Z. Physik B 35, 185–191 (1979)

Zeitschrift für Physik B

Manifolds of Equivalent Path Integral Solutions of the Fokker-Planck Equation

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Received September 14, 1978; Revised Version May 16, 1979

Path integral solutions of the multi-dimensional Fokker-Planck equation with variable dependent diffusion coefficients are deduced in a simple and exact manner. We show that the Onsager-Machlup function is not defined uniquely but is definable only together with the discretization prescription and the measure in the functional space. We present wide classes of mathematical equivalent path integral representations characterized by non-linear variable transformations $\mathbf{v}(\mathbf{q}', \mathbf{q})$ and the coefficients α_K of a linear combination, all giving exactly the same solution of the Fokker-Planck equation.

1. Introduction

Path integral solutions for the probability distribution of Markov processes as described by the Langevin equation with white noise or the stochastic equivalent [1] Fokker-Planck equation (1) have become of increasing interest in the last years [2–11]. Previously Onsager and Machlup [12] dealt with the probabilities for whole paths of linear diffusion processes. Extending to nonlinear Gaussian processes solution of the corresponding Fokker-Planck equations have been deduced in form of functional integrals yielding generalizations of the Onsager-Machlup function. A discussion about the uniqueness or the ambiguity, respectively, of the path integral representation has originated [8, 10], since a whole class of mathematical equivalent path integral solutions has been proposed at least for the one-dimensional Fokker-Planck equation [7].

Frequently the path integration solution of the Fokker-Planck equation is written in the form [10, 15]:

$$f(q,t) = \int_{q_0}^{q} D\mu(q) \cdot \exp\left[-\int_{t_0}^{t} \mathscr{L}(\dot{q}(t'), q(t'))\, dt'\right] f(q_0) \tag{1}$$

where $\mathscr{L}(\dot{q}, q)$ is called Onsager-Machlup function or sometimes Lagrangian and $D\mu(q)$ is the measure in the functional space. The expression (1) is just formal and we have to give a mathematically exact definition for it. Path integrals are defined as the limit of a well defined discrete form [16], i.e.

$$f(q_N, t) = \lim_{\substack{N\to\infty \\ N\tau = t - t_0}} \prod_{i=0}^{N-1} (\mu_i\, dq_i) \cdot \exp\left[-\tau \sum_{j=0}^{N-1} \mathscr{L}(q_{j+1}, q_j, \tau)\right] f(q_0). \tag{2}$$

Here we have chosen an equidistant lattice on the time axis.

We like to emphasize that only (2) is well defined and seems to be suitable for actual calculations. One should handle with the formal expression (1) carefully. It is not admissible to look on $\tau \sum \mathscr{L}(q_{j+1}, q_j, \tau)$ as an arbitrary Riemann sum of the integral $\int \mathscr{L}(\dot{q}, q)\, dt'$. Consider the well known case of a 1-dimensional linear Fokker-Planck equation:

$$\dot{f} = -\frac{d}{dq}(-\lambda q f) + \frac{1}{4}\frac{\partial^2 f}{\partial q^2}.$$

Here a common choise for the Onsager-Machlup function is [3, 4, 6, 10]:

$$\mathscr{L}(\dot{q}, q) = (\lambda q + \dot{q})^2 - \tfrac{1}{2}\lambda$$

taken together with the Wiener measure

$$\mu_i = (2\pi\tau\tfrac{1}{2})^{-\frac{1}{2}}.$$

0340-224X/79/0035/0185/$01.40

When $\dot{q}$ is defined [10, 15] by $\dot{q}=\frac{q_{i+1}-q_i}{\tau}$, a correct discrete form is (see Appendix C)

$$\mathscr{L}(q_{i+1},q_i)=\left[\lambda\tfrac{1}{2}(q_{i+1}-q_i)+\frac{1}{\tau}(q_{i+1}-q_i)\right]^2-\tfrac{1}{2}\lambda.$$

But we can see in Appendix C, that also the following discrete versions are correct i.e. it gives the same $f(q,t)$ in the limit $N\to\infty$, $\tau\to 0$:

$$\mathscr{L}(q_{i+1},q_i)=\left[\lambda(aq_{i+1}+bq_i)+\frac{1}{\tau}(q_{i+1}-q_i)\right]^2-a\lambda \tag{3}$$

with $a+b=1$. This ambiguity characterized by the number a does not arise from the ways in which a continuous function can be approximated by discrete ones [10]. For when we perform the formal limit from (2) to (1), we get

$$\mathscr{L}(\dot{q},q)=(\lambda q+\dot{q})^2-a\lambda. \tag{3a}$$

Therefrom we have to conclude, that the Onsager-Machlup function is not determined uniquely. Different $\mathscr{L}(\dot{q},q)$ demand different ways of discretization (3). Further this demonstrates that the formal continuous version (1) is meaningless when we do not specify how to come from (1) to the correct discrete version (2). Therefore we avoid the continuous form (1) which may be useful for abreviations.

Of course it is possible to remove the ambiguity in (3) by additional requirements [17] or special derivations of path integrals [7, 10, 11].

In this paper we show how the ambiguity pointed out in (3) is represented in the general case of the n-dimensional nonlinear Fokker-Planck-equation. We find in an exact manner wide classes of equivalent path integral representations all giving the same correct solution $f(\mathbf{q},t)$ of the Fokker-Planck equation. They are characterized by variable transformations $\mathbf{v}(\mathbf{q}',\mathbf{q})$ which may be nonlinear and by the coefficients α_k of a linear combination. We find that the Onsager-Machlup function $\mathscr{L}(\mathbf{q}_{i+1},\ q_i)$ is determined by the coefficients of the Fokker-Planck-equation in a simple way. In Sect. 2 we line out the procedure on principle how to come from the Fokker-Planck equation to a path integral representation of the solution. The necessary representations of the short time propagator are deduced in Sect. 3. The resulting path integral representations are given in Sect. 4 and discussed, especially for the case of a linear transformation $\mathbf{v}(\mathbf{q}',\mathbf{q})$. Additional manifolds of equivalent path integral solutions are found by a linear combination.

2. Procedure on Principle

Our starting point is the n-dimensional Fokker-Planck equation:

$$\frac{\partial f}{\partial t}=Lf \tag{4}$$

with

$$L=-\tfrac{1}{2}p_\nu p_\mu Q_{\nu\mu}(\mathbf{q})-ip_\nu K_\nu(\mathbf{q})+V(\mathbf{q}).$$

Here is

$$p_\nu=-i\frac{\partial}{\partial q_\nu}$$

and $f=f(\mathbf{q},t)$ is the probability density of the n-dimensional variable $\mathbf{q}$. We chose $f(\mathbf{q})$ to be at least continuous so that the Fokker-Planck equation is applicable.

Sum convention is used. The term $V(\mathbf{q})$ is introduced in order to compare with previous papers [8, 10] and to stress the connection to quantum mechanics.

A way of deducing a path integral form for the probability distribution f is to write the time evolution for infinitesimally small time in the following form:

$$f(\mathbf{q},t_0+\tau)=\int P_\tau(\mathbf{q}/\mathbf{q}_0)f(\mathbf{q}_0,t_0)\,dq_0 \tag{5}$$

where $P_\tau(\mathbf{q}/\mathbf{q}_0)$ is the conditional probability for small τ, also called short time propagator. Equation (5) is just the Chapman-Kolmogorov equation if we choose for $f(\mathbf{q},t)$ a conditional probability $P(\mathbf{q},t/\mathbf{q}')$. Taking the limit $N\to\infty$ of the N-times iteration of (5) we get

$$f(\mathbf{q}_N,t)=\lim_{\substack{N\to\infty\\ \tau\to 0}}\prod_{i=0}^{N-1}\{\int dq_i P_\tau(\mathbf{q}_{i+1},\mathbf{q}_i)\}f(\mathbf{q}_0,t_0). \tag{6}$$

The limit is taken so that $N\tau=t-t_0$ remains constant.

For $f(\mathbf{q}_0,t_0)$ we take continuous functions in accordance with $f(\mathbf{q})$ in (4).

The only problem to solve is to find a suitable form of the short time propagator $P_\tau(\mathbf{q}/\mathbf{q}')$ so that (6) yields the path integral solution of the Fokker-Planck equation of the form (2), i.e.

$$P_\tau(\mathbf{q}_{i+1}/\mathbf{q}_i)=\mu_i\exp[-\tau\mathscr{L}(\mathbf{q}_{i+1},\mathbf{q}_i)].$$

The limit $\tau \to 0$ is used only in the following steps of the procedure: for infinitesimally small τ the formal solution of (4) is

$$f(\mathbf{q}, t_0+\tau)=[1+\tau L+O(\tau^2)]f(\mathbf{q}, t_0). \tag{7}$$

There is no question that this is correct since in the derivation [1] of the Fokker-Planck equation (4) from the Chapman-Komogorov equation one gets directly (7) before one obtains therefrom the differential equation (4) (see also Appendix A). The N-times iteration of (7) yields (see Appendix A) in the limit $N\to\infty$, $\tau\to 0$:

$$f(\mathbf{q}, t)=\exp[L(t-t_0)]f(\mathbf{q}, t_0) \tag{8}$$

which is known as the formal solution of (4) for arbitrary times $t>t_0$.
From (7) directly we find the short time propagator

$$P_\tau(\mathbf{q}'/\mathbf{q})=\delta(\mathbf{q}'-\mathbf{q})[1+\tau L(\mathbf{q})+O(\tau^2)]. \tag{9}$$

We will bring (9) in a form appropriate for path integrals taking a suitable representation of the δ-function together with the operator L. Then the iteration will give us the path integral (2) instead of (8). In Appendix B it is shown that it is allowed to add arbitrary terms of the order $O(\tau^2)$ to $1+L\tau$ in (7) without effecting the result (8). The addition of terms of the order $O(\tau^2)$ in (9) will lead to different representations of the δ-function. In this step the mentioned ambiguity comes into play.
The resulting different short time propagators $P_\tau(\mathbf{q}'/\mathbf{q})$ are called "equivalent", because all of them are solutions of the Fokker Planck equation if applied on continuous functions in the limit $\tau\to 0$, and give the correct solution $f(\mathbf{q}_N, t)$ of the Fokker-Planck equation when inserted in (6).

3. Short Time Propagator

In order to find a suitable representation of the δ-function in (9) we will make a variable transformation and then a Fourier transformation in the one variable. At this point we will add terms of the order $O(\tau^2)$ and after that carry out the inverse of both of the transformations.
Using the form of L given in (1) we find from (9):

$$\begin{aligned}P_\tau(\mathbf{q}'/\mathbf{q})&=\tfrac{1}{2}\delta^{(\nu\mu)}(\mathbf{q}'-\mathbf{q})\,Q_{\nu\mu}(\mathbf{q})\tau\\&-\delta^{(\nu)}(\mathbf{q}'-\mathbf{q})\,K_\nu(\mathbf{q})\,\tau\\&+\delta(\mathbf{q}'-\mathbf{q})\,V(\mathbf{q})\,\tau+\delta(\mathbf{q}'-\mathbf{q})\end{aligned} \tag{10}$$

where $\delta^{(\nu\mu)}$ is the delta-function differentiated with respect to the ν-th and μ-the component of the argument. Now we make a variable transformation from $\mathbf{q}'$ and $\mathbf{q}$ to the new variables $\mathbf{u}$ and $\mathbf{v}$.

$$\begin{aligned}\mathbf{u}&=\mathbf{q}'-\mathbf{q}\\\mathbf{v}&=\mathbf{v}(\mathbf{q}',\mathbf{q}).\end{aligned} \tag{11}$$

The transformation $\mathbf{v}(\mathbf{q}',\mathbf{q})$ can be nonlinear but has to be one to one, i.e.:

$$\frac{\partial(\mathbf{u},\mathbf{v})}{\partial(\mathbf{q}',\mathbf{q})}>0.$$

The effect of the transformation is quite clear: In the δ-functions we have the argument $\mathbf{u}$ and in the other q-dependences we have to look at $\mathbf{q}$ as a function of $\mathbf{u}$ and $\mathbf{v}$ according to the inverse transformation of (11):

$$\mathbf{q}=\mathbf{q}(\mathbf{u},\mathbf{v}). \tag{12}$$

Using the well known formula for the n-times derivative of a δ-function.

$$f(x)\,\delta^{(n)}(x)=\sum_{r=0}^{n}\binom{n}{r}(-1)^r f^{(r)}(0)\,\delta^{(n-r)}(x)$$

we find:

$$\begin{aligned}P_\tau(\mathbf{u},\mathbf{v})&=\tau\,\delta(\mathbf{u})\tfrac{1}{2}Q^{(\nu\mu)}_{\nu\mu}(\mathbf{q}(\mathbf{v}))\\&-\tau\,\delta^{(\nu)}(\mathbf{u})\,Q^{(\mu)}_{\nu\mu}(\mathbf{q}(\mathbf{v}))+\tau\,\delta^{(\nu\mu)}(\mathbf{u})\tfrac{1}{2}Q_{\nu\mu}(\mathbf{q}(\mathbf{v}))\\&-\tau\,\delta^{(\nu)}(\mathbf{u})\,K_\nu(\mathbf{q}(\mathbf{v}))+\tau\,\delta(\mathbf{u})\,K^{(\nu)}_\nu(\mathbf{q}(\mathbf{v}))\\&+\tau\,\delta(\mathbf{u})\,V(\mathbf{q}(\mathbf{v}))+\delta(\mathbf{u})\end{aligned} \tag{13}$$

where we have defined corresponding to (12):

$$\begin{aligned}\mathbf{q}(\mathbf{v})&:=\mathbf{q}(\mathbf{u}=0,\mathbf{v})\\K^{(\nu)}_\nu(\mathbf{q}(\mathbf{v}))&=\left.\frac{\partial K_\nu(\mathbf{q}(\mathbf{u},\mathbf{v}))}{\partial u_\nu}\right|_{\mathbf{u}=0}.\quad\text{etc.}\end{aligned} \tag{14}$$

We have used $Q_{\nu\mu}=Q_{\mu\nu}$.
$P_\tau(\mathbf{u},\mathbf{v})$ is the short time propagator $P_\tau(\mathbf{q}/\mathbf{q}')$ expressed by the variables $\mathbf{u}$ and $\mathbf{v}$.
In the next step we perform the Fourier transformation of $P_\tau(\mathbf{u},\mathbf{v})$ with respect to $\mathbf{u}$:

$$P_\tau(\mathbf{u},\mathbf{v})=\int e^{i\mathbf{p}\mathbf{u}}\frac{dp}{(2\pi)^n}\tilde{P}_\tau(\mathbf{p},\mathbf{v}). \tag{15}$$

From (13) we get therefore:

$$\begin{aligned}\tilde{P}_\tau(\mathbf{p},\mathbf{v})&=1-\tfrac{1}{2}\tau p_\nu p_\mu Q_{\nu\mu}-i\tau p_\nu Q^{(\mu)}_{\nu\mu}\\&+\tfrac{1}{2}\tau Q^{(\nu\mu)}_{\nu\mu}-i\tau p_\nu K_\nu+\tau K^{(\nu)}_\nu+\tau V\end{aligned} \tag{16}$$

where the functions $Q_{\nu\mu}$ etc. have to be taken at $\mathbf{q}=\mathbf{q}(\mathbf{u}=0,\mathbf{v})$ as in (13).
At this point we will use the fact mentioned above (Appendix B) that we can add terms of the order

$O(\tau^2)$ to $P_\tau(\mathbf{q}'/\mathbf{q})$. This happens in writing:

$$\tilde{P}_\tau(\mathbf{p},\mathbf{v})\, e^{i\mathbf{p}\mathbf{u}}$$
$$=\exp\{-\tfrac{1}{2}\tau\, Q_{\nu\mu} p_\nu p_\mu - i p_\nu(\tau Q_{\nu\mu}^{(\mu)}$$
$$+\tau K_\nu - u_\nu) + \tau K_\nu^{(\nu)} + \tfrac{1}{2}\tau Q_{\nu\mu}^{(\nu\mu)} + \tau V\}. \tag{17}$$

Inserting this in the inverse Fourier transformation (15) we can carry out the integration over $\mathbf{p}$ with help of the quadratic completion and find the suitable form for the short time propagator:

$$P_\tau(\mathbf{q}'/\mathbf{q})$$
$$=(2\pi\tau)^{-n/2}\, Q^{-\frac{1}{2}} \exp\left\{-\tau\tfrac{1}{2}\left[Q_{\nu\lambda}^{(\lambda)} + K_\nu - \frac{q'_\nu - q_\nu}{\tau}\right]\right.$$
$$\left.\cdot\, Q_{\nu\mu}^{-1}\left[Q_{\mu\rho}^{(\rho)} + K_\mu - \frac{q'_\mu - q_\mu}{\tau}\right] + \tau K_\nu^{(\nu)} + \tfrac{1}{2}\tau Q_{\nu\mu}^{(\nu\mu)} + \tau V\right\}. \tag{18}$$

It is Q the determinat of $Q_{\nu\mu}$. In (18) we have performed the inverse (12) of the transformation (11). Therefore the functions K_ν, Q etc. have to be taken corresponding to (11) and (12) at

$$\mathbf{r}=\mathbf{q}(\mathbf{u}=0, \mathbf{v}(\mathbf{q}',\mathbf{q})). \tag{19}$$

Because we have set $\mathbf{u}=0$ the result of (19) is not the variable $\mathbf{q}$ as it would be for a one to one transformation without setting $\mathbf{u}=0$.
One can easily verify that the short time propagator is a solution of the Fokker Planck equation if applied on a continuous function. For this purpose one expands each q' dependence around q and omits terms which vanish in the limit $\tau\to 0$. One ends up with the equality of different representations of the δ-function. The special case of a linear transformation (20) is suitable to eluciate the derivation of (18). Thus let as choose:

$$\mathbf{v}=a\mathbf{q}'+b\mathbf{q} \tag{20}$$

with $a+b=1$.
The inverse transformation of (20) yields

$$\mathbf{q}=\mathbf{v}-a\mathbf{u}. \tag{21}$$

Then according to (19) the argument $\mathbf{r}$ of the functions K_ν, Q etc. is determined from (21) by setting $\mathbf{u}=0$ and inserting (20), i.e.:

$$\mathbf{r}=a\mathbf{q}'+b\mathbf{q}. \tag{22}$$

From (14) we find with help of (21) and (22) that for $K_\nu^{(\nu)}$ etc. we have to write:

$$K_\nu^{(\nu)}=\frac{\partial K_\nu(\mathbf{q}(\mathbf{u},\mathbf{v}))}{\partial q_\nu}\frac{\partial q_\nu}{\partial u_\nu}\bigg|_{\substack{\mathbf{u}=0\\ \mathbf{v}=\mathbf{v}(\mathbf{q}',\mathbf{q})}} = -a\frac{\partial K_\nu(\mathbf{r})}{\partial r_\nu}. \tag{23}$$

Therefrom we find the short time propagator for this case:

$$P_\tau(\mathbf{q}'/\mathbf{q})=(2\pi\tau)^{-n/2}\, Q^{-\frac{1}{2}}(\mathbf{r})$$
$$\cdot\,\exp\left\{-\tau\tfrac{1}{2}\left[-aQ_{\nu\lambda}^{(\lambda)}(\mathbf{r}) + K_\nu(\mathbf{r}) - \frac{q'_\nu - q_\nu}{\tau}\right]\right.$$
$$\cdot\, Q_{\nu\mu}^{-1}(\mathbf{r})\left[-aQ_{\mu\rho}^{(\rho)}(\mathbf{r}) + K_\mu(\mathbf{r}) - \frac{q'_\mu - q_\mu}{\tau}\right]$$
$$\left.-a\tau K_\nu^{(\nu)}(\mathbf{r}) + \tfrac{1}{2}a^2\tau Q_{\nu\mu}^{(\nu\mu)}(\mathbf{r}) + \tau V(\mathbf{r})\right\}. \tag{24}$$

The choise $a=0$ makes all derivatives of the K_ν and $Q_{\nu\mu}$ disappearing. That means that the differentiations of the coefficients in (4) are included in the representation of the δ-functions. The choice $a=1$ means that these differentiations are carried out before the representation is constructed on the way from (10) to (18). A choice $0<a<1$ means that these differentiations are carried out partially and are partially contained in the representation of the δ-function s.

4. Path Integral

The short time propagator (18) has the suitable form so that we can insert it in (6) and get the path integral (2). We find the measure in the functional space:

$$\mu_i\, dq_i=(2\pi\tau)^{-n/2}\, Q(\mathbf{r}_i)^{-\frac{1}{2}}\, dq_i \tag{25}$$

The Onsager-Machlup function is

$$\mathscr{L}(\mathbf{q}_{i+1},\mathbf{q}_i)$$
$$=\tfrac{1}{2}\left[Q_{\nu\lambda}^{(\lambda)}(\mathbf{r}_i) + K_\nu(\mathbf{r}_i) - \frac{q_{\nu,i+1} - q_{\nu,i}}{\tau}\right]$$
$$\cdot\, Q_{\nu\mu}^{-1}(\mathbf{r}_i)[\;]_\mu - \tau K_\nu^{(\nu)}(\mathbf{r}_i)$$
$$-\tfrac{1}{2}\tau Q_{\nu\mu}^{(\nu\mu)}(\mathbf{r}_i) - \tau V(\mathbf{r}_i). \tag{26}$$

The arguments $\mathbf{r}_i$ are given correspondingly to (19) by:

$$\mathbf{r}_i=\mathbf{q}(\mathbf{u}=0, \mathbf{v}(\mathbf{q}_{i+1},\mathbf{q}_i)) \tag{27}$$

$[\;]_\mu$ means the same bracket as before but with the index μ instead of ν. The derivatives $K_\nu^{\nu}(\mathbf{r}_i)$ are defined by (14) but with insertion $\mathbf{v}=\mathbf{v}(\mathbf{q}_{i+1},\mathbf{q}_i)$.
We have found a wide class of equivalent path integral representations (2), (25) and (26) of the solution of the Fokker-Planck equation (4). They are characterized by a transformation $\mathbf{v}(\mathbf{q}',\mathbf{q})$ (see (11)) which can also be non-linear but must be one to one. They have arisen from the different ways by which a δ-function can be represented. The equivalence means that all these path integrals give the same correct

solution of the Fokker-Planck-equation. For a special case this is demonstrated in the Appendix C.

This ambiguity survives if we perform the formal limit from (2) to (1). The resulting continuous form of the Onsager-Machlup function contains this ambiguity further on. We do not write down this form because it is meaningless in our opinion. One example (3a) should be enough to demonstrate this.

The ambiguity in (2) can be removed be additional requirements [17] or special ways of derivations [7, 10, 11]. That different operator orderings [11] can give different equivalent results becomes clear when we take into account the correspondence [13] of the transformation $\mathbf{v}(\mathbf{q}',\mathbf{q})$ (11) to special operator orderings. The choice of a linear transformation (20) with $a=0$ gives the simplest form corresponding to (24) because all derivatives of the K_ν and $Q_{\nu\mu}$ disappear and one ends up with a quadratic form for the Onsager-Machlup function (26). This should be the most suitable form to determine the most probable way. Instead of the path integral representation in the configuration space (2) we can get the representation in the phase space [11] if we do not carry out the inverse Fourier transformation (15).

In addition to the class of equivalent path integrals pointed out in (25) and (26) we can find further manifolds by a linear combination of different transformations (11). That means the following:

We put $P_\tau(\mathbf{q}'/\mathbf{q})$ in (9) to pieces by

$$P_\tau(\mathbf{q}'/\mathbf{q})=\sum_k \alpha_k P_\tau(\mathbf{q}'/\mathbf{q}) \tag{28}$$

with $\sum_k \alpha_k=1$.

Each part $\alpha_k P_\tau(\mathbf{q}'/\mathbf{q})$ is handled as described by the procedure from (10) to (18), but with different variable transformations (11) which we characterize by the index k, i.e.

$$\mathbf{v}=\mathbf{v}_k(\mathbf{q}',\mathbf{q}). \tag{29}$$

The only consequence is that we get in (18) instead of the functions K_ν, Q etc. a linear combination with different $\mathbf{r}$ corresponding to (19):

$$K_\nu=\sum_k \alpha_k K_\nu(\mathbf{r}_k) \qquad \text{etc.} \tag{30}$$

with

$$\mathbf{r}_k=\mathbf{q}_k(\mathbf{u}=0,\mathbf{v}_k(\mathbf{q}',\mathbf{q})). \tag{31}$$

The corresponding result is got for the measure and the Onsager-Machlup function in (25), (26) and (27). We will demonstrate this by the example of the linear combination of the two linear transformation (20) with $a=0$ and $a=1$. We take

$$\mathbf{v}_1=\mathbf{q}' \qquad (a=1),$$
$$\mathbf{v}_2=\mathbf{q} \qquad (a=0).$$

Corresponding to (23) we do not get derivatives of K_ν and $Q_{\nu\mu}$ in the part $k=2$ and in the part $k=1$ for each differentiation we get a factor (-1). The result is the following:

The measure is instead of (25):

$$\mu_i dq_i=(2\pi\tau)^{-n/2}\,\|\alpha_1 Q_{\nu\mu}(\mathbf{q}_{i+1})+\alpha_2 \mathbf{Q}_{\nu\mu}(\mathbf{q}_i)\|^{-\frac{1}{2}}. \tag{32}$$

The Onsager-Machlup function is instead of (26):

$$\begin{aligned}\mathscr{L}(\mathbf{q}_{i+1},\mathbf{q}_i)=\tfrac{1}{2}\Big[&-\alpha_1 Q^{(\lambda)}_{\nu\lambda}(\mathbf{q}_{i+1})+\alpha_1 K_\nu(\mathbf{q}_{i+1})\\ &+\alpha_2 K_\nu(\mathbf{q}_i)-\frac{q_{\nu,i+1}-q_{\nu,i}}{\tau}\Big]\\ &\cdot(\alpha_1 Q_{\nu\mu}(\mathbf{q}_{i+1})+\alpha_2 Q_{\nu\mu}(\mathbf{q}_i))^{-1}\\ &\cdot[\ \ ]_\mu+\alpha_1 K^{(\nu)}_\nu(\mathbf{q}_{i+1})-\tfrac{1}{2}\alpha_1 Q^{(\nu\mu)}_{\nu\mu}(\mathbf{q}_{i+1})\\ &-\alpha_1 V(\mathbf{q}_{i+1})-\alpha_2 V(\mathbf{q}_i).\end{aligned} \tag{33}$$

The expression (32) and (33) should not be mixed up with that which we get from (24) when we set $\alpha_1=a$ and $\alpha_2=b$. In (26) we get from (24) that the arguments of the functions have to be taken (22) at $\mathbf{r}=a\mathbf{q}_{i+1}+\mathbf{b}\mathbf{q}_i$ unlike to (33).

For the 1-dimensional case with constant Q we get from (33):

$$\mathscr{L}(q_{i+1},q_i)=\tfrac{1}{2}Q^{-1}\left(\alpha_1 K(q_{i+1})+\alpha_2 K(q_i)-\frac{q_{i+1}-q_i}{\tau}\right)^2+\alpha_1 K'(q_{i+1}).$$

This is in complete agreement with Ref. [7] disregarding a sign error there and omitting the unnecessary replacement $K'(q)\Rightarrow K'(q')$ at the end.

Appendix A

We like to make sure, that (7) is consistent with (8) as it should be. Since we handle with one operator L only commutation relations do not play a rôle. The N-times iteration of (7) gives

$$(1+\tau L)^N f.$$

Since (see at Eq. (6)) $N=\dfrac{t-t_0}{\tau}$

$$(1+\tau L)^N\to\exp[L(t-t_0)] \tag{A1}$$

for $\tau \to 0$ [14]. In Appendix B we show that we can omit the term $O(\tau^2)$ in (7).

In order that we can apply the method in [14] we have to make sure that arbitrary powers of L exist and give a finite contribution. This may restrict the possible initial conditions f at the time t_0. We choose f out of the space $\mathscr{S}=\left\{f \left| \frac{\partial^n f}{\partial q^n} \right.\text{ continous for all } n, \max_q \left| q^s \frac{\partial^r f}{\partial q^r} \right| < \infty \text{ for all } s \text{ and } r \right\}$ since L contains differentiations. The operator L does not lead out of $\mathscr{S}$ and therefore arbitrary powers of L exist and $L^n f$ remains finite.

If one likes to take a δ-function for f as it appears for the conditional probability density $P(q,t|q_0,t_0)$ at $t=t_0$ it seems that one comes into trouble [15]. For $t-t_0=\tau$ one has a typical spread of P of the order $\sqrt{\tau}$. Since each L applied on P gives a factor $1/\tau$, one can not say $L\tau$ to be a small quantity and (A1) should be wrong. To overcome this problem we remember that the δ-function is a distribution (linear continuous functional) in the mathematically strict sense. For the δ-function as a (tempered) distribution on $\mathscr{S}$ the n-th derivative exist for any n, since here the properties of the test functions only are of interest. Therefore $P(q,t|q_0,t_0)$ is a distribution (linear continuous functional) in the limit $t-t_0 \to 0$ which is defined only together with a test function, i.e. only the following expression is defined:

$$\lim_{t \to t_0} P(q,t|q_0 t_0) f(q_0)\, dq_0. \tag{A2}$$

If we like to apply the operator L, we can do this only after the integration in (A2) is performed since L applied on the distribution P alone is not defined. Taking test functions out of the physical interesting space $\mathscr{S}$ we will have functions (A2) of finite spread only and L applied on (A2) gives a finite contribution. Generally we will not get any difficulty if we extent the possible initial functions f to tempered distributions.

At first sight the necessity to take f out of $\mathscr{S}$ seems to be a restriction. But $\mathscr{S}$ is dense in the space $\mathscr{L}_1$ of the absolutely integrable functions (normalization!). Therefore we can use the unique defined continuation of the short time propagator which is an integral operator for the physically interesting functions out of $\mathscr{L}_1$. It may be questionable if the limit appearing there can be interchanged with the limit $\tau \to 0$ in the propagator. The simplest way to show this is the proof that the resulting short time propagator (18) solves the Fokker-Planck equation (4) what we have mentioned in Sect. 3.

In Appendix C we see for a simple example that we do not need the test function $f(q_0)$ for the concrete calculation. It is only necessary in order to know which mathematical operation are allowed.

Appendix B

$$\left[1+\frac{1}{n}+O\left(\frac{1}{n^2}\right)\right]^n$$

$$=\left[1+\frac{1}{n}\right]^n+\sum_{\nu=1}^{n}\left(1+\frac{1}{n}\right)^{n-\nu}\left[O\left(\frac{1}{n^2}\right)\right]^\nu \frac{n!}{(n-\nu)!\,\nu!}.$$

Since $\left(1+\frac{1}{n}\right)^{n-\nu} \leqq \left(1+\frac{1}{n}\right)^n < 3$ (see [14]) we have:

$$0 \leqq \sum_{\nu=1}^{n}\left(1+\frac{1}{n}\right)^{n-\nu}\left[O\left(\frac{1}{n^2}\right)\right]^\nu \frac{n!}{(n-\nu)!\,\nu!}$$

$$\leqq 3\cdot n\, O\left(\frac{1}{n^2}\right)+\sum_{\nu=2}^{n} 3\frac{n^\nu}{\nu!}\left[O\left(\frac{1}{n^2}\right)\right]^\nu$$

$$\leqq 3\cdot n\, O\left(\frac{1}{n^2}\right)+\sum_{\nu=2}^{n} 3\left[O\left(\frac{1}{n}\right)\right]^\nu$$

$$\leqq 3\cdot n\, O\left(\frac{1}{n^2}\right)+n\cdot 3\left[O\left(\frac{1}{n}\right)\right]^2 \to 0$$

so that

$$\left[1+\frac{1}{n}+O\left(\frac{1}{n^2}\right)\right]^n \to \left[1+\frac{1}{n}\right]^n \to e \quad \text{q.e.d.}$$

Appendix C

Here we show by a simple example that indeed different path integral representations give the same exact result. We take the 1-dimensional case with $Q=\frac{1}{2}$, $K=-\lambda q$ and $V\equiv 0$. The equivalence class is chosen to be given by the linear transformation (20). From (24) and (6) we find with $f(q_0,t_0)=\delta(q_0)$

$$f(q,t)=\lim_{\substack{N\to\infty\\ N\tau=t-t_0}} \prod_{i=1}^{N-1}\left[(\pi\tau)^{-\frac{1}{2}}dq_i\right](\pi\tau)^{-\frac{1}{2}} \cdot \exp\left[-\tau\sum_{j=0}^{N-1}\mathscr{L}(q_{j+1},q_j)\right] \tag{C1}$$

with

$$\mathscr{L}(q_{j+1},q_j) =\left[\lambda(a q_{i+1}+b q_i)+\frac{1}{\tau}(q_{i+1}-q_i)\right]^2-\lambda a'. \tag{C2}$$

It is $q_N=q$ and $q_0=0$. We have written $\lambda a'$ instead of λa in order to show that only $a'=a$ is correct.

We perform the integration in (C1) by the method given in Ref. 16. Therefore we write for the quadratic form:

$$\tau \sum_{j=0}^{N-1} \mathscr{L}(q_{j+1}, q_j) = \sum_{i,j=1}^{N-1} a_{ij} q_i q_j - 2 q q_{N-1} \frac{\beta}{\tau} + A$$

with

$$a_{ii} = \frac{\alpha}{\tau} := \tau \left(\lambda a + \frac{1}{\tau}\right)^2 + \tau \left(-\lambda b + \frac{1}{\tau}\right)^2$$

$$a_{i,i+1} = a_{i+1,i} = \frac{\beta}{\tau} := -\tau \left(\lambda a + \frac{1}{\tau}\right)\left(-\lambda b + \frac{1}{\tau}\right)$$

$$A = -t a' \lambda + \tau \left(\lambda a + \frac{1}{\tau}\right)^2 q^2. \tag{C3}$$

Using the formula 1.28 of Ref. 16 we get

$$f(q,t) = [\pi \tau \det(\tau a_{ij})]^{-\frac{1}{2}} \exp\left(\frac{c^2}{4} - A\right)$$

with

$$C^2 = 4(a^{-1})_{N-1,N-1} q^2 \frac{\beta^2}{\tau^2}.$$

In order to determine $\det(\tau a_{ij})$ and $(a^{-1})_{N-1,N-1}$ in the limit $\tau \to 0$ we define $D_{N-1} = \det(\tau a_{ij})$ and D_K as the corresponding principle minor of the K-th order. From (C3) we get the difference equation:

$$D_{K+1} = \alpha D_K - \beta^2 D_{K-1}$$
$$D_1 = \alpha$$
$$D_2 = \alpha^2 - \beta^2. \tag{C4}$$

Defining $\tau D_K = B_K = B(K\tau)$ we get for fixed $t' = K\tau$ in the limit $\tau \to 0$ instead of (C4) the differential equation

$$\frac{\partial^2 B}{\partial t'^2} = 2\lambda(a-b)\frac{\partial B}{\partial t'} + 4ab\lambda^2 B$$

with $B(0) = 0$ and $B'(0) = 1$. Using $a + b = 1$ the solution is:

$$B(t) = \frac{1}{2\lambda}(e^{2\lambda a t'} - e^{-2\lambda b t'}) = \lim_{\substack{\tau \to 0 \\ N \to \infty}} \tau \det(\tau a_{ij}).$$

Using $(a^{-1})_{N-1,N-1} = \frac{\tau D_{N-2}}{D_{N-1}}$ we get in the limit $N \to \infty$

$$f(q,t) = (2\pi\sigma^2)^{-\frac{1}{2}} \exp\left[-\frac{1}{2}\frac{q^2}{\sigma^2}\right]$$

with $\sigma^2 = \dfrac{1 - e^{-2\lambda t}}{4\lambda}$

which is the well known solution of the corresponding Fokker-Planck equation. The arising additional factor $e^{\lambda t(a'-a)}$ disappears since we choose $a' = a$ in (C2).

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