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PLANCK EQUATIONS

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PATH INTEGRAL APPROACH TO THE SOLUTION OF FOKKER-PLANCK EQUATIONS

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Abstract:

The classical transport equation of the Fokker-Planck type is transformed into a path integral formulation and solved within the saddle point approximation. The numerical results are compared with the exact solution and with the approximation gained by applying a moment expansion for some simple drift potentials and constant diffusion. The limitations of the present approach as well as general problems connected with the saddle point approximation are discussed.

In the last years nuclear physicists have gained current interest in the dynamics of stochastic processes and successfully applied classical transport equations of the Fokker Planck type to slow collective nuclear motion such as heavy ion reactions in the energy range of a few MeV/n above the Coulomb barrier [1] and induced nuclear fission [2,3]. While exact solutions of these equations presently are only available for the one-dimensional problem [4,5], the standard approximation scheme is to apply a moment expansion up to second order [3,6]. This is sufficient for harmonic driving potentials, but turns out to be very crucial in actual cases [3,7] due to the occurrence of instability points where the moment expansion tends to diverge. In addition physics require non-harmonic driving potentials in order to allow for a proper understanding of the experimental data [8].

In this letter we want to draw attention to and stimulate discussion on an approximate solution of the Fokker Planck equation within the path integral formalism. There has been an intensive discussion on the proper definition of a Lagrangian in statistical physics in the late 70th connected with the ordering problem of operators [9,10] but nobody really has developed the techniques and performed calculations except for the anharmonic oscillator in an analytical investigation [11]. We want to propose a way similar in spirit to ref. [9] and derive pseudo classical equations of motion for the various paths and the corresponding Gelfand-Yaglom determinant [12]. The application to a simple driving potential will give us some insight into the validity of the present approach.

In this initial study we focus our intention on a Fokker Planck equation of the type

$$\frac{\partial}{\partial t} f(x, t) = - \frac{\partial}{\partial x} v(x) f(x, t) + D \frac{\partial^2}{\partial x^2} f(x, t) \quad (1)$$

with constant diffusion coefficient D and a general drift potential $v_d(x)$ with $v(x)$ given by

$$v(x) = - \frac{\partial}{\partial x} V_d(x) \quad (2)$$

For later purposes we rewrite $f(x, t)$ in the form

$$f(x, t) = \exp \left\{ \int_0^x \alpha(x') dx' \right\} g(x, t) \quad (3)$$

where $g(x, t)$ obeys

$$\frac{\partial}{\partial t} g(x, t) = - H_r(x, -i \frac{\partial}{\partial x}) g(x, t) \quad (4)$$

with

$$H_r(x, p) = g(x) + i v_r(x) p + D p^2,$$

$$g(x) = \frac{\partial v}{\partial x}(x) + v(x) \alpha(x) - D \frac{\partial^2}{\partial x^2} \alpha(x) - D \alpha(x)^2,$$

$$v_r(x) = v(x) - 2D\alpha(x)$$

and the convention that all differential operators appear on the right of each product. Iterative application of the evolution in ϵ time steps

$$\begin{aligned} g(x, t+\epsilon) &= \int \frac{dp dx'}{2\pi} \{ 1 - \epsilon H_r(x, -i \frac{\partial}{\partial x}) e^{ip(x-x')} \} g(x', t) \\ &= \int \frac{dp dx'}{2\pi} \exp \{ -\epsilon H_r(x, p) + ip(x-x') \} g(x', t) \end{aligned} \quad (5)$$

gives the full time evolution from 0 to t in form of a path integral (Hamiltonian form)

$$g(x, t) = \int D[x(t)] D[p(t)] \exp \left\{ - \int_0^t (H_r(x, p) - ip(x-x')) dt \right\} g(x_0, 0) \quad (6)$$

The formal way of writing $g(x, t)$ in eq. (6) has to be understood as the following[†] limit $N \rightarrow \infty$, $\epsilon = t/N$,

$$g(x, t) = \lim_{N \rightarrow \infty} \int \frac{dx_0 dp_0}{2\pi} \dots \int \frac{dx_{N-1} dp_{N-1}}{2\pi} \exp \left\{ - \sum_{j=1}^N (H_r(x_j, p_{j-1}) - i p_{j-1}(x_j - x_{j-1})) \right\} g(x_0, 0) \quad (7)$$

$$x = x_N, \quad \dot{x}_j = (x_j - x_{j-1})/\epsilon.$$

As the Hamiltonian action is quadratic in the pseudo momenta p_j we can perform these integrations and are left with the Lagrangian form[#] of the propagator as a sum over all paths from x_0 to x

$$G(x, x_0; t) = \lim_{N \rightarrow \infty} \int \frac{dx_1}{\sqrt{4\pi D \epsilon}} \dots \int \frac{dx_{N-1}}{\sqrt{4\pi D \epsilon}} \quad (8)$$

$$\exp \left\{ - \sum_{i=1}^N L \left(x_i, \frac{x_i - x_{i-1}}{\epsilon} \right) \right\} = \int D[x(t)] e^{-\int_0^t L_r(x, \dot{x}) dt}$$

$$\text{where } L_r(x, \dot{x}) = H_r(x, p) - p\dot{x}$$

$$\dot{x} = \frac{\partial H_r}{\partial p},$$

or explicitly

$$L_r(x, \dot{x}) = \beta(x) + \frac{1}{4D} (\dot{x} - \gamma(x))^2. \quad (9b)$$

[†]note, that due to the freedom in choosing the order of the operators in (4) the continuous form (6) is in fact an unsatisfactory notation as it is only uniquely defined together with its explicit discretization (7). The freedom to replace

$\frac{\partial}{\partial x} \gamma(x)$ by $(1 - \bar{\alpha}(x)) \frac{\partial}{\partial x} \gamma(x) + \bar{\alpha}(x) \gamma'(x) \frac{\partial}{\partial x}$ with arbitrary $\bar{\alpha}(x)$ corresponds to a local gauge transformation [10] and the variety of path integral forms obtained in this way is identical to those obtained here by the choice (4) and varying the 'gauge factor' $\exp \left\{ \int_0^x \alpha(x') dx' \right\}$ in (3).

[#] note, that the path integral representations (6-7) or (8) are still exact.

Through the saddle point approximation to eq. (8) the propagator

$$G(x, x_0; t) \approx \frac{1}{\sqrt{d(x, t)}} \cdot \exp \left\{ - \int_0^t L_r(x_c, \dot{x}_c) dt \right\} \quad (10)$$

is built up by the pseudo classical paths that link x_0 with x . They are determined via

$$\delta \int L_r(x, \dot{x}) dt = 0; \quad x(0) = x_0, \quad x(t) = x$$

$$\text{or} \quad \ddot{x}_c = - \frac{\partial}{\partial x} U(x) \quad (11)$$

$$\text{with } U(x) = - \frac{\gamma^2(x)}{2} - 2D\beta(x).$$

Some more care has to be attributed to the calculation of the fluctuations around the classical path, i.e. the determinant[†] $d(t)$. It can only be constructed from the discretized version of the action

$$S(N, \epsilon) = \epsilon \sum_{j=1}^N L_\epsilon(x_j, \dot{x}_j) \quad (12)$$

Following Gelfand and Yaglom [12] we introduce the determinant of second order derivatives up to the I^{th} time step by

$$d(I, \epsilon) = \det_I \left\{ \frac{\partial^2 S}{\partial x_i \partial x_k} \right\} = \frac{\epsilon^I}{2\pi} \left(\frac{\partial^2 L_1}{\partial \dot{x}_1^2} \dots \frac{\partial^2 L_I}{\partial \dot{x}_I^2} \right)^{-1} \quad (13)$$

for $0 < I < N$ and $i, k \leq I$

[†]In contrast to conventional Schrödinger mechanics the determinant is no longer given by the dispersion of the paths, i.e. $d(t) = \det \left(\frac{\partial x}{\partial x_0} \right)$ due to the ordering problem of the term proportional to $\dot{x}$ in the Lagrangian (9b). Only by choosing $\alpha(x) = \frac{\gamma(x)}{2D}$ this property of $d(t)$ can be retained. In fact ordinary methods of the calculus (e.g. $\int_t^x \gamma(x') dx' = \frac{1}{\epsilon} \sum_{j=1}^N \gamma(x_j) \epsilon$) cannot be applied to the action integral as the discretization limit $N \rightarrow \infty$ applies for both simultaneously, for the action and the integrations $\int dx_1 \dots dx_N$.

with the aim of deriving a recursion relation of d in I . Expanding the determinant with respect to the last line (or column) and comparing equal powers in ϵ yields

$$d(I \cdot \epsilon) = \epsilon \cdot \frac{\partial^2 S}{\partial x_I^2} / \frac{\partial^2 L_I}{\partial x_I^2} \cdot d((I-1) \cdot \epsilon) - \epsilon^2 \frac{\partial^2 S}{\partial x_I \partial x_{I-1}} / \left(\frac{\partial^2 L_I}{\partial x_I^2} \cdot \frac{\partial^2 L_{I-1}}{\partial x_{I-1}^2} \right) \cdot d((I-2) \cdot \epsilon). \quad (14)$$

Going over to the continuous limit in time eq. (14) becomes an ordinary second order differential equation in time,

$$\begin{aligned} \ddot{d}(t) &= \left(\frac{\partial^2 L}{\partial x^2} / \frac{\partial^2 L}{\partial x^2} - \left(\frac{\partial^2 L}{\partial x \partial x} / \frac{\partial^2 L}{\partial x^2} \right)^2 \right) \cdot d(t) \\ &+ 2 \frac{\partial^2 L}{\partial x \partial x} / \frac{\partial^2 L}{\partial x^2} \cdot \dot{d}(t) \\ &= (2Dg''(x) - \dot{x}y''(x) + y(x)y''(x)) d(t) \\ &- 2y'(x) \dot{d}(t) \end{aligned} \quad (15)$$

with $d(0) = 0$ and $\dot{d}(0) = 1$.

Here the primes and dots denote the derivatives with respect to x and t , respectively. The equations (11,16) entirely determine the time evolution of the approximate propagator (10) of the Fokker Planck equation (1). Within this approach the initial problem has been transformed to the solution of simple differential equations in time, i.e. the pseudo classical equations of motion, which can be done using conventional computational techniques.

Going over to the more technical side of the problem we have to fix the function $\alpha(x)$, which up to now has been free and should be optimized in such a way that the solution of the path integral approach within the saddle

point approximation (SPIA) comes close to the exact distribution function. There are four different choices for $\alpha(x)$ which correspond to specific limits. For

$$\alpha(x) = 0, \quad (17a)$$

i.e. $f(x,t) = g(x,t)$, we found out within various models for $Y(x)$, that the SPIA becomes very poor for longer times. Other choices, which simplify the Lagrangian (9b) essentially, require $\beta(x) = 0$ or $\gamma(x) = 0$ or $U(x) = 0$ leading to

$$\alpha(x) = \frac{V(x)}{D}, \quad (17b)$$

$$\alpha(x) = \frac{V(x)}{2D} \quad \text{and} \quad (17c)$$

$$\alpha(x) = \int_0^x \left(\frac{V^2(x')}{4D^2} + \frac{V'(x')}{D} \right) dx' \quad (17d)$$

respectively. We obtained the best results with the choice (17b) because for $t \rightarrow \infty$ $g(x,t)$ has to approach a constant value for all x . In general the choice of $\alpha(x)$ influences the occurrence of caustics which will be discussed later.

In order to show some application we choose the drift potential

$$V(x) = \pm (2 \cosh(x))^{-1} \quad (18)$$

and $D = 0.2$

in units of the universe time scale, where x is dimensionless. The attractive potential is able to cover essential differences from the harmonic oscillator (where the saddle point approximation is exact) and the repulsive potential may well simulate the situation met in induced nuclear fission.

We first consider the attractive case with the initial condition $f(x,0) = \delta(x-1)$.

The approximate solutions for various times displayed in fig. 1a) (dotted line) are compared with the exact solutions (full line) and with the gaussians obtained from a moment expansion of eq. (1) (dashed line). Noticable deviations from the exact solution come in for $t > 0.4$ for the gaussian approximation and for $t > 2$ for the SPIA. While the gaussian approximation essentially fails in reproducing the tails of the distribution the SPIA still works fairly well in this region. Thus the variance of the distribution $\sigma_x(t)$ (full line) is sufficiently well reproduced in the SPIA (dotted line) in contrast to the gaussian approach (dashed line) (fig. 2a).

The same statements hold in case of the repulsive driving potential where the initial distribution was chosen to be placed on the instability point at $x=0 : f(x,0) = \delta(x)$. The respective time evolution of the distributions $f(x,t)$ is displayed in fig. 1b). The deviations of the gaussian approximation become more apparent for longer times because the exact distribution splits into two parts which essentially are reproduced by the SPIA. Again the SPIA nicely fits the tails of the distribution but becomes rather poor for longer times in the central region. This type of deviation does not significantly influence the variance $\sigma_x(t)$ as can be seen from fig. 2b).

In summary the numerical studies convey, that the SPIA remains valid for much longer times than the gaussian approach and essentially gives good results for the tails of the distributions. The latter phenomena promises an application to nuclear fission within the SPIA because the fission probability delicately depends on the high energy tail of the corresponding distribution function [2].

We still have to discuss the problem of choosing the function $\alpha(x)$ in eq. (3) as it is intimately related with the occurrence of caustics through the properties of the pseudo potential $U(x)$ in eq. (11). For illustration $U(x)$ is displayed in fig. 3) for the attractive drift potential $V_d(x)$ for three different choices (17a-c). All paths start with $x(0) = 1$ and $\dot{x}(0)$ ranging from $-\infty$ to $+\infty$. The interesting paths which build up the final distribution in the central region are those with $\dot{x}^2(0) \approx 2U(0)$. All paths with $\dot{x}^2(0) < 2U(0)$ will be reflected after a finite time and thus cross in time with another path. These crossings denoted as caustics cause the saddle point approximation to break down [12]. It is thus important to choose $\alpha(x)$ in such a way that $U(x)$ becomes rather shallow (dotted line) which pushes the occurrence of caustics to later times. In this respect (17d) would be the optimal choice for $\alpha(x)$ because no caustics occur, but it turns out, that the approximation for the Gelfand-Yaglom determinant (14) becomes rather poor.⁺ The SPIA thus cannot provide good solutions for all times within the present treatment.

In conclusion we can summarize that the path integral approach proposed in this letter provides a rather simple technical method for solving classical transport equations of the Fokker Planck type for small times. For the problems studied the SPIA gives a sufficient description for times which are about one order of magnitude larger than those times for which the moment expansion method remains valid. It further describes the tail regions fairly well. In spite of the technical advantages obtained we clearly have to point out that the simple saddle point limit breaks down after a finite time due to the caustic problem.

⁺for precision: for ordinary integrals the various choices of $\alpha(x)$ would correspond to a transformation $\int d\xi e^{S(\xi)}$ to $\int d\eta a(\eta) e^{S(\eta)}$ where the saddle point approximation is only applied to the respective actions and $a(\eta)$ is assumed to be smooth.

Nevertheless the integral formulation opens further refinements of approximations that may overcome the present difficulties. Here one might think of uniform approximations [13] that care about the occurrence of several classical paths or an extension to complex paths [14] as well as schemes that treat those long wavelength modes $x(t)$ explicitly that are governing the caustic problem. Some work has to be done along this line in future. Still an application of the present approach to nuclear fission appears promising.

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Figure captions:

Fig. 1: Comparison of the time evolution of the distribution function for the attractive drift potential (l.h.s) and repulsive drift potential (r.h.s).
 exact solution (full line)
 gaussian approximation (dashed line)
 path integral approach (dotted line)

Fig. 2: Comparison of the resulting standard deviations as function of time for the attractive and repulsive drift potential.
 exact solution (full line)
 gaussian approximation (dashed line)
 path integral approach (dotted line)

Fig. 3: Illustration of the pseudo potential $U(x)$ for three different choices of $\alpha(x)$
 17a) (full line)
 17b) (dotted line)
 17c) (dashed line)

Fig. 1

Fig. 2

Fig. 3