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PATH INTEGRALS FOR INERTIALESS CLASSICAL PARTICLES UNDERGOING RAPID STOCHASTIC TREMBLING (II. GENERAL THEORY)

VIKTOR BEZÁK*, Bratislava

A thorough analysis is given in order to elucidate delicate differences between the usage of the Feynman path integrals in quantum mechanics (or quantum statistics) and in classical probabilistic applications. The analysis, when relating to a non-linear Langevin dynamic equation, holds for the white-noise approximation. A generalization directed beyond the white-noise approximation is also suggested, with discussing difficulties connected with it. Finally, a generalization is mentioned concerning an inertialess Brownian system of d degrees of freedom.

ИНТЕГРАЛЫ ПО ТРАЕКТОРИЯМ ДЛЯ НЕИНЕРЦИОННЫХ ЧАСТИЦ, ПОДВЕРГАЮЩИХСЯ БЫСТРОМУ СЛУЧАЙНОМУ ВЫБРАЦИОННОМУ ВОЗДЕЙСТВИЮ (II. ОБЩАЯ ТЕОРИЯ)

Проводится подробный анализ тонкостей в различиях между применениями фейнмановских интегралов по траекториям в квантовой механике (или в квантовой статистике) и в классической теории случайных процессов. Анализ нелинейного уравнения Ланжевена в динамике проводится только в приближении белого шума, хотя рассматривается также общий случай и обсуждаются возникающие при этом математические трудности. Последним упоминается обобщение, касающееся системы броуновских неинерционных частиц с d степенями свободы.

I. INTRODUCTION

This paper represents the second part of the preceding one (Part I, [1]). We intend to be more general and more abstract than in Part I. The main aim of this paper is to introduce some mathematical criticism of careless manipulations with exponents in probabilistic applications of Feynman's path integrals. Four Appendices are enclosed. The first of them (Appendix I) refers to linear Langevin equations only. We have included it here (and not in Part I) in order to make manifest the sharp contrast between possibilities rendered by the linear theory and shortage of such possibilities in more general, nonlinear theories.

* Katedra všeobecnej fyziky PFUK, Mlynská dolina, CS-816 31 Bratislava.

II. LANGEVIN EQUATION WITH A GENERAL DETERMINISTIC FORCE AND SMOLUCHOWSKI EQUATION

Without specifying the meaning of the variable x, let us investigate the Langevin equation

$$\gamma\dot{x} + F(x) = f(t), \tag{1}$$

where $f(t)$ is a Gaussian white-noise function:

$$\langle f(t)\rangle = 0, \quad \langle f(t')\,f(t'')\rangle = \eta^2\delta(t'-t''). \tag{2}$$

For simplicity, let no boundaries be present. The nonlinearity of equation (1) makes the formulation of the corresponding path integral somewhat ambiguous. This ambiguity is delicate and we will discuss it at the end of the present paper (in Appendix IV following other elucidations). The simplest form to which the path integrals can be reduced is

$$P(x, t|x_0) = \int_{x_0,0}^{x,t} \mathscr{D}x(\tau)\exp\left\{-\frac{1}{2\eta^2}\int_0^t d\tau[\gamma\dot{x}(\tau) - F(x(\tau))]^2\right\}. \tag{3}$$

This seemingly plain formula requires extraordinary caution when we deal with the exponent. Namely, when we decompose the exponent, one of this terms is

$$\int_0^t d\tau\dot{x}(\tau)\,F(x(\tau)) = \int_{x_0}^{x} dx(\tau)\,F(x(\tau)). \tag{4}$$

Then, if we have chosen a potential $V(x)$ such that

$$F(x) = -dV/dx, \tag{5}$$

it is tempting to put (4) equal to the expression $V(x_0) - V(x)$. Nevertheless this would be fallacious and we must accept the inequality

$$-\int_{x_0}^{x} dx(\tau)\left[\frac{dV}{dx}\right]_{x=x(\tau)} \neq V(x_0) - V(x), \tag{6}$$

since the subintegral in the l.h.s. of (6) is not an ordinary differential. This circumstance reflects the property — well-known to connoisseurs of the Wiener theory of the Brownian motion — that the paths $x(\tau)$ are so highly irregular that they do not possess derivatives $\dot{x}(\tau)$ in a classical sense. Notwithstanding, the concept of the path integral (3) may still be used but one must know how to path-integrate correctly.

To elucidate the path integration, let us use the transition property of the conditional probability density $P(x, t|x_0)$ and write first the obvious equation

$$P(x, t+\tau|x_0) = \int_{-\infty}^{\infty} d\xi P(x, \tau|\xi)\,P(\xi, t|x_0) = \int_{-\infty}^{\infty} d\xi\, P(x, \tau|x-\xi)\times \tag{7}$$

$$\times P(x-\xi, t|x_0)$$

at once recognizable as the Chapman-Kolmogorov equation[1]. The second step is to let τ tend to zero ($\tau>0$) so that the path integral representing $P(x, \tau|x-\xi)$ in accordance with formula (3) may be reduced to the simple expression

$$P(x, \tau|x-\xi)=\left(\frac{\gamma^2}{2\pi\eta^2\tau}\right)^{1/2} \exp\left\{-\frac{\tau}{2\eta^2}\left[\gamma\frac{\xi}{\tau}-F(x-\xi)\right]^2\right\}. \tag{8}$$

As the time variable τ is infinitesimal, all relevant values of the integration variable ξ in the r.h.s. of equation (7) are infinitesimal as well. If we put expression (8) into equation (7), we must leave the vital Gaussian factor

$$g(\xi, \tau)=\left(\frac{\gamma^2}{2\pi\eta^2\tau}\right)^{1/2} \exp\left\{-\frac{\gamma^2\xi^2}{2\eta^2\tau}\right\} \tag{9}$$

of function (8) intact while developing everything remaining into the Taylor series up to the first order in τ and the second order in ξ. Afterwards, the integration with respect to ξ gives terms proportional to τ that must be equalized with the term $\tau\,\partial P(x, t|x_0)/\partial t$ from the l.h.s. of equation (7). The unique result of such equalization is the Fokker-Planck equation reduced into the form known as the Smoluchowski equation:

$$\frac{\partial P(x, t|x_0)}{\partial t}=\frac{\eta^2}{2\gamma^2}\frac{\partial^2 P(x, t|x_0)}{\partial x^2}-\frac{1}{\gamma}\frac{\partial}{\partial x}[F(x)\,P(x, t|x_0)]. \tag{10}$$

This equation — in our case concerning the massless particle in the "x-space" — parallels the Fokker-Planck equation for a true mass particle in the "velocity space" that has become somewhat more widely known in statistical physics. For completeness, we are presenting the Fokker-Planck equation for the "velocity space" in Appendix II, taking $F=0$, in accordance with Ref. [2].

In connection with the function $F(x-\xi)$ in expression (8) let us point out that it *does not respect* Feynman's suggestion for approximation of expressions like $d\tau x(\tau)A(x(\tau))$ in the exponent of path integrals. Such expressions, linear in the velocity $\dot{x}(\tau)$, are approximated according to Feynman's theory (see his original article [3]) by expressions like $(x_{i+1}-x_i)\times A_x\left(\frac{1}{2}(x_{i+1}+x_i)\right)$ or $(x_{i+1}-x_i)\frac{1}{2}[A_x(x_{i+1})+A_x(x_i)]$ ("trapezoidal rule"). If we followed Fenman's

[1] It would be historically more just to call the Chapman-Kolmogorov equation, as some authors did, the Smoluchowski equation. Nevertheless, we will use in agreement with other authors (cf. e.g. [2]) the name Smoluchowski equation for a specified form of the Fokker-Planck equation (cf. equ. (10) and corresponding equations in Part I). Let us point out, moreover, that even the Fokker-Planck equation itself represents a specified form of one of the well-known Kolmogorov equations so that one may also speak of the Fokker-Planck-Kolmogorov equation. However, it is quite unfair to replace, as some cybernetical references do, the name Fokker-Planck equation simply by the Kolmogorov equation.

usage — which is undoubtedly correct in quantum-mechanical and quantum-statistical context with path integrals involving a vector potential $\mathbf{A}(\mathbf{r})$ — we should be misled when using, with $x_{i+1}=x$, $x_i=x-\xi$, rather the function $F\left(x-\frac{1}{2}\xi\right)$ or $\frac{1}{2}[F(x)+F(x-\xi)]$, respectively, instead of using the function $F(x-\xi)$, which is really correct in formula (8). To make this peculiarity more clear, we are enclosing Appendix III.

This "discrepancy" can simply be explained as follows.

In quantum-mechanical usage, the ultimate requirement which must be borne in mind is that the position x and momentum p_x be noncommuting operators satisfying the Heisenberg commutation rules[2]. These rules, when applied to the operator $(\mathbf{p}-e\mathbf{A})^2$, give rise to a term $\sim$ div $\mathbf{A}$ that would be absent in the Hamiltonian if it were derived from the path integral defined with an exponent containing a sum of expressions $(x_{i+1}-x_i)\,A_x(x_i)=\xi A_x(x-\xi)$, in analogy to formula (8). A way how to recover from the quantum-mechanical path integral the correct Hamiltonian in full is just given by using, for instance, the expressions

$$(x_{i+1}-x_i)\,A_x\left(\frac{1}{2}(x_{i+1}+x_i)\right)=\xi A_x\left(x-\frac{1}{2}\xi\right).$$

On the other hand, the ultimate requirement which must be respected in the probabilistic usage of the path integrals is that the transition probability density (8) be Markovian, i.e. that the value of the function $P(x_{i+1}, t|x_i)$ for the infinitesimal time $t=\tau$ in the next state $x_{i+1}=x$ be solely determined by the previous state $x_i=x-\xi$ at $t_0=0$. Thus, for any fixed value ξ, the only function of x which may be expected *a priori* to occur in expression (8) must be a function of the variable $x-\xi$ but not of the variable x, separately or in another combination with ξ.

III. A GENERALIZATION DIRECTED BEYOND THE WHITE-NOISE APPROXIMATION

We will briefly show difficulties met in any attempt to go, in case of presence of a general deterministic force $F(x)$, beyond the assumption that the autocorrelation function $\langle f(t')\,f(t'')\rangle$ be of the white-noise type. For brevity, we assume a one-dimensional formulation. In the stochastic (Langevin) equation

$$\gamma\dot{x}-F(x)=\tilde{f}(t) \tag{11}$$

[2] For a path-integral derivation of these rules, cf. § 9 in [3].

the fluctuating force $\tilde{f}(t)$ remains to be Gaussian of zero mean but the autocorrelation function is some general function

$$\langle \tilde{f}(t')\,\tilde{f}(t'')\rangle = W(t', t''). \tag{12}$$

Now, the path integral implied by the stochastic process described by equation (11) is

$$P(x, t|x_0) = \int_{x_0,0}^{x,t} \mathscr{D}x(\tau)\, \exp\left\{-\frac{1}{2}\int_0^t\int_0^t d\tau'\, d\tau''[\gamma\dot{x}(\tau') - F(x(\tau'))]\, W^{-1}(\tau', \tau'')\, [\gamma\dot{x}(\tau'') - F(x(\tau''))]\right\}, \tag{13}$$

where $W^{-1}(\tau', \tau'')$ is the solution to the integral equation

$$\int_{-\infty}^{\infty} d\tau\; W(t', \tau)\; W^{-1}(\tau, t'') = \delta(t' - t''). \tag{14}$$

Let us show first that there exists a transformation $\{x(\tau)\} \to \{x'(\tau)\}$ of the paths leading to a simple Wienerian ("kinetic-energy") term $\int_0^t d\tau\, \dot{x}'^2(\tau)$ in the exponent of the path integral (13). For this objective we introduce a function $U_t(\tau, \tau_0)$ defined by the integral equation

$$\int_0^t\int_0^t d\tau_0'\, d\tau_0''\; U_t(\tau_0', \tau')\; W^{-1}(\tau_0', \tau_0'')\; U_t(\tau_0'', \tau'') = \delta(\tau' - \tau''). \tag{15}$$

If we were able to solve this equation — and notice that even prior to having started solving it we should have to have solved equation (14) — we could use the function

$$T_t(\tau, \tau_0) = -\frac{\partial}{\partial \tau_0}\int_0^{\tau} d\tau'\; U_t(\tau', \tau_0). \tag{16}$$

Then, the transformation in question is

$$x'(\tau) = \int_0^t d\tau_0[T_t(\tau, \tau_0) - T_t(t, \tau_0)]\, x(\tau_0) + (x' - x_0')\, \tau/t + x_0'. \tag{17}$$

By differentiating equation (17), using integration by parts and taking into account definition (16), we obtain the transformation of the velocities:

$$\dot{x}'(\tau) = \int_0^t d\tau_0 U_t(\tau, \tau_0)\, \dot{x}(\tau_0) - U_t(\tau, t)\, x' + (x' - x_0')/t. \tag{18}$$

After inserting expression (18) into formula (13), remembering definition (14), we obtain the path integral in the form

$$P(x', t|x_0') = \int_{x_0',0}^{x',t} \mathscr{D}x'(\tau)\, \exp\left\{-\frac{\gamma^2}{2}\int_0^t d\tau\, \dot{x}'^2(\tau) + \int_0^t\int_0^t d\tau'\, d\tau''(\ldots)\right\}. \tag{19}$$

The integrand (...) in the double integral of the exponent depends linearly on the velocity $\dot{x}'(\tau)$. We have on purpose not written the expression (...) explicitly, as we ought to find the inverse transform to (17) first. No simple partial differential equation of the Fokker-Planck type is possible since the time variable t occurs also as a parameter in the function $T_t(\tau, \tau_0)$ (and hence in the kernel of the inverse transformation to (17), too). In addition, any derivation of such an equation is impeded by the presence of the *double* integral $\int_0^t\int_0^t d\tau'\, d\tau''$ (...) in the exponent of the path integral (19).

Fortunately, as long as the deterministic component $F(x)$ of the force is either x-independent or proportional to x, a fairly general stochastic theorizing, independent of the concept of path integrals, is well manageable, as we have already mentioned (Appendix I). No such possibility seems to exist for a general, nonlinear function $F(x)$, unless for small enough values of $W(t, t)$ when an approximation analogical to the WKB approximation of the quantum mechanics could still be used. Generally, therefore, we may proclaim that the white-noise assumption is indeed an essential secret of success and not following it means encountering complications.

IV. CONCLUDING REMARKS

We can unify all the examples given in Part I of the present paper [1], as well as further examples, into a more general scheme as follows.

Let us realize a Brownian particle whose stochastic motion is described by the equation

$$\mathbf{\Gamma}\cdot\dot{\mathbf{r}} - \mathbf{F}(\mathbf{r}) = \mathbf{f}(t), \tag{20}$$

where $\mathbf{\Gamma}$ is some constant tensor, $\mathbf{F}(\mathbf{r})$ some deterministic vector function that is not explicitly dependent on t, and $\mathbf{f}(t)$ some spatially uniform but temporally highly fluctuating force defined as a Gaussian random function of zero mean ($\langle \mathbf{f}(t)\rangle = 0$) with a white-noise autocorrelation function

$$\langle \mathbf{f}(t')\,\mathbf{f}(t'')\rangle = \mathbf{\Lambda}\delta(t' - t''). \tag{21}$$

The product $\mathbf{ff}$ is meant as dyadic and $\mathbf{\Lambda}$ is a positively definite tensor.

The tensor $\mathbf{\Gamma}$ corresponds to friction but may contain (in case of the particle being charged) also components of the magnetic field. To formulate the functional path integral corresponding to equation (20), it is necessary to assume that $\mathbf{\Gamma}^T\mathbf{\Lambda}^{-1}\mathbf{\Gamma}$ is a positively definite tensor, too. ($\mathbf{\Gamma}^T$ is given by transposition of $\mathbf{\Gamma}$ and $\mathbf{\Lambda}^{-1}$ is inverse to $\mathbf{\Lambda}$). Then the desired path integral is

$$P(\mathbf{r}, t|\mathbf{r}_0) = \int_{\mathbf{r}_0,0}^{\mathbf{r},t} \mathscr{D}\mathbf{r}(\tau)\, \exp\left\{-\frac{1}{2}\int_0^t d\tau[\dot{\mathbf{r}}(\tau)\,\mathbf{\Gamma}^T - \mathbf{F}(\mathbf{r}(\tau))]\,\mathbf{\Lambda}^{-1}[\mathbf{\Gamma}\dot{\mathbf{r}}(\tau) - \mathbf{F}(\mathbf{r}(\tau))]\right\}. \tag{22}$$

The probability density $P(\mathbf{r}, t|\mathbf{r}_0)$ satisfies the equation

$$\frac{\partial P(\mathbf{r}, t|\mathbf{r}_0)}{\partial t}=\frac{1}{2}\nabla\mathbf{\Gamma}^{-1}\mathbf{\Lambda}(\mathbf{\Gamma}^{-1})^T\nabla P(\mathbf{r}, t|\mathbf{r}_0)-\nabla\mathbf{\Gamma}^{-1}[\mathbf{F}(\mathbf{r})\,P(\mathbf{r}, t|\mathbf{r}_0)], \tag{23}$$

$$P(\mathbf{r}, +0|\mathbf{r}_0)=\delta(\mathbf{r}-\mathbf{r}_0), \tag{23a}$$

which may be termed the Fokker-Planck (or Smoluchowski) equation related to a stochastic (Langevin) equation (20). Equation (23) displays a tensor diffusion coefficient

$$\mathbf{D}=\frac{1}{2}\mathbf{\Gamma}^{-1}\mathbf{\Lambda}(\mathbf{\Gamma}^{-1})^T. \tag{24}$$

The problem can easily be generalized to the case of Brownian motion of inertialess system of any number d of degrees of freedom. If Ξ denotes a vector in the corresponding d-dimensional Euclidian space, the consideration may run along the same line:

1 — dynamic stochastic (Langevin) equation for $\Xi(t)$
↓
2 — path integral for $P(\Xi, t|\Xi_0)$
↓
3 — differential (Fokker-Planck) equation for $P(\Xi, t|\Xi_0)$
↓
4 — solution $P(\Xi, t|\Xi_0)$.

The solution must fulfil the initial condition

$$P(\Xi, +0|\Xi_0)=\delta(\Xi-\Xi_0). \tag{25}$$

In case of the absence of boundaries, or in case when the boundaries are ideally reflecting (i.e. not absorbing), condition (25) implies the normalization condition

$$\int d^d\Xi P(\Xi, t|\Xi_0)=1 \tag{26}$$

for all values of Ξ_0 and $t\geq 0$.

It was evident from our analysis that in order to have, for a general case of the deterministic force $F(\Xi)$, the path integral in the Wiener (or Feynman-Kac) form, it was truly vital to consider the fluctuating force $f(t)$ as a Gaussian random function. Moreover, as we have stressed in Section III, it is almost inevitable to accept the white-noise approximation in order to guarantee at least partial simplicity.

The step $2\rightarrow 3$ is not compulsory and may be ignored whenever we can calculate the path integral directly. Unfortunately, generally such a calculation is likely to succeed only numerically.

Analytic calculations are possible when the exponent of the path integral is quadratic. Then the direct way how to calculate the Ξ- and Ξ_0-dependences of the

function $P(\Xi, t|\Xi_0)$ is to calculate the "classical path (s)" and insert it (them) into the exponent of the path integral for $P(\Xi, t|\Xi_0)$. The result of such a calculation is still uncertain in a multiplication factor $\mathcal{N}(t)$ independent of Ξ and Ξ_0, but dependent on t. The factor $\mathcal{N}(t)$ may be calculated by the functional path integration over closed paths or from the Fokker-Planck (Smoluchowski) equation. Alternatively, the normalization condition (26), if applicable (e.g. for the case of ideally reflecting boundaries), yields also a possibility to calculate the factor $\mathcal{N}(t)$ directly without using either the path integration or the Fokker-Planck (Smoluchowski) equation. Let us recall, however, that the analytically calculable path integrals correspond to linear Langevin equations for which, as we have suggested, there are other, and even better, methods.

We may conclude, therefore, that the path integrals have an opportunity to prove their potency rather in connection with nonlinear Langevin equations. We believe that the opportunity will soon become real as far as numerical methods for calculating the path integrals (preferably of a Monte Carlo type) will become a common-place in libraries of programs at contemporary computer centres.

APPENDIX I

Let us consider the linear Langevin equation without boundaries

$$\gamma\dot{x}+kx=f(t), \tag{I.1}$$

where γ, k are positive constants and $f(t)$ is a random function — not necessarily specified either as Gaussian or even as of the white-noise type — and let the function $f(t)$ be defined with zero mean,

$$\langle f(t)\rangle=0, \tag{I.2}$$

and with some general autocorrelation function

$$\langle f(t')\,f(t'')\rangle=W(t', t''). \tag{I.3}$$

Owing to the linearity, we can write generally the solution to equation (I.1) in the form

$$x(t)=\left[x(0)+\frac{1}{\gamma}\int_0^t d\tau\, f(\tau)\exp\left(\frac{k}{\gamma}\tau\right)\right]\exp\left(-\frac{k}{\gamma}t\right). \tag{I.4}$$

Thus, we can directly derive the variance

$$\langle[x(t)-x(0)]^2\rangle=\frac{1}{\gamma^2}\int_0^t\int_0^t d\tau'\,d\tau''\,W(\tau', \tau'')\exp\left(\frac{k}{\gamma}(\tau'+\tau'')\right)\times \\ \times\exp\left(-\frac{2k}{\gamma}t\right). \tag{I.5}$$

In particular, if we take into account the well-known relation

$$\langle [x(t)-x(0)]^2\rangle = 2Dt \tag{I.6}$$

defining the diffusion coefficient D, we shall obtain, for $W(t', t'') = \eta^2\delta(t'-t'')$ and $k=0$, the value $D=\frac{1}{2}\eta^2/\gamma^2$ without resort to a path integral at all. The consideration can be generalized directly for higher statistical moments $\langle [x(t)-x(0)]^n\rangle$ $(n>2)$ provided that the random function $f(t)$ is sufficiently well defined by higher correlation functions or cumulants.

APPENDIX II

The best-known form of the Langevin equation for a free Brownian particle of mass m is

$$m\dot{v} + \gamma v = f(t), \tag{II.1}$$

where v is the velocity and the remaining symbols γ, $f(t)$ have the same meaning as in Appendix I. Evidently, the line of argument given in Appendix I may be repeated by simply changing the notation. We will briefly reproduce, however, the derivation of the Fokker-Planck equation [2] — cf. also the collection of papers [3], pp. 33—35 — for the case of $f(t)$ being a Gaussian random function of the white-noise type. We start from the (Chapman-Kolmogorov) equation

$$P(v, t+\tau|v_0) = \left(\frac{m^2}{2\pi\eta^2\tau}\right)^{1/2}\int_{-\infty}^{\infty} \mathrm{d}\xi \exp\left\{-\frac{\tau}{2\eta^2}\left[m\frac{\xi}{\tau} + \gamma(v-\xi)\right]^2\right\} P(v-\xi, t|v_0) \tag{II.2}$$

for the infinitesimal time $\tau>0$. Denoting

$$g(\xi, \tau) = \left(\frac{m^2}{2\pi\eta^2\tau}\right)^{1/2} \exp\left\{-\frac{m^2\xi^2}{2\eta^2\tau}\right\} \tag{II.3}$$

we may rewrite equation (II.2) into the form

$$P(v, t+\tau|v_0) = \int_{-\infty}^{\infty} \mathrm{d}\xi g(\xi, \tau) \exp\left\{-\frac{m\gamma}{\eta^2}\xi(v-\xi) - \frac{\gamma^2\tau}{2\eta^2}(v-\xi)^2\right\}\times \tag{II.4}$$
$$\times P(v-\xi, t|v_0).$$

After expressing the l.h.s. as $P(v, t|v_0) + \tau\partial P(v, t|v_0)/\partial t + O(\tau^2)$, developing the integrand, except the function $g(\xi, \tau)$, of the r.h.s. into the Taylor series up to the first order in τ and second order in ξ, performing the integration and finally

comparing all the terms proportional to τ, we shall obtain the Fokker-Planck equation

$$\frac{\partial P(v, t|v_0)}{\partial t} = \frac{\eta^2}{2m^2}\frac{\partial^2 P(v, t|v_0)}{\partial v^2} + \frac{\gamma}{m}\frac{\partial}{\partial v}[vP(v, t|v_0)], \tag{II.5}$$

which reveals a "diffusion coefficient" in the velocity space

$$D_v = \frac{\eta^2}{2m^2}. \tag{II.6}$$

APPENDIX III

Similarly as in the case of equation (II.4) of Appendix II we may rewrite equation (7) in the form

$$P(x, t+\tau|x_0) = \int_{-\infty}^{\infty} \mathrm{d}\xi g(\xi, \tau) \exp\left\{\frac{\gamma}{\eta}\xi F(x-\xi) - \frac{\tau}{2\eta^2}F^2(x-\xi)\right\}\times \tag{III.1}$$
$$\times P(x-\xi, t|x_0).$$

If we complete all the steps which led us from equation (II.4) to equation (II.5), we shall obtain, in a perfect analogy, the Smoluchowski equation (10). It may be pointed out, anyway, that the correct Smoluchowski equation could equally well be obtained even if the expression $F^2(x-\xi)$ were replaced by $F^2(x)$; namely, when expressions of the order $\tau\xi$ in the exponent of integral (III.1) are taken into account, the integration in equation (III.1) gives only terms of the order $O(\tau^{3/2})$, i.e. the order which we were neglecting. The only significant point is to write the τ-independent term in the form $(\gamma/\eta)\,\xi F(x-\xi)$.

Of course, it is of interest to show what happens when the τ-independent term is written in agreement with Feynman's rule. Then we have to investigate the equation

$$\Pi(x, t+\tau|x_0) = \int_{-\infty}^{\infty} \mathrm{d}\xi\, g(\xi, \tau) \exp\left\{\frac{\gamma}{\eta}\xi F\left(x-\frac{1}{2}\xi\right) - \frac{\tau}{2\eta^2}F^2(x)\right\}\times \tag{III.2}$$
$$\times \Pi(x-\xi, t|x_0).$$

Again, by following the procedure that has led us to the Smoluchowski equation, we shall obtain the equation

$$\frac{\partial \Pi(x, t|x_0)}{\partial t} = \frac{\eta^2}{2\gamma^2}\frac{\partial^2 \Pi(x, t|x_0)}{\partial x^2} - \frac{1}{2\gamma}\left(\frac{\partial F}{\partial x}\right)\Pi(x, t|x_0) - \tag{III.3}$$
$$-\frac{1}{\gamma}F\frac{\partial \Pi(x, t|x_0)}{\partial x}.$$

This equation differs from the Smoluchowski equation in a term $(1/2\gamma)\times(\partial F/\partial x)\,\Pi(x,t|x_0)$.

What is very interesting is the fact that if the inequality (6) were reversed into an innocently looking equality, i.e. in other words, if the path integral (3) were decomposed into the form

$$\Pi(x,t|x_0)=\exp\left\{\frac{\gamma}{\eta^2}(V(x_0)-V(x))\right\}\int_{x_0,0}^{x,t}\mathscr{D}x(\tau)\exp\left\{-\frac{1}{2\eta^2}\times\right. \quad \text{(III.4)}$$
$$\left.\times\int_0^t d\tau[\gamma\dot{x}^2(\tau)+F^2(x(\tau))]\right\},$$

then the value of the path integral would be exactly the same as if the Feynman rule were used. That is why we had the right to denote on purpose this path integral by the same symbol $\Pi(x,t|x_0)$, and not $P(x,t|x_0)$; since if we juxtapose correctly the corresponding differential equation to it — and this is indeed an easy problem since the integrand in the exponent reminds a sum of a kinetic and potential energies so that we may recollect the Bloch equation for the canonical density matrix — we shall obtain exactly equation (III.3). Naturally, in general $P(x,t|x_0)\neq\Pi(x,t|x_0)$.

Thus, we may conclude that Feynman's treatment of the path integrals — although properly corresponding to the possibility of performing usual integrations in the exponent of quantum-mechanical path integrals — is not automatically transferable into probabilistic applications.

If we wished to be formally rigorous, we ought to use, in case of the probabilistic function $P(x,t|x_0)$, a different symbol from $\int$, say M.p. $\int$ (a deliberate proposal, as M.P. is abbreviation for the "Markov process") in the exponent of the path integral (3), reserving the symbol $\int$ (understood in its traditional meaning) for the exponent in the path integral representing the function $\Pi(x,t|x_0)$ and, of course, for exponents of quantum mechanical, or quantum statistical, path integrals. Thus, we should write, instead of formula (3), the path integral

$$P(x,t|x_0)=\int_{x_0,0}^{x,t}\mathscr{D}x(\tau)\exp\left\{-\frac{1}{2\eta^2}\,\text{M.p.}\int_0^t d\tau[\gamma\dot{x}(\tau)-F(x(\tau))]^2\right\}=$$
$$=\int_{x_0,0}^{x,t}\mathscr{D}x(\tau)\exp\left\{\frac{\gamma}{\eta^2}\,\text{M.p.}\int_0^t d\tau\dot{x}(\tau)\,F(x(\tau))\right\}\times \quad \text{(III.5)}$$
$$\times\exp\left\{-\frac{1}{2\eta^2}\int_0^t d\tau[\gamma^2\dot{x}^2(\tau)+F^2(x(\tau))]\right\}.$$

The second form is also correct, as the integrals $\int$ and M.p. $\int$ are essentially different only for integrands dependent linearly on the velocity $\dot{x}(\tau)$. Similarly, we ought to write M.p. in front of the integral in relation (6), i.e. distinguish explicitly the relations

$$-\text{M.p.}\int_{x_0}^{x}dx(\tau)\left[\frac{\partial V}{\partial x}\right]_{x=x(\tau)}\neq V(x_0)-V(x) \quad \text{(III.6)}$$

and

$$-\int_{x_0}^{x}dx(\tau)\left[\frac{\partial V}{\partial x}\right]_{x=x(\tau)}=V(x_0)-V(x). \quad \text{(III.7)}$$

The same careful formal distinction between the symbols $\int$ and M.p. $\int$ should be made in the corresponding exponents of path integrals dealt with in Sections IV and V. (Namely, the integrals in the exponents of formulae (13), (19) and (22) have obligatorily to be understood in the sense of "Markov process integrals",

APPENDIX IV

In the preceding appendix, we have discussed rules of the proper path integration provided that a path integral (integral (3)) was already put forward before. Now we will scrutinize the way how the path integrals corresponding to nonlinear Langevin equations can be derived. The chief difference between the present and former derivation (which was given in Section III.1 of Part I) is in the point that now the Jacobian $J=|\delta f(\tau)/\delta x(\tau)|$ may be, owing to the nonlinearity of equation (1), path-dependent. To show this, we may discretize the time interval $(0,t)$ by dividing it into N equal subintervals so that $0<t_1<\ldots<t_{N-1}<t_N=t$ and rewrite the Langevin equation (1) as a difference equation. According to a recent paper by Kitahara and Metiu [5], generally the discrete transcription of the Langevin equation (1) may be taken in the form

$$\gamma\frac{x_{i+1}-x_i}{\tau}-[\mu F(x_{i+1})+(1-\mu)\,F(x_i)]=f_{i+1}, \quad \text{(IV.1)}$$

where $i=0,1,\ldots,N-1$; $x_i=x(t_i)$, $f_i=f(t_i)$, $\tau=t_{i+1}-t_i=t/N$. If $\tau\to0$, equation (IV.1) goes over into equation (1) for any value of μ. Nevertheless, we would rather call, for $\mu\neq0$, the stochastic process described by equation (IV.1) pseudo-Markovian. For a pure Markov process we require $\mu=0$, following the philosophy of the Markov processes that a next state x_{i+1} actualized after elapsing an infinitesimal time τ must be determinable, respecting the deterministic force F, purely from the present state x_i. In other words, we find it difficult from the point of view of classical causality to accept a definition of a dynamic Markov process whose next state x_{i+1} is dependent on *itself* via the *causal* influence $F(x_{i+1})$, in addition to the influence $F(x_i)$. Such an argument, of course, does not apply to the random force $f(t)$, which is assumed to operate independently as a deus ex machina. There is no other reason but convention that we have written, following Ref. [5], f_{i+1}, and not f_i, on the r.h.s. of equation (IV.1). For the proper definition of the corresponding path integral, however, it is not at all immaterial whether we use the discretized Langevin equation in the form

$$\gamma \frac{x_{i+1}-x_i}{\tau} - F(x_i) = f_{i+1} \tag{IV.2}$$

or

$$\gamma \frac{x_{i+1}-x_i}{\tau} - F(x_i) = f_i . \tag{IV.3}$$

Indeed, the Jacobian

$$J = \left| \frac{\partial(f_1, f_2, \ldots, f_{N-1})}{\partial(x_1, x_2, \ldots, x_{N-1})} \right| = \prod_{i=1}^{N-1} \left| \frac{\partial f_i}{\partial x_i} \right|$$

has different values, respectively:

$$J = \left(\frac{\gamma}{\tau}\right)^{N-1}, \tag{IV.4}$$

$$J = \left(\frac{\gamma}{\tau}\right)^{N-1} \exp\left\{\frac{1}{\gamma}\int_0^t \mathrm{d}\tau \left[\frac{\partial F(x)}{\partial x}\right]_{x=x(\tau)}\right\}. \tag{IV.5}$$

To prove the last expression, we may divide the number of the subintervals into N/n blocks so that $n \to \infty$ and also $N/n \to \infty$ when $N \to \infty$, and $\partial F/\partial x$ may be approximated as a constant within each block consisting of n adjacent subintervals. Then we may use the limiting procedure $(1+a/n)^n \to e^a$ that gives, for $a = (\Delta t/\gamma)\, \partial F/\partial x$, where $\Delta t = \tau n$, the expression $\exp\{(\Delta t/\gamma)\, \partial F/\partial x\}$. After exhausting all the blocks, we obtain the exponential (IV.5).).

The expression (IV.5) and the corresponding equation (IV.3) are, in fact, equivalent to the Kitahara-Metiu relation (IV.1) with $\mu = -1$.

It is not difficult to define suitable rules for the path integration respecting the transformation (IV.1). When introducing (in the spirit of Appendix III) a special notation M. p. $(\mu) \int$ defined by the formula

$$\mathrm{M.p.}\,(\mu) \int_0^t \mathrm{d}\tau\, \dot{x}(\tau)\, F(x(\tau)) = \sum_{i=1}^{N-1} (x_{i+1}-x_i)\, F((1-\mu)\, x_{i+1} + \mu x_i), \tag{IV.6}$$

we may write the path integral (3) in the form

$$P(x, t|x_0) = \int_{x_0,0}^{x,t} \mathscr{D}x(\tau) \exp\left\{-\frac{\mu}{\gamma}\int_0^t \mathrm{d}\tau \left[\frac{\partial F}{\partial x}\right]_{x=x(\tau)}\right\} \times \tag{IV.7}$$

$$\times \exp\left\{-\frac{1}{2\eta^2}\,\mathrm{M.p.}\,(\mu)\int_0^t \mathrm{d}\tau [\gamma \dot{x}(\tau) - F(x(\tau))]^2\right\}.$$

For the transition probability function $P(x, \tau|x-\xi)$ with an infinitesimal value τ, we have thus, as a counterpart to formula (8), the expression

$$P(x, \tau|x-\xi) = \left(\frac{\gamma^2}{2\pi\eta^2\tau}\right)^{1/2} \exp\left\{-\frac{\mu\tau}{\gamma}\frac{\partial F}{\partial x}\right\} \exp\left\{-\frac{1}{2\eta^2}\left[\gamma\frac{\xi}{\tau} - F(x-\mu\xi)\right]^2\right\}. \tag{IV.8}$$

(since $x_{i+1} = x$, $x_i = x - \xi$). The apparent μ-dependence is irrelevant, as the Chapman-Kolmogorov equation (7) gives, whichever value μ in function (IV.8) is used, the Smoluchowski equation (10) that is not anymore dependent — as a well-defined physical equation — on the nonphysical, arbitrary parameter μ. In this way, we have shown that in order to eschew any confusion (or at least superfluous ambiguities mentioned in Ref. [5]), it is sufficient to make a simple formal distinction between symbols used for integrals occurring in the exponents of the path integrals.

Finally, notice the formal identities

$$\mathrm{M.p.}\,(0) = \mathrm{M.p.} \int, \tag{IV.9}$$

$$\mathrm{M.p.}\left(\frac{1}{2}\right) \int = \int, \tag{IV.10}$$

directly deducible by comparing the definitions of Appendix III with the definition given by formula (IV.6).

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