REDUCED KINETIC EQUATIONS: AN INFLUENCE FUNCTIONAL APPROACH

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ABSTRACT

A scheme for obtaining reduced descriptions of multivariate kinetic equations, based on the 'influence functional' method of Feynmann, is presented. It is applied to the case of Fokker-Planck equations, showing the form that results for the reduced equation. The possibility of Markovian or non-Markovian reduced description is discussed. As a particular example, the reduction of the Kramers equation to the Smoluchwski equation in the limit of high friction is also discussed.

1. INTRODUCTION

In the context of the kinetic or transport description of physical phenomena, there is a wide range of situations, in physics as well as in other sciences, where it is desirable to describe the problem not in terms of a full set of (N) 'macroscopic' variables, but only via a

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small set (K<N) of 'relevant' variables. A few examples include kinetic of multicomponent chemical reactions, cluster growth in homogeneous nucleation, kinetics of phase transitions, in heavy ion reactions at low energies, magnetic resonance absorption, etc [1].

One of the problems to be faced if one starts from the 'full' description, is to find the form of the reduced one, that is, the reduced kinetic equation and its solution. Sometimes there is a well defined separation of time scales, with some of the variables varying over a time scale which is characteristically very much shorter than that of the rest. When dissipation is present, it is possible for the fast variables to relax to a quasistationary state, in which their values follow the values of the slow variables (Haken's slaving principle[2]).

This problem has been recently treated by means of an adiabatic elimination of variables[3]. However, if the above mentioned separation in time scales is not strictly fulfilled, such elimination procedure is not so obvious.

In this contribution we present a different method which is based on Feynman's influence functional method[4]. The starting point is the assumption that the complete description is Markovian. This is a necessary step in order to have, via the Chapman-Kolmogorov equation, a representation of its solution in terms of a path integral. We will consider the case of multivariate Fokker-Planck equations, although we expect that this approach could be also applied to other kinetic schemes, if the Markovianicity previously referred to is satisfied.

2. THE METHOD

We will use the same notation and some of the results of ref.[5]. There, it was shown the uniqueness of the thermodynamic Lagrangian associated to generalized Langevin or Fokker-Planck equations. We will not discuss such questions here. Instead, we start with the multivariate Fokker-Planck equation given by:

$$\frac{\partial}{\partial t} P(x,t \mid x_0,t_0) = -\sum_j \frac{\partial}{\partial x_j}\left(h_j(x) P\right) + \frac{1}{2} \sum_{jl} D_{jl} \frac{\partial^2}{\partial x_j \partial x_l} P \qquad (1a)$$

where $x = (x_1, x_2, \ldots\ldots x_N)$. In an obvious short hand notation we have:

$$\frac{\partial}{\partial t} P(x,t \mid x_0,t_0) = -\frac{\partial}{\partial x}\left(h(x) P\right) + \frac{1}{2} \frac{\partial}{\partial x} \hat{D} \frac{\partial}{\partial x} P \qquad (1b)$$

$P(x,t \mid x_0,t_0)$ being the conditional probability for reaching the 'point' x at time t, if we have started from x_0 at t_0

Following ref.[5], the 'short time propagator' (or conditional probability) is given by:

$$P(x_j, t_{j-1}+\tau \mid x_{j-1}, t_{j-1}) = \frac{1}{\sqrt{2\pi\tau D}} \exp\left\{-\frac{1}{2}\left[\frac{x_j - x_{j-1}}{\tau} - h(x_{j-1})\right] \hat{D}^{-1} \left[\frac{x_j - x_{j-1}}{\tau} - h(x_{j-1})\right]^t\right\} \qquad (2a)$$

where τ is a very short time interval as usual, and D is the determinant of $\hat{D}$ ($D_{ij} = D_{ij}$) . By acting reiteratively with the short time propagator, and taking the limit $\tau \to 0$, $n\tau = t_f - t_0$ we arrive at the full propagator.

$$P(x_f, t_f \mid x_0, t_0) = \int_{x(t_f) = x_f} \mathcal{D}[x(\tau)] \exp\left\{-\frac{1}{2}\int_{t_0}^{t_f} d\tau \left\{\left[\dot{x}(\tau) - h(x)\right] \hat{D}^{-1} \left[\dot{x}(\tau) - h(x)\right]^t + \frac{\partial}{\partial x} h(x)\right\}\right\} \qquad (2b)$$

the measure being given by:

$$\mathcal{D}[x(\tau)] \sim \lim_{\substack{n\to\infty \\ n\tau = t_f - t_0}} \frac{1}{\sqrt{2\pi\tau D}} \prod_{j=1}^{n-1} \frac{dx_j}{\sqrt{2\pi\tau D}} \qquad (2c)$$

We introduce now the idea of the subset of 'relevant' variables, assuming that:

$$\{x\} = \{\{\pi\}, \{\$\}\} \tag{3a}$$

$\{\pi\}$ being the subset of 'relevant' variables, and $\{\$\}$ the subset of the remaining variables. Similarly, we write:

$$\{h(x)\} = \{\{h_r(x)\}, \{h_s(x)\}\} \tag{3b}$$

and also adopting the separation:

$$h_r(x) = h_{r,0}(\pi) + h_{r,1}(\pi, \$) \tag{3c}$$

Then the full Lagrangian:

$$\mathcal{L}(\dot{x}, x) = \tfrac{1}{2}\left[\dot{x} - h(x)\right] \hat{D}^{-1} \left[\dot{x} - h(x)\right]^t + \tfrac{1}{2} \frac{\partial}{\partial x} h(x) \tag{4}$$

can be writen as the sum of three contributions:

$$\mathcal{L}(\dot{x}, x) = \mathcal{L}_r(\dot{\pi}, \pi) + \mathcal{L}_s(\dot{\$}, \$, \pi) + \mathcal{L}_{int}(\dot{x}, x)$$

which are given by:

$$\mathcal{L}_r(\dot{\pi}, \pi) = \tfrac{1}{2}\left[\dot{\pi} - h_{r,0}(\pi)\right] \hat{d}_r \left[\dot{\pi} - h_{r,0}(\pi)\right]^t + \tfrac{1}{2} \frac{\partial}{\partial \pi} h_{r,0}(\pi)$$

$$\mathcal{L}_s(\dot{\$}, \$, \pi) = \tfrac{1}{2}\left[\dot{\$} - h_s(\$, \pi)\right] \hat{d}_s \left[\dot{\$} - h_s(\$, \pi)\right]^t + \tfrac{1}{2} \frac{\partial}{\partial \$} h_s(\$, \pi)$$

$$\mathcal{L}_{int}(\dot{x}, x) = \mathcal{L}_{int}(\dot{\pi}, \pi, \dot{\$}, \$) = \text{rest} \tag{5}$$

where we have used the following definitions:

$$\hat{D}^{-1} = \begin{pmatrix} d_r & d_{rs} \\ d_{sr} & d_s \end{pmatrix} \tag{6}$$

At this point we define the marginal (or 'inclusive') conditional probability by means of:

$$P(\pi_f, t_f \mid \pi_0, t_0) = \int d\$_f \int d\$_0 \, \tilde{P}(\$_0) \, P(x_f, t_f \mid x_0, t_0) \qquad (7)$$

where we have taken a weighted average on the initial distribution of the subset $\{\$_0\}$, and summed over all possible final values $\{\$_f\}$ as usual. In order to make the connection with the Feynman approach, the marginal probability can be written as:

$$P(\pi_f, t_f \mid \pi_0, t_0) = \int \mathcal{D}[\pi(\tau)] \; \exp\left\{-\int_{t_0}^{t_f} d\tau \, \mathcal{L}_r(\dot{\pi}, \pi)\right\} F(\dot{\pi}, \pi) \qquad (8a)$$

where the functional $F(\dot{\pi}, \pi)$ is given by:

$$F(\dot{\pi}, \pi) = \int d\$_f \int d\$_0 \, \tilde{P}(\$_0) \int_{\$_f} \mathcal{D}[\$(\tau)] \; \exp\left\{-\int_{t_0}^{t_f} d\tau \left[\mathcal{L}_\$(\dot{\$}, \$, \tau) + \mathcal{L}_{int}(\dot{x}, x)\right]\right\} \qquad (8b)$$

This has the form of Feynman's 'influence functional'[4], although the latter arose in a different context (it must be remarked that Feynman's influence functional is, in fact, a double path integral).

In the same spirit of Feynman's scheme, we wrote:

$$F(\dot{\pi}, \pi) = \exp\left\{-\int_{t_0}^{t_f} d\tau \, \Phi(\dot{\pi}, \pi)\right\} \qquad (8c)$$

In order to simplify the notation, in what follows we will consider only one relevant variable: x . Then eqs. (8a) through (8c) reduce to:

$$P(x_f, t_f \mid x_0, t_0) = \int_{x(t_f)=x_f} \mathcal{D}[x(\tau)] \; \exp\left\{-\frac{1}{2}\int_{t_0}^{t_f} d\tau \left\{ \frac{[\dot{x}(\tau) - h(x(\tau))]^2}{D_x} + \frac{d}{dx} h_0(x(\tau)) \right\}\right\} F(\dot{x}, x) \qquad (9a)$$

and correspondingly for $F(\dot{x}, x)$. One of the questions we can ask is about the stationary path. It is obtained as the solution of:

$$\frac{d}{dt}\frac{\partial}{\partial \dot{x}}\mathcal{L}_x - \frac{\partial \mathcal{L}_x}{\partial x} = -\left\{\frac{d}{dt}\frac{\partial}{\partial \dot{x}}\bar{\Phi} - \frac{\partial}{\partial x}\bar{\Phi}\right\} = \Psi(\dot{x},x) \qquad (10a)$$

which, taking $\dot{v} = \ddot{x}$, can be written as:

$$\dot{v} = -\frac{\partial}{\partial x}U_{eff}(x) + D_x\Psi(\dot{x},x) \qquad (10b)$$

We can exploit the stochastic character of the processes at hand, and assume that the effect of $D_x\Psi$ is stochastic in nature and, following previous authors [6], that it has the form:

$$-\int_{t_0}^{t}\alpha(t-\tau)\,\dot{x}(\tau)\,d\tau + f_{fl}(t) \qquad (11a)$$

where $f_{fl}(t)$ is a fluctuating (Langevin-like) contribution, with a given probability distribution $\bar{P}[f]$, and the rest is a systematic effect. If the memory is short, such a systematic contribution becomes

$$-\alpha_0\,\dot{x}(t) \qquad (11b)$$

Now, we must consider an average of the functional over its distribution:

$$F_{av}(\dot{x},x) = \int \mathcal{D}f_{fl}\;\bar{P}[f_{fl}]\;F_{fl}(\dot{x},x)$$

Assuming a Gaussian distrition such an average gives the result [4]

$$F(\dot{x},x) = \exp\left\{-\int_{t_0}^{t}d\tau\, f_0(\tau)\,\chi(t) + \frac{1}{2}\int_{t_0}^{t}d\tau\int_{t_0}^{\tau}d\tau'\,\chi(\tau)\,\chi(\tau')\,C(\tau,\tau')\right\} \qquad (12)$$

where $C(\tau,\tau') = \langle f_{fl}(\tau),\, f_{fl}(\tau')\rangle$ is the correlation function and $f_0(\tau) = \langle f_{fl}(\tau)\rangle$ is the mean value.

3. EXAMPLES

We can discuss further how to exploit the above assumptions, along the line followed in ref. [6]. Nevertheless, we would like to

find out what kind of reduced equation governs the evolution of (9a) with $F(\dot{x},x)$ given by (12). In order to find this out we must analyze the following limit:

$$\lim_{\varepsilon\to 0}\ \frac{1}{\varepsilon}\left\{P(x,t+\varepsilon\,|\,x_0,t_0)-P(x,t\,|\,x_0,t_0)\right\}= \tag{13}$$
$$=\frac{1}{\varepsilon}\left\{\int\mathcal{D}[x(\tau)]\ e^{-\int_{t_0}^{t+\varepsilon}\cdots}-\int\mathcal{D}[x(\tau)]\ e^{-\int_{t_0}^{t}\cdots}\right\}$$

If we expand the r.h.s. up to terms of first order in ε, we will end with the desired equation. Furthermore, if we adopt the "Markovian-case", that is the short memory situation of eq. (11b), we will find that

$$F(\dot{x},x)=\exp\left\{\frac{T\alpha_0}{2}\,x(t)^2-f_0(t)\,x(t)\right\} \tag{14}$$

leading to the effective Lagrangian:

$$\mathcal{L}_{eff}(\dot{x},x)= \tag{15}$$
$$\frac{1}{2D_x}\left[\dot{x}-h_0(x)\right]^2+\frac{1}{2}\frac{d}{dx}h_0(x)+f_0(t)x(t)-\alpha_0\,x(t)\dot{x}(t)-\frac{\alpha_0}{2}T\,x(t)^2$$

Replacing in (13) and going to the limit $\varepsilon\to 0$, we arrive at:

$$\frac{\partial}{\partial t}P(x,t\,|\,x_0t_0)=g_0(x)P-\frac{\partial}{\partial x}\left[g_1(x)P\right]+\frac{D_x}{2}\frac{\partial^2}{\partial x^2}P \tag{16}$$

where

$$g_0(x)=-\left\{\left[f_0(t)-\alpha_0 h_0(x)\right]x(t)-\frac{\alpha_0}{2}\left[T+\alpha_0 D_x\right]x(t)^2-\frac{\alpha_0 D_x}{2}\right\}$$
$$g_1(x)=h_0(x)+\alpha_0 D_x\,x(t) \tag{17}$$

A trivial result is the one corresponding to the situation $\alpha_0=0$ and $f_0(t)=0$. Then, there is no interaction between both sets of variables, and we get

$$\frac{\partial P}{\partial t}=-\frac{\partial}{\partial x}\left[h_0(x)P\right]+\frac{D_x}{2}\frac{\partial^2}{\partial x^2}P \tag{18}$$

as expected. In general, the linear term will work as a probability 'source' or 'sink', depending on the sign of $g_0(x)$. The former case will imply that the remaining variables will contribute positively to the process. While the latter case implies that the effect of such a set has a dissipative character.

Now we want to discuss the application of the previous scheme to a situation that has been extensively studied by other approaches. This is the Kramers-Chandrsekhar equation[8] , very well known from studies of Brownian motion. It is given by:

$$\frac{\partial}{\partial t} P_K(y,v,t \mid y_0,v_0,t_0) = -\frac{\partial}{\partial y}[v P_K] + \frac{\partial}{\partial v}[(U'(y)+\gamma v) P_K] + \gamma \frac{\partial^2}{\partial x^2} P_K \qquad (19a)$$

where y is the 'spatial' variable, v the associated 'velocity', γ the friction constant and U(y), the potential in which the Brownian particle is diffusing. It has been shown [8] , that in the limit of very high friction this equation reduces to the also very well known Smoluchowski's equation [8] . This equation has the form:

$$\frac{\partial}{\partial t} P_S(y,t \mid y_0,t_0) = \frac{1}{\gamma}\frac{\partial}{\partial y}\left[U'(y) P_S\right] + \frac{1}{\gamma}\frac{\partial^2}{\partial y^2} P_S \qquad (19b)$$

We will give directly the expression of the path integral solution of both equations, the details of its derivation will be given elsewhere [9] . For the Kramers' equation we have:

$$P_K(y_f,v_f,t_f \mid y_0,v_0,t_0) = \int_{\substack{v_0,v_f \\ y_0,y_f}} \mathcal{D}[y(\tau)]\, \exp\left\{-\frac{\gamma}{4}\int_{t_0}^{t_f} d\tau \left[\ddot{y}(\tau)+\frac{U'(y(\tau))}{\gamma}+\frac{\dddot{y}(\tau)}{\gamma}\right]^2\right\} \qquad (20a)$$

and for Smoluchowski's it is:

$$P_S(y_f,t_f \mid y_0,t_0) = \int_{y_0} \mathcal{D}[y(\tau)]\, \exp\left\{-\frac{\gamma}{4}\int_{t_0}^{t_f} d\tau \left[\dot{y}(\tau)+\frac{U'(y(\tau))}{\gamma}\right]^2\right\} \qquad (20b)$$

In reference [9] we have discussed how, by means of the definition in eq. (7) and by means of a kind of perturbational expansion in terms of the parameter $1/\gamma$, we can obtain the result (20b), starting from

(20a), up to terms of zero-th order in the expansion parameter. We expect that higher order terms will give the known contributions[8] This is a problem currently under study.

4. DISCUSSION

In this communication we have presented a scheme of elimination of irrelevant variables from multivariable kinetic equations, based on Feynman's influence functional method. We have discussed the particular situation of Fokker-Planck equations, even though we expect this method to be applicable to other kinetic descriptions. The starting point of the scheme is that the full description must be Markovian. This is a necessary step in order to have, via a Chapman-Kolmogorov relation, a path integral representation of its solution. We feel that this method could be useful not only in those situations where two very different time scales can be defined, but also for more general situations. For instance, in the case of a short memory effect of the remaining variables over the relevant ones (eq.(11b)), we have shown that we arrive at an essentially Markovian result. But, if instead of such a short memory effect we assume the 'non-Markovian' case of eq. (11a), and repeat the same procedure, what we can expect is to arrive to a non-Markovian equation. This is the case, with the non-Markovianicity arising in the linear term. In order to find more 'conventional' forms of non-Markov equations[7] , we would need to consider more elaborate forms of the influence functional, situations where the original transport coefficients are time-dependent, or incorporating a space dependence into the diffusion tensor. All these points are currently under investigation.

Another situation of interest is the inverse problem, that is to study the corresponding 'backward' or 'adjoint' equation. This is a relevant problem in many situations where we want to find out the most adequate initial conditions (or their weight) in order to reach a desired final condition (for instance, this is extensively exploited in neutron transport problems by means of the neutron 'importance'[10]

or to evaluate the distribution of escape times from a given region. The latter result is relevant, for obtaining mean first passage times, which is of great importance in the decay of metastable states (e.g. nuclear fission)[8)]

In short, we expect to continue studying this problem, extending the analysis to other kinetic equations, and applying the results in those nuclear problems that are usually described in the framework of transport theoretical methods.

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