\beta} \right] P_2(q, t/q_0, t_0).$$

Equation (4.1'), as it has been already stated, describes a pseudo-Markovian stochastic process, in the limit  $t - t_0 \gg 1/\beta$ . The steady-state solution of this equation with vanishing flux of particles is

$$(4.2) \quad P_e(q) \propto \exp\left\{-\frac{U(q)}{T}\right\},$$

which is assumed to be real. Then, on putting

$$(4.3) \quad P_2(q, t) = \psi(q, t)P_e(q)^{1/2} = \psi(q, t)\psi_e(q),$$

there results from (4.1') that  $\psi(q)$  obeys, to the same order of approximation, the equation similar to the heat equation:

$$(4.4) \quad -\frac{2T^2}{m\beta^2}\psi''(q, t) + \left[\frac{U'^2}{2m\beta^2} - \frac{TU''}{m\beta^2}\right]\psi(q, t) = -\frac{2T}{\beta}\frac{\partial\psi}{\partial t},$$

which has the same form of the Schroedinger equation, with the only difference that the coefficient of the time-derivative is real. Then, upon looking for solutions of the form

$$(4.5) \quad \frac{\partial\psi}{\partial t} = -\lambda\beta\psi,$$

Eq. (4.4) is transformed into the eigenvalue equation

$$(4.6) \quad -\frac{2T^2}{m\beta^2}\psi''(q) + \left[\frac{U'^2}{2m\beta^2} - \frac{TU''}{m\beta^2}\right]\psi(q) = 2T\lambda\psi(q),$$

whose eigenvalues  $2T\lambda_n$  are assumed to be bounded from below and discrete, the function  $\psi_e(q)$  corresponding to the lowest eigenvalue  $\lambda_0 = 0$  [27]. The solution to Eq. (4.4) with boundary conditions  $\delta(q - q_0)$  as  $t \rightarrow t_0$  is representable as a linear combination of normalized eigenfunctions

$$(4.7) \quad k(q, t/q_0, t_0) = \sum_{n=0}^{\infty} \psi_n(q)\bar{\psi}_n(q_0)\exp\{-\lambda_n\beta(t - t_0)\},$$

where  $\bar{\psi}_n$  is the time-reversed solution to Eqs. (4.4), (4.5). This requires a reversed sign on the rhs of those equations. Since the boundary conditions are real,  $\bar{\psi}_n$  is the c.c. to  $\psi_n$ , so that it satisfies Eq. (4.6) with c.c. coefficients. The corresponding propagator for Eq. (4.1') is

$$(4.8) \quad K(q, t/q_0, t_0) = \sum_{n=0}^{\infty} \psi_n(q)\bar{\psi}_n(q_0)\frac{\bar{\psi}_e(q)}{\bar{\psi}_e(q_0)}\exp\{-\lambda_n\beta(t - t_0)\},$$

which satisfies the proper boundary conditions. Following R. FEYNMAN and A. HIBBS [14], the kernel (4.7) is representable as a path integral:

$$(4.9) \quad k(q, t/q_0, t_0) = \int_{q_0, t_0}^{q, t} \mathcal{D}q(\alpha) \exp \left\{ -\frac{m\beta}{4T} \int_{t_0}^t d\alpha \left[ \dot{q}^2 + \frac{2}{m} V(q(\alpha)) \right] \right\},$$

where

$$(4.10) \quad V(q) = \frac{U'^2}{2m\beta^2} - \frac{TU''}{m\beta^2}.$$

There results from (4.9) the path-integral representation

$$(4.11) \quad K(q, t/q_0, t_0) = \int_{q_0, t_0}^{q, t} \mathcal{D}q(\alpha) \exp \left\{ -\frac{m\beta}{4T} \int_{t_0}^t d\alpha \left[ \dot{q}^2 + \frac{2}{m} V(q(\alpha)) \right] - \frac{1}{2T} \int_{t_0}^t d\alpha \dot{q} \frac{dU}{dq(\alpha)} \right\}.$$

By applying Roncadelli's identity [22] to the rhs of Eq. (4.11), there results

$$(4.12) \quad K(q, t/q_0, t_0) = \int_{q_0, t_0}^{q, t} \mathcal{D}q(\alpha) \exp \left\{ -\frac{m\beta}{4T} \int_{t_0}^t d\alpha \left[ \dot{q} + \frac{1}{m\beta} \frac{dU}{dq(\alpha)} \right]^2 + \frac{\beta}{2T} \int_{t_0}^t d\alpha \left[ \frac{1}{2m\beta^2} \left( \frac{dU}{dq(\alpha)} \right)^2 - V(q(\alpha)) \right] \right\} \\ = \int_{q_0, t_0}^{q, t} \mathcal{D}q(\alpha) \exp \left\{ -\frac{m\beta}{4T} \int_{t_0}^t d\alpha \left[ \dot{q} + \frac{1}{m\beta} \frac{dU}{dq(\alpha)} \right]^2 + \frac{1}{2m\beta} \int_{t_0}^t d\alpha \frac{d^2U}{dq(\alpha)^2} \right\}.$$

Some remarks are in order for Eqs. (4.11), (4.12). Equation (4.11) is the path-average of the "action-production" integral, multiplied by the weight factor

$$\exp \left\{ -\frac{1}{2T} (U(q) - U(q_0)) \right\},$$

which is of course path-independent [15, 19, 20]. It is formally the same as the averaged exponential of the entropy-production integral introduced by L. ONSAGER [12, 28], and extended to dissipative dynamical systems by S. MACHLUP and L. ONSAGER [13, 20, 21], except for a constant factor with dimension of time.

The second term in the argument of the exponential of the rhs of Eq. (4.12) plays a role in the correct definition of the path integral, as it will be explained in the next paragraph. Surprisingly enough, it does not appear in RONCADELLI's developments [22], and is disregarded as "unphysical" by B. H. LAVENDA [19]. From the definition (4.10) of the potential  $V(q)$  it follows trivially that  $\varphi_e(q)$  must obey a Hamilton–Jacobi–Riccati equation with potential energy  $V(q)$ . However notice that, from the definition of  $\varphi_e(q)$  adopted here (Eqs. (2.6), (3.2') (3.8)), follows that

$$(4.13) \quad V(q) = -U(q) - \beta\varphi_e(q) + O\left(\frac{1}{\beta^4}\right),$$

which yields an interpretation of the Onsager–Machlup Lagrangian for the process described by Eqs. (4.1'), (4.9) through the HJYR Eq. (2.6), and *vice-versa*. In fact, given a potential energy function  $V(q)$  and requiring that (4.13) should be satisfied, implies

$$(4.14) \quad \frac{1}{2m\beta^2} \left(\frac{dU}{dq}\right)^2 - \frac{T}{m\beta^2} \frac{d^2U}{dq^2} + U(q) + \beta\varphi_e(q) = O\left(\frac{1}{\beta^4}\right),$$

so that  $\varphi_e(q)$  satisfies a HJYR equation up to  $O(1/\beta^2)$ .

The identification (4.13) is not trivial since the two members of the equality have been obtained following the completely independent arguments: the lhs from the Smoluchowski or the related heat equation, the rhs from Hamilton–Jacobi–Yasue theory of equations of motion, with the adopted definition of  $g(q)$  in order to eliminate memory terms. It is therefore remarkable that Eq. (4.14) yields the exact expansion of  $\varphi_\varepsilon(q)$  up to  $O(1/\beta^3)$ , since this is a direct consequence of Eqs. (2.6), (3.2'), (3.8) without having recourse to the Smoluchowski equation, which may be derived by entirely independent arguments. This proves that the definition of  $g(q)$  which has been adopted is the correct one. Insertion of these terms into Eq. (4.1') determines corrections to the diffusion coefficient, by the condition that the equilibrium probability distribution should be proportional to  $\exp\{-U(q)/T\}$  and in turn, new terms of the drift can be obtained, by a recursive procedure. In this way it may be obtained (terms  $O(1/\beta^2)$  in  $D(q)$  have been put equal to zero):

$$(4.15) \quad D(q) = \frac{T}{m\beta} + \frac{T}{m^2\beta^3}U''(q) + \text{h.o.t.}$$

and by substituting into the derivative of Eq. (2.6)

$$(4.16) \quad p(q) = -\frac{U'}{\beta} - \frac{1}{m\beta^3}(U'U'' - TU''') \\ - \frac{1}{m^2\beta^5}(U'^2U''' + 2U'U''^2 - 2TU'U'''' - 5TU''U''' + T^2U''''').$$

The leading terms of this expansion were first obtained by G. WILEMSKI [31], by projection of the full phase-space Fokker–Planck equation onto the configuration space. A more exhaustive deduction directly in coordinate space was carried out in [9, 10].

## 5. Discretization of the path integral

The path-integral averages which are introduced in Eqs. (4.11), (4.12) need to be defined as the proper limit of multidimensional integrals, by subdividing the interval  $(t_0, t)$  into a finite number of segments, whose maximum length is made decreasing toward zero. It is assumed for simplicity that all the  $N$  segments have equal length  $\varepsilon$ . The origin of each segment is numbered from zero to  $N - 1$ . The path function  $q(\alpha)$ ,  $t_0 \leq \alpha \leq t$ , is then approximated by a polygonal curve, while the derivative  $\dot{q}(\alpha)$  assumes the value of the slope of the straight line connecting two contiguous points  $q(\alpha_i)$ ,  $q(\alpha_{i+1})$ . Then, Eq. (4.11) is written as follows:

$$\begin{aligned}
 (5.1) \quad K(q, t/q_0, t_0) &= \lim_{\varepsilon \rightarrow 0} \int_{-\infty}^{+\infty} dq_1 \dots \int_{-\infty}^{+\infty} dq_{N-1} \mathcal{N}^N \\
 &\times \exp \left\{ -\frac{m\beta}{4T} \sum_{i=0}^{N-1} \varepsilon \left[ \left( \frac{q_{i+1} - q_i}{\varepsilon} \right)^2 + \frac{V(q_{i+1}) + V(q_i)}{m} \right] \right. \\
 &\quad \left. - \frac{1}{4T} \sum_{i=0}^{N-1} (q_{i+1} - q_i)(U'(q_{i+1}) + U'(q_i)) \right\} \\
 &= \lim_{\varepsilon \rightarrow 0} \int_{-\infty}^{+\infty} d\eta_0 \dots \int_{-\infty}^{+\infty} d\eta_{N-2} \left( \frac{4\pi T \varepsilon}{m\beta} \right)^{-N/2} \\
 &\times \exp \left\{ -\frac{m\beta}{4T} \sum_{i=0}^{N-1} \varepsilon \left[ \left( \frac{\eta_i}{\varepsilon} \right)^2 + \frac{V(q_{i+1}) + V(q_i)}{m} \right] \right. \\
 &\quad \left. - \frac{1}{4T} \sum_{i=0}^{N-1} \eta_i (U'(q_{i+1}) + U'(q_i)) \right\},
 \end{aligned}$$

where  $q_i$  is shorthand for  $q(\alpha_i)$  and

$$(5.1') \quad \begin{cases} q_{i+1} = q_0 + \sum_{j=0}^i \eta_j, & i = 0, \dots, N-1, \\ q_N = q, \end{cases}$$

$$(5.1'') \quad \left| \frac{\partial(\eta_0, \dots, \eta_{N-2})}{\partial(q_1, \dots, q_{N-1})} \right| = 1,$$

$\mathcal{N}$  being the normalization factor, which has been fixed so as to be correct for leading order in the limit  $\varepsilon \rightarrow 0$ . For every partition into  $N$  segments, integration of the expression under integral sign in (5.1) over one single variable  $q_i$  yields, because of the Chapman–Kolmogorov equation, a reduced probability density in  $N - 2$  variables:

$$\begin{aligned}
 (5.2) \quad & \int_{-\infty}^{+\infty} dq_i \exp \left\{ -\frac{m\beta}{4T} \varepsilon \left[ \left( \frac{q_{i+1} - q_i}{\varepsilon} \right)^2 + \frac{V(q_{i+1}) + V(q_i)}{m} \right] \right\} \\
 & \times \exp \left\{ -\frac{m\beta}{4T} \varepsilon \left[ \left( \frac{q_i - q_{i-1}}{\varepsilon} \right)^2 + \frac{V(q_i) + V(q_{i-1})}{m} \right] \right\} \\
 = & \int_{-\infty}^{+\infty} dq_i \exp \left\{ -\frac{m\beta}{4T} \left[ \frac{2}{\varepsilon} \left( q_i - \frac{q_{i+1} + q_{i-1}}{2} \right)^2 + \frac{1}{2\varepsilon} (q_{i+1} - q_{i-1})^2 \right. \right. \\
 & \left. \left. + \varepsilon \frac{V(q_{i+1}) + V(q_{i-1}) + 2V(q_i)}{m} \right] \right\} \\
 = & \left[ \frac{2\pi T \varepsilon}{\beta(m + \varepsilon^2 \bar{V}_i'')} \right]^{1/2} \\
 & \times \exp \left\{ -\frac{m\beta}{4T} 2\varepsilon \left[ \left( 1 - \frac{\varepsilon^2}{2m} \bar{V}_i'' \right) \left( \frac{q_{i+1} - q_{i-1}}{2\varepsilon} \right)^2 + \frac{V(q_{i+1}) + V(q_{i-1})}{m} \right] \right\} \\
 & \times \exp \left\{ \frac{\beta \varepsilon^3}{4T} \frac{\bar{V}_i'^2}{(2m + \varepsilon^2 \bar{V}_i'')} \right\},
 \end{aligned}$$

where

$$(5.2') \quad \bar{V}_i = V \left( \frac{q_{i+1} + q_{i-1}}{2} \right)$$

has been expanded up to second-order in the argument. By repeating this procedure, a family of multivariate probability densities is deduced, which shows that Kolmogorov compatibility conditions for a multivariate probability distribution function [32] are satisfied, as it is necessary, in the limit  $\varepsilon \rightarrow 0$ . Upon subdivision of each interval into two equal subintervals repeatedly, the procedure may be continued to  $\varepsilon$  so small at will, which shows that *in this limit*, an underlying stochastic process possibly exists for the infinite family of compatible probability distribution functions, from the fundamental theorem of A. N. KOLMOGOROV [32].

A proof for the convergence (simple convergence [33]) of this multiple-integral to a probability distribution function, which is an average upon the Wiener measure over the paths, may be found in [34] under mild conditions of regularity

upon  $V(q)$ . The proof is based on measurability properties of the functional to be averaged, proved by N. Wiener. Convergence rates in the mean square error norm were estimated in [35].

The evolution equation for the kernel  $K(q, t/q_0, t_0)$  is to be evaluated as follows [14], taking into account the fact that the  $\eta_i$  are independent random variables, the process being Markovian [36] (or rather pseudo-Markovian [29, 30]) in the configurational variable  $q$ : the Chapman–Kolmogorov [36] equation for the kernel  $K(q, t/q_0, t_0)$ , whose validity in the limit  $\varepsilon \rightarrow 0$  has been established above, is written

$$\begin{aligned}
(5.3) \quad & K(q, t/q_0, t_0) \\
&= \lim_{\varepsilon \rightarrow 0} \sqrt{\frac{m\beta}{4\pi T\varepsilon}} \int_{-\infty}^{+\infty} d\eta_{N-1} \\
&\quad \times \exp \left\{ -\frac{m\beta\varepsilon}{4T} \left[ \left( \frac{\eta_{N-1}}{\varepsilon} \right)^2 + \frac{V(q) + V(q_{N-1})}{m} \right] - \eta_{N-1} \frac{U'(q) + U'(q_{N-1})}{4T} \right\} \\
&\quad \times K(q_{N-1}, t - \varepsilon/q_0, t_0) \\
&= \lim_{\varepsilon \rightarrow 0} \sqrt{\frac{m\beta}{4\pi T\varepsilon}} \int_{-\infty}^{+\infty} d\eta_{N-1} \exp \left\{ -\frac{m\beta}{4T\varepsilon} \eta_{N-1}^2 \right\} \\
&\quad \times \left\{ 1 - \frac{\beta\varepsilon}{4T} (V(q) + V(q - \eta_{N-1})) - \frac{1}{4T} \eta_{N-1} (U'(q) + U'(q - \eta_{N-1})) \right. \\
&\quad \left. + \frac{1}{32T^2} \eta_{N-1}^2 (U'(q) + U'(q - \eta_{N-1}))^2 + \text{h.o.t.} \right\} K(q - \eta_{N-1}, t - \varepsilon/q_0, t_0).
\end{aligned}$$

It is required that the above equality holds up to  $O(\varepsilon)$ . Therefore,

$$\begin{aligned}
(5.4) \quad & K(q, t/q_0, t_0) - K(q, t - \varepsilon/q_0, t_0) \\
&= \sqrt{\frac{m\beta}{4\pi T\varepsilon}} \int_{-\infty}^{+\infty} d\eta \exp \left\{ -\frac{m\beta}{4T\varepsilon} \eta^2 \right\} \left\{ -\eta K'(q, t/q_0, t_0) + \frac{1}{2} \eta^2 K''(q, t/q_0, t_0) \right. \\
&\quad - \frac{\beta\varepsilon}{2T} V(q) K(q, t/q_0, t_0) - \frac{1}{2T} \eta U'(q) [K(q, t/q_0, t_0) - \eta K'(q, t/q_0, t_0)] \\
&\quad \left. + \frac{1}{4T} \eta^2 U'' K(q, t/q_0, t_0) + \frac{1}{8T^2} \eta^2 U'^2 K(q, t/q_0, t_0) + \text{h.o.t.} \right\} \\
&= \varepsilon \left\{ \frac{T}{m\beta} \frac{\partial^2}{\partial q^2} + \frac{1}{m\beta} \frac{\partial}{\partial q} \frac{\partial U}{\partial q} \right\} K(q, t/q_0, t_0) + \text{h.o.t.}
\end{aligned}$$

There follows, by going to the limit  $\varepsilon \rightarrow 0$  in Eq. (5.4), that  $K(q, t/q_0, t_0)$  defined as the limit as  $\varepsilon \rightarrow 0$  in Eq. (5.3) after integrating first over  $d\eta_{N-1}$ , verifies

Eq. (4.1'), and consequently, the Kolmogorov consistency conditions for multivariate distribution functions of the limiting process are verified in agreement with Eq. (5.2).

The following remark is in order about the discretization procedure: the last factor in Eq. (4.11) is path-independent, therefore its average is independent of the measure and must give an invariant result, consequently the time-derivative of this factor is equally known from the heat equation (4.4). These properties require that the weights should be assigned as in Eq. (5.1). Therefore the definition (5.1) of the path integral is correct, and may be applied to the rhs of Eq. (4.12) in order to obtain the desired generalization of the Onsager principle. The calculations have been displayed in some detail in order to compare this path integral representation of the propagator with the following one, which has been remodeled into the form of Onsager theory of minimum entropy production.

## 6. Generalized Onsager–Machlup principle

Using the rhs of Eq. (4.12), and considering the leading constant part of the diffusion coefficient as in Eq. (4.1'), the alternative discretized formulation of the kernel  $K(q, t/q_0, t_0)$  results:

$$\begin{aligned}
 (6.1) \quad & K(q, t/q_0, t_0) \\
 &= \lim_{\varepsilon \rightarrow 0} \left\langle \exp \left\{ -\frac{m\beta}{4T} \sum_{i=0}^{N-1} \varepsilon \left[ \frac{q_{i+1} - q_i}{\varepsilon} + \frac{U'(q_{i+1}) + U'(q_i)}{2m\beta} \right]^2 \right. \right. \\
 & \qquad \qquad \qquad \left. \left. + \sum_{i=0}^{N-1} \frac{\varepsilon}{4m\beta} (U''(q_{i+1}) + U''(q_i)) \right\} \right\rangle \\
 &= \lim_{\varepsilon \rightarrow 0} \int_{-\infty}^{+\infty} d\eta_0 \dots \int_{-\infty}^{+\infty} d\eta_{N-2} \left( \frac{4\pi T\varepsilon}{m\beta} \right)^{-N/2} \exp \left\{ -\frac{m\beta}{4T} \sum_{i=0}^{N-1} \left[ \frac{\eta_i^2}{\varepsilon} + \frac{\varepsilon}{m^2\beta^2} U'(q_i)^2 \right] \right. \\
 & \qquad \qquad \qquad \left. - \frac{1}{2T} \sum_{i=0}^{N-1} \left[ \eta_i U'(q_i) + \frac{1}{2} \eta_i^2 U''(q_i) \right] + \sum_{i=0}^{N-1} \frac{\varepsilon}{2m\beta} U''(q_i) + o(\varepsilon) \right\},
 \end{aligned}$$

where only one out of the  $\eta_i$ ,  $i = 1, 2, \dots, N - 1$  (at free choice) is defined by Eqs. (5.1'). The convergence of the integrals requires bounds upon the derivatives of the potential energy function  $U(q)$ :

$$(6.1') \quad \frac{m\beta}{\varepsilon} > U''(q_i), \quad \forall i.$$

Therefore it can be deduced (see Appendix B)

$$(6.2) \quad K(q, t/q_0, t_0) = \lim_{\varepsilon \rightarrow 0} \int_{-\infty}^{+\infty} d\eta_0 \dots \int_{-\infty}^{+\infty} d\eta_{N-2} \left( \frac{4\pi T\varepsilon}{m\beta} \right)^{-N/2} \\ \times \exp \left\{ -\frac{m\beta}{4T} \sum_{i=0}^{N-1} \varepsilon \left[ \frac{\eta_i}{\varepsilon} + \frac{1}{m\beta} U'(q_i) \right]^2 \right\}$$

where, according to (5.1')

$$(6.2') \quad \eta_{N-1} = q - q_0 - \sum_{i=0}^{N-2} \eta_i, \quad t = t_0 + N\varepsilon.$$

The exactness of Eq. (6.2) may be proved straightforwardly by evaluating the time-derivative of the kernel, which yields the same equation (4.1') or (5.4), in the limit  $\varepsilon \rightarrow 0$ . In order to prove the assertion, Eq. (6.2) is rewritten in the form of Chapman–Kolmogorov equation, where terms are retained up to  $O(\varepsilon)$ .

$$(6.3) \quad K(q, t/q_0, t_0) \\ = \left( \frac{4\pi T\varepsilon}{m\beta} \right)^{-1/2} \int_{-\infty}^{+\infty} d\eta_{N-1} \exp \left\{ -\frac{m\beta}{4T\varepsilon} \left[ \eta_{N-1} + \frac{\varepsilon}{m\beta} U'(q_{N-1}) \right]^2 \right\} \\ \times K(q - \eta_{N-1}, t - \varepsilon/q_0, t_0) \\ = \left( \frac{4\pi T\varepsilon}{m\beta} \right)^{-1/2} \int_{-\infty}^{+\infty} d\eta \left\{ -\frac{m\beta}{4T\varepsilon} \eta^2 \right\} \\ \times \left\{ 1 - \frac{\eta}{2T} U'(q - \eta) - \frac{\varepsilon}{4Tm\beta} U'(q - \eta)^2 + \frac{\eta^2}{8T^2} U'(q - \eta)^2 + o(\varepsilon) \right\} \\ \times \left\{ K(q, t/q_0, t_0) - \eta K'(q, t/q_0, t_0) \right. \\ \left. + \frac{\eta^2}{2} K''(q, t/q_0, t_0) - \varepsilon \frac{\partial}{\partial t} K(q, t/q_0, t_0) + o(\varepsilon) \right\} \\ = K(q, t/q_0, t_0) \left( 1 + \frac{\varepsilon}{m\beta} U''(q) \right) + \frac{\varepsilon}{m\beta} U'(q) K'(q, t/q_0, t_0) \\ + \frac{T\varepsilon}{m\beta} K''(q, t/q_0, t_0) - \varepsilon \frac{\partial}{\partial t} K(q, t/q_0, t_0) + o(\varepsilon),$$

which is Eq. (5.4) in the limit  $\varepsilon \rightarrow 0$ . Consequently, the path average in the rhs of Eq. (6.2) obeys, in the limit  $\varepsilon \rightarrow 0$ , the same second-order partial differential

equation in the variables  $q$  and  $t$  than the path average in the rhs of Eq. (5.1). Given the same boundary conditions, these averages are therefore identical by virtue of the existence and uniqueness theorem due to S. V. KOVALEVSKAIA [37].

The interest in Eq. (6.2) is that it may be rewritten:

$$(6.5) \quad K(q, t/q_0, t_0) = \lim_{\varepsilon \rightarrow 0} \left( \frac{4\pi mT}{\beta\varepsilon} \right)^{-N/2} \\ \times \int_{-\infty}^{+\infty} \dots \int_{-\infty}^{+\infty} d\tilde{\pi}(\alpha_0) \dots d\tilde{\pi}(\alpha_{N-2}) \exp \left\{ -\frac{\beta\varepsilon}{4mT} \sum_{i=0}^{N-1} \tilde{\pi}(\alpha_i)^2 \right\},$$

where it has been put

$$(6.6) \quad \frac{q(\alpha_{i+1}) - q(\alpha_i)}{\varepsilon} = -\frac{1}{m\beta} U'(q(\alpha_i)) + \frac{1}{m} \tilde{\pi}(\alpha_i).$$

The family of normally distributed random variables  $\tilde{\pi}(\alpha_i)$  verify the Kolmogorov consistency conditions [32] and therefore, they define a Wiener process  $\tilde{w}(\alpha)$  [34, 35, 36]. Consequently, Eq. (6.6) may be rewritten [35, 38]:

$$(6.6') \quad dq = -\frac{1}{m\beta} U'(\alpha) d\alpha + \frac{1}{m} d\tilde{w}(\alpha).$$

The random increment  $d\tilde{w}(\alpha)$  is denoted by differential notation  $\tilde{\pi}(\alpha)d\alpha$  with the limiting property

$$(6.6'') \quad \langle \tilde{\pi}(\alpha) \tilde{\pi}(\gamma) \rangle = \frac{2mT}{\beta} \delta(\alpha - \gamma),$$

$\tilde{\pi}(\alpha)$  being a Gaussian random variable with zero mean and variance  $2mT/\beta$ , which is *uncorrelated with position* (see Appendix C)<sup>4</sup>. These properties follow from the definition of the Feynman path integral in Eqs. (4.11), (5.1). Its identification with  $\tilde{p}(q(t), Q, t)$  of Eq. (2.7) would necessitate a proof that all these requirements are satisfied by that variable. Consequently, there is in general a certain sort of inconsistency between the representation of the stochastic process developed here through Eqs. (2.7) and the following ones, and the different one appearing in the path integral formulation, because Eq. (3.1) would give vanishing diffusive term if equation of motion (6.6') is used in place of (2.7). It is however not surprising that (2.7) with definitions (4.1) and (6.6'), correspond to

<sup>4</sup>These properties are similar to those of  $\xi(t)$  in Eq. (2.4). It should be appreciated however that  $\xi(t)$  is intended to represent a real physical variable, while  $\tilde{\pi}(t)$  is a purely abstract tool, notationally convenient, without obvious physical counterpart (see [12]). In fact, almost all realizations of  $\tilde{w}(t)$  are nowhere differentiable [34].

the same differential equation for the evolution of the probability density, since it is well known that the Ito and Stratonovich interpretation of stochastic calculus are equivalent for purely additive stochastic differential equations. It is therefore obvious that a different type of calculus is needed in order to handle equations like (6.6') [38].

In going from (5.1) to (6.2), the terms proportional to  $U''$  have been preaveraged over the Maxwellian distribution of velocities. This does not modify the value of the path average (see Appendix B).

The maximum value of the exponent in Eq. (6.5) is of course attained for  $\tilde{\pi}(\alpha)$  identically zero, which is also the most probable value. This value is also stationary. However, the stationary values of the arguments of exponentials in Eqs. (5.1) and (6.2) are exactly the same only in the limit of low temperature, because the preaveraged term vanishes in this limit.

The stationary value of the argument of exponential in the rhs of Eq. (4.11) follows from the Euler–Lagrange equation<sup>5)</sup>

$$(6.7) \quad \frac{d}{dt} \frac{\partial \mathcal{L}}{\partial \dot{q}} - \frac{\partial \mathcal{L}}{\partial q} = 0,$$

$$(6.7') \quad \mathcal{L} = \frac{m}{2} \left[ \dot{q}^2 + \frac{2}{m} V(q) \right]$$

and leads to the equation of motion

$$(6.8) \quad \ddot{q} = \frac{1}{m} V'(q) = - \frac{\partial}{\partial q} [U(q) + \beta \varphi_e(q, Q)] + O\left(\frac{1}{\beta^4}\right)$$

because of (4.13). The same result is obtained by the stationary condition applied to (4.12). Therefore the equations of motion read

$$(6.9) \quad \ddot{q} = \frac{1}{m^2 \beta^2} (U'' U' - T U'''),$$

Equation (6.9) characterizes the paths where the action is stationary, which are the paths followed by the spontaneous evolution of the system from a given configuration (minimum entropy production), or the paths joining two arbitrary points in configuration space (arbitrary fluctuations). The spontaneous evolution from a given configuration follows, on the average, Eq. (4.1), whose time derivative yields, averaging each infinitesimal step, Eq. (6.9), because<sup>6)</sup>

<sup>5)</sup>The Euler–Lagrange equations presuppose that the integration over time in the exponent may be interchanged with path average.

<sup>6)</sup>If the probability density distribution is concentrated in one point, then the averaged fluctuating velocity vanishes there, because of Eq. (3.4) and the boundary conditions. But  $\tilde{p}(t)$  is still correlated with position, so that the average change of  $p(q)$  in one infinitesimal step is given by (6.10).

$$\begin{aligned}
 (6.10) \quad \langle \ddot{q}(t)\delta(q(t) - q) \rangle &= \left\langle \left[ \frac{d}{dt} \frac{1}{m} p(q) \right] \delta(q(t) - q) \right\rangle \\
 &= \frac{1}{m^2} p'(q) p(q) \langle \delta(q(t) - q) \rangle + \frac{1}{m^2} \langle p'(q) \tilde{p}(t) \delta(q(t) - q) \rangle \\
 &= \frac{1}{m^2} [p'(q) p(q) + \hat{D}_q^{\infty \text{tr}} p''(q)] \langle \delta(q(t) - q) \rangle \\
 &= \frac{1}{m^2} [p'(q) p(q) - g(q)] \langle \delta(q(t) - q) \rangle.
 \end{aligned}$$

In Eq. (6.10) it has been used the fact that, as  $t - t_0 \rightarrow +\infty$ , after cancellation of the memory terms

$$(6.11) \quad \langle \tilde{p}(t)\delta(q(t) - q) \rangle = \langle \delta(q(t) - q) \rangle \hat{D}_q^{\infty \text{tr}} \frac{\partial}{\partial q}$$

in the sense of distribution theory [33]. Using (4.1), this yields Eq. (6.9). At variance with this result, upon averaging and differentiating Eq. (6.6') over time the last term would be missing, because  $\tilde{\pi}(t)$  is not correlated with position. In fact, preaveraging in Eq. (6.2) has changed the stationary paths.

## 7. Connection with Machlup–Onsager theory

The Hamilton–Jacobi–Yasue equation (2.4) yields, by the condition of stationarity of the action, the second-order differential equation which may be written, following [13], in a form reminiscent of Eq. (2.7):

$$(7.1) \quad \dot{q} = -\frac{U'}{m\beta} - \frac{1}{m\beta} [m\ddot{q} - \xi(t)].$$

On putting  $\xi(t) = 0$  and substituting from (6.9) the first-order equation with respect to time, follows

$$(7.2) \quad \dot{q} = -\frac{U'}{\beta} - \frac{1}{m^2\beta^3} (U'U'' - TU''').$$

Upon comparing this equation with (4.14), it is possible to identify  $mdq/dt$  with the drift  $p_e(q)$ , expanded up to  $O(1/\beta^3)$ . The solutions to Eq. (7.2) are the curves which, at each infinitesimal step, regress from a given configuration with the average velocity, which is the drift (see footnote 6)). This type of regression is different from that which was defined in [12], except for the linear case.

Equation (6.9) is a second-order equation, therefore the solutions are able to connect two arbitrary points in configuration space. By retaining  $\xi(t)$  in (7.1) it

is possible to identify, by combining (2.7) and (4.1), the equation with

$$(7.3) \quad \dot{q} = \frac{1}{m}[p(q) + \tilde{p}(t)] = -\frac{U'}{m\beta} + \frac{1}{m}\tilde{p}(t) + O(\beta^{-3}).$$

These trajectories spread around the most probable one (6.9) and yield, upon averaging over the paths, the exponential of the action (4.11) or (4.12), the fundamental solution of the asymptotic diffusion equation (4.1'), which is (4.8).

At variance with this result, L. ONSAGER and S. MACHLUP [12] write Eq. (6.6'), where  $\tilde{\pi}(t)$  is *assumed* to be uncorrelated with position. The propagator is then given by (6.2) as a path average and the most probable path satisfying the boundary conditions is

$$(7.4) \quad \ddot{q} = \frac{1}{m^2\beta^2}U''U',$$

which is symmetrical under time inversion.

S. MACHLUP and L. ONSAGER [13] write the Lagrangian function

$$(7.5) \quad \mathcal{L}_{\text{MO}} = m\beta \left( \dot{q} + \frac{U'}{\beta} + \frac{\ddot{q}}{\beta} \right)^2,$$

whose minimum value yields the equation of motion (7.1) (with vanishing random force, yielding the regression curve), while the Euler–Lagrange equation results in a fourth-order equation in time, whose solutions verify both Eq. (7.1) with vanishing  $\xi(t)$ , and its mirror image by time inversion. As it is well known, their approach is bound to consider only linear systems, however, Lagrangian (7.5) does not appear to be exempt from interpretation ambiguities.

## 8. Summary and conclusions

In this work, a classical mechanical system acted upon by frictional forces and stochastic random forces has been considered in the limit of large frictional coefficient. The system is subjected to boundary conditions at time  $t'_0 \rightarrow -\infty$ , such that at the time  $t_0$  is found in a definite configuration, in equilibrium with the random field [8].

The velocity is split into a deterministic plus a fluctuating random component, accordingly the flux of particles is evaluated by stochastically averaging over each component, inside a small spatial interval. The moments of the fluctuating random velocity may in principle be computed in terms of stochastic averages over the trajectories, from which the entire probability distribution follows. It is found that the averaged fluctuating component of velocity at time  $t$  and position  $q$  is in general dependent upon the total probability distribution

in configuration space, plus a memory term, which is an average over the trajectories from  $q_0$  to  $q$ . In the limit of short correlation time of velocities, it is proven that this term can be made vanishing identically by forcing the drift to obey a Hamilton–Jacobi–Yasue equation (see (2.4)), supplemented by a term of Riccati type (Eqs. (2.6), (3.8)). This term can be interpreted as an averaged stochastic kinetic energy density of the system, interacting with the environment. In fact, from Eq. (3.5) it is obtained

$$(8.1) \quad \frac{1}{m} \langle p(q(t), Q) \tilde{p}(q(t), Q, t) \delta(q(t) - q) \rangle \\ = -p(q, Q) \frac{\partial}{\partial q} \hat{D}(q) \langle \delta(q(t) - q) \rangle + \text{memory terms.}$$

Leading order coefficients of the operator  $\hat{D}(q)$  up to  $1/\beta^3$  are [10]

$$(8.2) \quad D(q) = \frac{T}{m\beta} \left( 1 + \frac{1}{m\beta^2} U''(q) \right),$$

therefore by an integration by parts, using the boundary conditions at infinity, there results the kinetic energy density

$$(8.3) \quad \frac{1}{m} \langle p(q(t), Q) \tilde{p}(q(t), Q, t) \delta(q(t) - q) \rangle \\ = \frac{T}{m\beta} \left( 1 + \frac{U''(q)}{m\beta^2} \right) p'(q, Q) \langle \delta(q(t) - q) \rangle \\ = -G(q, Q) \langle \delta(q(t) - q) \rangle + O\left(\frac{1}{\beta^4}\right),$$

because the memory terms cancel exactly to this order of approximation. Thus this energy acts as a potential energy density term in the equation for the drift velocity (2.6), but only to the leading order. There does not seem to be an obvious interpretation for this limitation.

There follows that the average value of the total velocity cannot vanish and therefore the velocity distribution cannot be Maxwellian, unless the system has reached configurational equilibrium, because the velocity distribution in a given point is, generally speaking, dependent upon the total probability distribution in configuration space at the same value of time. In other words, the velocity probability distribution depends not only on the configurational coordinate of the particle, but upon the coordinate distribution of the whole ensemble of particles under consideration. This is somewhat in contradiction with the Maxwell–Boltzmann law, which postulates the complete independence of velocity distribution from localization in configuration space, because in the present framework

the equilibrium probability distribution of velocities requires the contemporary equilibrium distribution of configurations.

The cancellation of memory terms allows to write a memoryless Markovian equation governing the evolution of probability density from time  $t_0$  onwards, but only in the limit of large time<sup>7)</sup>.

The fundamental solution of this limiting equation may assume the form of a Feynman path integral, whose Lagrangian contains a potential energy which is a function of the drift velocity and its derivatives (Onsager–Machlup potential), such that the drift velocity satisfies a HJ-Riccati equation with this potential. This equation results to be matching exactly the equation previously derived for the drift under the identification (4.13), so it is possible to claim that the true modified Hamilton–Jacobi equation characterizing the drift has been obtained.

The Feynman path integral can be transformed, using an identity due to M. RONCADELLI [22] (see also [19]), into that form belonging to the formulation of the ONSAGER and MACHLUP–ONSAGER [12, 13, 28] minimum entropy production principle, in such a way that the most probable path is varied, but the result of functional integration is invariant. We have therefore obtained a genuinely pseudo-Markovian representation of the stochastic process, which is valid in the limit of large time. The corresponding Langevin equation is (6.6'), which is to be confronted with (2.7). It should be noticed that the steps which lead from (2.7) to the large-time asymptotic Smoluchowski equation (4.1'), and consequently to the Feynman integral representation of the fundamental solution (4.11) or (5.1), involve several approximations, consequently the equations of motion (2.7) and (6.6') need not be completely equivalent.

The singular solution that we have used (Eq. (4.1)) is the one which is commonly used in overdamped diffusive systems, and was studied in [2] including the time-dependent case. However, it was proven in [30] that also other solutions play a role in the description of diffusive systems. Actually, an equation with time-dependent coefficients obtained in [39] was shown [30] to be linear combination of equations obtained from different solutions of the HJYR equation (2.6).

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<sup>7)</sup>Time-dependent  $g(q, t)$  might be considered, but it is out of scope in this work.

**Appendix A. Proof of Equation (2.11)**

Using eq. (2.9), there follows that

$$(A.1) \quad \langle \tilde{p}(t)\tilde{p}(s) \rangle = \int_{-\infty}^t d\tau \int_{-\infty}^s d\sigma \langle \mathcal{G}(t, \tau)\mathcal{G}(s, \sigma)[k(\tau) - g(q(\tau))][k(\sigma) - g(q(\sigma))] \rangle;$$

now, upon substitution from (4.1), (2.9') we obtain

$$(A.2) \quad \mathcal{G}(t, \tau) = \exp \left\{ -\beta(t - \tau) + O\left(\frac{|U''|}{\beta}\right) \right\}$$

and similarly for  $\mathcal{G}(s, \sigma)$ . Consequently, on substituting from (3.8), we obtain

$$(A.3) \quad \begin{aligned} \langle \tilde{p}(t)\tilde{p}(s) \rangle &= \int_{-\infty}^t d\tau \int_{-\infty}^s d\sigma \exp \left\{ -\beta(t + s - \tau - \sigma) + O\left(\frac{|U''|}{\beta}\right) \right\} \\ &\times \left[ \langle \xi(\tau)\xi(\sigma) \rangle + \frac{T}{m\beta} \langle \xi(\tau)p''(q(\sigma)) \rangle + \frac{T}{m\beta} \langle \xi(\sigma)p''(q(\tau)) \rangle \right. \\ &\left. + \left(\frac{T}{m\beta}\right)^2 \langle p''(q(\tau))p''(q(\sigma)) \rangle \right]. \end{aligned}$$

Making use of Furutsu–Novikov theorem [40, 41], we obtain:

$$(A.4) \quad \begin{aligned} \langle \xi(\tau)p''(q(\sigma)) \rangle &= 2m\beta T \int_{-\infty}^t dt_1 \delta(t_1 - \tau) \int_{-\infty}^t dt_2 \left\langle p'''(q(\sigma)) \frac{\delta q(\sigma)}{\delta \xi(t_2)} \right\rangle \delta(t_1 - t_2) \\ &= 2m\beta T \left\langle p'''(q(\sigma)) \frac{\delta q(\sigma)}{\delta \xi(\tau)} \right\rangle. \end{aligned}$$

We are interested in the evaluation of expression (A.3) in the limit  $t \gg t_0$ , and consequently, the initial data may be neglected, by considering only time coordinates posterior to  $t_0$ . Using Eq. (4.6) of [11] it follows

$$(A.5) \quad \frac{\delta q(\sigma)}{\delta \xi(\tau)} = \frac{1 - e^{-\beta(\sigma - \tau)}}{m\beta} h(\sigma - \tau) + O\left(\frac{|U''|}{\beta^2}\right),$$

where  $h(\alpha)$  is a heaviside function of argument  $\alpha$ . Upon introducing this expression into Eq. (A.3), and simplifying the boundary conditions as explained above, there follows

$$\begin{aligned}
(A.6) \quad & \int_{t_0}^t d\tau \int_{t_0}^s d\sigma \exp \left\{ -\beta(t+s-\tau-\sigma) + O\left(\frac{|U''|}{\beta}\right) \right\} \left\langle p'''(q(\sigma)) \frac{\delta q(\sigma)}{\delta \xi(\tau)} \right\rangle \\
&= \frac{-T}{2m^2\beta^4} \int_{t_0}^{\min(t,s)} d\sigma \langle U'''(q(\sigma)) \rangle \exp\{-\beta(t+s-2\sigma)\} \\
&\quad - \frac{T}{m^2\beta^4} \int_t^s d\sigma \langle U'''(q(\sigma)) \rangle [\exp\{-\beta(s-\sigma)\} - \exp\{-\beta(s-t)\}] h(s-t) \\
&\quad + \text{h.o.t.}
\end{aligned}$$

In a similar way the remaining terms of Eq. (A.3) can be evaluated, so there is left, to the leading order

$$(A.7) \quad \langle \tilde{p}(t)\tilde{p}(s) \rangle \sim mT \exp\{-\beta|t-s|\} \xrightarrow{\beta \rightarrow +\infty} \frac{2mT}{\beta} \delta(t-s),$$

where simple convergence is understood in sense of the distribution theory [33].

## Appendix B. Proof of Equation (6.2)

As  $\varepsilon \rightarrow 0$ , the constraint (6.2') does not modify significantly the Gaussian distribution of the  $N-1$  remaining variables  $\eta_i$ 's, (like in a perfect gas, the total fixed momentum does not modify appreciably the Maxwellian distribution of the velocities of each particle). Accordingly, it is licit to integrate over the variables free from constraints, and consequently, two sums in the argument of the exponential in the rhs of Eq. (6.1) average out to zero, leaving the sum in Eq. (6.2).

Substituting from (6.2'), Eq. (6.1) is rewritten in the following form, by choosing variables  $\eta_0, \eta_1, \dots, \eta_{N-2}, q$  in place of  $\eta_0, \eta_1, \dots, \eta_{N-1}$ , where the Jacobian of the linear transformation is of modulus 1:

$$\begin{aligned}
(B.1) \quad & K(q, t/q_0, t_0) = \lim_{\varepsilon \rightarrow 0} \int_{-\infty}^{+\infty} d\eta_0 \dots \int_{-\infty}^{+\infty} d\eta_{N-2} \left( \frac{4\pi T\varepsilon}{m\beta} \right)^{-N/2} \\
&\quad \times \exp \left\{ -\frac{m\beta}{4T\varepsilon} \sum_{i=0}^{N-1} \left[ \eta_i + \frac{\varepsilon}{m\beta} U'(q_i) \right]^2 + \sum_{i=0}^{N-1} \left( \frac{\varepsilon}{2m\beta} - \frac{\eta_i^2}{4T} \right) U''(q_i) \right\}
\end{aligned}$$

and making use of the algebraic identity:

$$\begin{aligned}
(B.2) \quad & \exp \left\{ -\frac{m\beta}{4T\varepsilon} \left[ (\eta_{N-n-1} + a_n)^2 + \frac{1}{n} (\eta_{N-n-1} + b_n)^2 \right] \right\} \\
&= \exp \left\{ -\frac{(n+1)m\beta}{4nT\varepsilon} \left[ \eta_{N-n-1} + \frac{1}{n+1} (na_n + b_n) \right]^2 + \frac{m\beta}{4nT\varepsilon} (a_n - b_n)^2 \right\},
\end{aligned}$$

where it has been defined

$$(B.2') \quad \begin{cases} a_n = \frac{\varepsilon}{m\beta} U'(q_{N-n-1}), \\ -b_n = q - q_{N-n-1} + \frac{\varepsilon}{m\beta} \sum_{i=1}^n U'(q_{N-i}). \end{cases}$$

The above expression may be recast into the form

$$(B.3) \quad K(q, t/q_0, t_0) = \lim_{\varepsilon \rightarrow 0} \int_{-\infty}^{+\infty} d\eta_0 \dots \int_{-\infty}^{+\infty} d\eta_{N-2} \left( \frac{4\pi T\varepsilon}{m\beta} \right)^{-N/2} \\ \times \prod_{n=1}^{N-1} \exp \left\{ -\frac{(n+1)m\beta}{4nT\varepsilon} \left[ \eta_{N-n-1} + \frac{n\varepsilon}{(n+1)m\beta} U'(q_{N-n-1}) \right. \right. \\ \left. \left. - \frac{1}{n+1} \left( q - q_{N-n-1} + \frac{\varepsilon}{m\beta} \sum_{i=1}^n U'(q_{N-i}) \right) \right]^2 \right\} \\ \times \exp \left\{ -\frac{m\beta}{4NT\varepsilon} \left[ q - q_0 + \frac{\varepsilon}{m\beta} \sum_{i=1}^N U'(q_{N-i}) \right]^2 \right\} \\ \times \exp \left\{ \sum_{i=0}^{N-1} \left( \frac{\varepsilon}{2m\beta} - \frac{\eta_i^2}{4T} \right) U''(q_i) \right\}.$$

Expression (B.3) is exact. It shows that the statistical distribution of the  $\eta_i$  is somewhat narrowed by the imposed constraint (5.1'), by a factor close to one, and moreover it is polarized in the direction of the final configuration, by an amount which is dependent on  $n$ , differing from the perfect gas model, in which all the molecules are a priori equivalent<sup>8)</sup>. Moreover, there is introduced by the constraints, a small correlation between the variables  $\eta_i$ 's, originating from the term  $(\varepsilon/(n+1)) \sum_{i=1}^n U'(q_{N-i})$ . This correlation is considered negligible in the following. Therefore it is obtained, for  $n = 1, 2, \dots, N-1$ :

$$(B.4) \quad \int_{-\infty}^{+\infty} d\eta \eta_{N-n-1}^2 \exp \left\{ -\frac{(n+1)m\beta}{4Tn\varepsilon} \left[ \eta_{N-n-1} + \frac{n}{n+1} a_n + \frac{1}{n+1} b_n \right]^2 \right\} \\ = \left( \frac{4\pi Tn\varepsilon}{(n+1)m\beta} \right)^{1/2} \left[ \frac{2Tn\varepsilon}{m\beta(n+1)} + \left( \frac{n}{n+1} a_n + \frac{1}{n+1} b_n \right)^2 \right].$$

<sup>8)</sup>It would be different if the velocities of the molecules were measured successively, practically at the same instant of time. Then the distribution of velocities would be similar to (B.3), with  $U' = \text{const}$ . Conditional Wiener integrals were also considered in [34].

The rhs of Eq. (B.3) may be evaluated by expanding the last factor in cumulants up to  $O(\varepsilon)$ . This yields

$$\begin{aligned}
(B.5) \quad K(q, t/q_0, t_0) &= \lim_{\varepsilon \rightarrow 0} \int_{-\infty}^{+\infty} d\eta_0 \dots \int_{-\infty}^{+\infty} d\eta_{N-2} \left( \frac{4\pi T \varepsilon}{m\beta} \right)^{-N/2} \\
&\times \exp \left\{ \sum_{i=0}^{N-1} \left[ \frac{\varepsilon \langle U''(q_i) \rangle}{(N-i)2m\beta} + \left\langle \left( \frac{q - q_i}{N-i} + O(\varepsilon) \right)^2 \frac{U''(q_i)}{4T} \right\rangle \right] \right\} \\
&\times \prod_{n=1}^{N-1} \exp \left\{ -\frac{(n+1)m\beta}{4nT\varepsilon} \left[ \eta_{N-n-1} + \frac{n\varepsilon}{(n+1)m\beta} U'(q_{N-n-1}) \right. \right. \\
&\quad \left. \left. - \frac{1}{n+1} \left( q - q_{N-n-1} + \frac{\varepsilon}{m\beta} \sum_{i=1}^n U'(q_{N-i}) \right) \right]^2 \right\} \\
&\times \exp \left\{ -\frac{m\beta}{4NT\varepsilon} \left[ q - q_0 + \frac{\varepsilon}{m\beta} \sum_{i=1}^N U'(q_{N-i}) \right]^2 \right\}.
\end{aligned}$$

In the evaluation of Eq. (B.5), the  $\eta_i$  are considered as independent random variables, normally distributed with mean values determined by the constraints.

Considering that the system coordinate has bounded second moments [35], there follows the estimate

$$\begin{aligned}
(B.6) \quad \left| \left\langle \sum_{i=1}^{(1-\mu)N} \left( \frac{q - q_i}{N-i} \right)^2 U''(q_i) \right\rangle \right| &\leq \sum_{k=\mu N}^N \left| \left\langle \left( \frac{q - q_{N-k}}{k} \right)^2 U''(q_{N-k}) \right\rangle \right| \\
&\leq \sup_{N-k} | \langle (q - q_{N-k})^2 U''(q_{N-k}) \rangle | \sum_{k=\mu N}^N \frac{1}{k^2} \\
&< \frac{1}{\mu^2 N} \sup_{N-k} | \langle (q - q_{N-k})^2 U''(q_{N-k}) \rangle |,
\end{aligned}$$

which shows that

$$(B.6') \quad \left\langle \sum_{i=1}^{(1-\mu)N} \left( \frac{\varepsilon}{2m\beta} - \frac{\eta_i^2}{4T} \right) U''(q_i) \right\rangle \xrightarrow{N \rightarrow \infty} 0, \quad \forall \mu, \quad 0 < \mu < 1.$$

On the other hand, the process being purely continuous [36], there follows that the sum

$$\begin{aligned}
 \text{(B.7)} \quad & \sum_{k=1}^{\mu N} \frac{|\langle (q - q_{N-k})^2 U''(q_{N-k}) \rangle|}{k^2} \\
 & \leq \sum_{k=1}^{\mu N} \frac{2T}{m\beta} \frac{k\varepsilon + o(k\varepsilon)}{k^2} \sup_{N-k} |U''(q_{N-k})| \\
 & = \frac{2T \sup_{N-k} |U''(q_{N-k})|}{m\beta} \sum_{k=1}^{\mu N} \frac{\varepsilon + o(\varepsilon)}{k} \\
 & \leq \frac{2T[\varepsilon + o(\varepsilon)] \sup_{N-k} |U''(q_{N-k})|}{m\beta} \sum_{k=1}^{\mu N} \frac{1}{k} \xrightarrow{\varepsilon \rightarrow 0} 0.
 \end{aligned}$$

The notation “ $\sup_{N-k}$ ” means: supremum value over all the subdivisions and realizations of the process (see Eq. (6.1'))<sup>9</sup>. Therefore, the rhs can be made small at will by choosing  $\mu$  and  $\varepsilon$  sufficiently small (if  $\mu N$  is not an integer, the nearest integer number should be substituted in its place).

In order to check the change of variables that has been introduced, we write down the expression for the kernel (6.1). If  $U'(q) = \text{const}$ , the integrations may be performed immediately, yielding:

$$\begin{aligned}
 \text{(B.8)} \quad & K(q, t/q_0 t_0) \\
 & = \lim_{\varepsilon \rightarrow 0} \left( \frac{4\pi T \varepsilon}{m\beta} \right)^{-N/2} \prod_{n=1}^{N-1} \left( \frac{(n+1)m\beta}{4\pi T n \varepsilon} \right)^{-1/2} \\
 & \quad \times \exp \left\{ -\frac{m\beta}{4NT\varepsilon} \left[ q - q_0 + \frac{\varepsilon}{m\beta} \sum_{i=1}^N U'(q_{N-i}) \right]^2 \right\} \\
 & = \left( \frac{4\pi T(t-t_0)}{m\beta} \right)^{-1/2} \exp \left\{ -\frac{m\beta}{4T(t-t_0)} \left[ q - q_0 + \frac{U'}{m\beta}(t-t_0) \right]^2 \right\},
 \end{aligned}$$

where it has been put:  $N\varepsilon = t - t_0$ . It is remarkable that all the exponential factors, except for the last one, in the rhs of Eq. (B.5), converge to  $\delta$ -functions of the arguments, while the last factor represents a Gaussian whose width is independent of  $\varepsilon$ , therefore the integrations can be performed immediately, by considering the last factor as a constant in the relevant integration range. It is therefore possible to argue that this expression for the kernel would be useful in more complicated potentials, though its use is out of scope in this work.

<sup>9</sup>The necessity of smoothness conditions on the potential  $U(q)$  was also pointed out in [31, 42].

### 9. Appendix C. Proof of Equations (6.6), (6.6')

From Eq. (5.1') it is obtained

$$(C.1) \quad q_{i+1} - q_i = \eta_i,$$

then from Eq. (6.6)

$$(C.2) \quad \varepsilon \tilde{\pi}_i = m\eta_i + \frac{\varepsilon}{\beta} U'(q_i);$$

consequently

$$(C.3) \quad \begin{aligned} \langle \tilde{\pi}_i \tilde{\pi}_j \rangle &= \int_{-\infty}^{+\infty} d\eta_0 \dots \int_{-\infty}^{+\infty} d\eta_{N-1} \left( \frac{4\pi T \varepsilon}{m\beta} \right)^{-N/2} \left[ \frac{m\eta_i}{\varepsilon} + \frac{1}{\beta} U'(q_i) \right] \\ &\quad \times \left[ \frac{m\eta_j}{\varepsilon} + \frac{1}{\beta} U'(q_j) \right] \exp \left\{ -\frac{m\beta}{4T} \sum_{k=0}^{N-1} \varepsilon \left[ \frac{\eta_k}{\varepsilon} + \frac{1}{m\beta} U'(q_k) \right]^2 \right\} \\ &= \frac{2mT}{\beta\varepsilon} \delta_{ij} \xrightarrow{\varepsilon \rightarrow 0} \frac{2mT}{\beta} \delta(t_i - t_j), \end{aligned}$$

with  $t_k = t_0 + k\varepsilon$ ,  $k = 1, 2, \dots, N-1$ . Convergence is understood as simple in the sense of the distribution theory [33]. The same limit is obtained if the time coordinates are kept fixed while the subdivision of the interval is made finer. In the same way it is proven that  $\tilde{\pi}(t_j)$  is uncorrelated with any function of  $q(t_j)$ :

$$(C.4) \quad \begin{aligned} \langle f(q_j) \tilde{\pi}_j \rangle &= \int_{-\infty}^{+\infty} d\eta_0 \dots \int_{-\infty}^{+\infty} d\eta_{N-1} \left( \frac{4\pi T \varepsilon}{m\beta} \right)^{-N/2} f(q_j) \\ &\quad \times \left[ \frac{m\eta_j}{\varepsilon} + \frac{1}{\beta} U'(q_j) \right] \exp \left\{ -\frac{m\beta}{4T} \sum_{i=0}^{N-1} \varepsilon \left[ \frac{\eta_i}{\varepsilon} + \frac{1}{m\beta} U'(q_i) \right]^2 \right\} = 0, \end{aligned}$$

because  $q_j$  does not depend upon  $\eta_k$ , for  $k \geq j$ .

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