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THE KRAMERS-MOYAL EXPANSION FOR THE FOKKER-PLANCK EQUATION

BY

Sorinel Adrian OPRISAN♣

ABSTRACT: This paper presents a unitary approach to the scaling problem of the solution for the Fokker-Planck equation. These results have been obtained within the framework of the stochastic canonical theory, which is more general than the Ito's stochastic theory.

1. INTRODUCTION

It is well known that the usual way to study the stochastic behavior of a statistical system is the Ito formalism. In this framework appear a major difficulty related to the Ito definition of the collision integrals [1,2,5]. On the other hand, the stochastic canonical theory shows flexibility and generality concerning the problem of the Ornstein-Uhlenbeck processes [1,5]. In agreement with the basic ideas of the stochastic canonical theory [2,4], it is assumed that the time derivative of an extensive variable can be described by the following formula:

$$\frac{dn}{dt} = \sum_k \omega_k \left(V_k^+ - V_k^- \right), \tag{1}$$

where: ω is the vector which indicates the total change of the quantity n after the k elementary process,

V_k^+ or V_f^- are the elementary transition rates of the k process.

In order to find explicit form of the probability distribution of fluctuations for the extensive variable x, we will consider the following scaling relation:

$$x - \bar{x} = qV^{\beta} , \tag{2}$$

where x=n/V is the density of the considered extensive variable, V is the volume of the system, β is the scaling factor, q is the density of the extensive scaled variable. It will furthermore be assumed that all processes which we consider are Markovian and then, in order to give a complete description of the system's fluctuations, we have to compute only the two time conditional probability $P_{2(n_0,t_0|n,t)}$ and the single-time probability density $W_{1(n,t)}$ [2,5]. We can easily find the two time conditional probability in respect to the scaled variable q, using (2):

♣ Department of Theoretical Physics, Faculty of Physics, "Al. I. Cuza" University, Iasi, 6600, ROMÂNIA
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$$P(q,t) = V^{-\beta} P_{2(n_0,t_0|n,t)} \tag{3}$$

where $P(q,0)=\delta(q)$. As a consequence of this relation, we write the time derivative of the two time conditional probability in the form:

$$\frac{\partial P}{\partial t} = V^{-\beta}\left(\frac{\partial P_2}{\partial t} + \frac{\partial P_2}{\partial x}\frac{dx}{dt}\right) = V^{-\beta}\left(\frac{\partial P_2}{\partial t} + \frac{\partial}{\partial q}\left(P\sum_k \omega_k\left(v_k^+ - v_k^-\right)\right)\right) \tag{4}$$

where $v_k^{\pm} = \frac{V_k^{\pm}}{V}$. Let us consider in more detail the equation (4), having in mind two fundamental assumptions: first, the asymptotic expression for the single time probability density, namely:

$$W_{1(n)} = \lim_{t\to\infty} P_{2(n_0,t_0|n,t)} \tag{5}$$

second, the master equation for the stochastic processes [2.5]:

$$\frac{dW_{1(n)}}{dt} = \sum_k V^+_{k(n-\omega_k)} W_{1(n-\omega_k,t)} + \sum_k V^-_{k(n+\omega_k)} W_{1(n+\omega_k,t)} - \\ - \sum_k V^+_{k(n)} W_{1(n,t)} dt - \sum_k V^-_{k(n)} W_{1(n,t)} dt \tag{6}$$

2. THEORETICAL RESULTS

In this section we adopt the Kramers-Moyal hypothesis, namely that ω_k=0 or ±1 in every elementary process and, furthermore, $n >> \omega$. This allow us to perform a Taylor series expansion on the right-hand side of (6) to obtain:

$$\frac{dW_{1(n)}}{dt} = -\frac{\partial}{\partial n}\left(W_{1(n)}\sum_k \omega_k\left(V_k^+ - V_k^-\right)\right) + \\ + \frac{1}{2!}\frac{\partial^2}{\partial n \partial n^T}\left(W_{1(n)}\sum_k \omega_k\left(V_k^+ - V_k^-\right)\omega_k^T\right) + \ldots \tag{7}$$

Introducing relation (5) into this equation , one obtains:

$$\frac{dP_2}{dt} = -\frac{\partial}{\partial x}\left(P_2\sum_k \omega_k\left(v_k^+ - v_k^-\right)\right) + \\ + \frac{1}{2!}V^{-1}\frac{\partial^2}{\partial x \partial x^T}\left(P_2\sum_k \omega_k\left(v_k^+ + v_k^-\right)\omega_k^T\right) + \ldots \tag{8}$$

Now it is possible to obtain the Kramers-Moyal like expansion for the probability density of the scaled extensive variable from (4) and (8) in the form:

$$\frac{\partial P}{\partial t} = -\frac{\partial}{\partial q}\left(PV^{\beta}\left(\frac{\partial h}{\partial x}qV^{\beta} + \frac{1}{2!}\frac{\partial^2}{\partial x \partial x^T}V^{2\beta}qq^T + \ldots\right)\right) + \\ + \frac{1}{2}\frac{\partial^2}{\partial q \partial q^T}\left(PV^{-1-2\beta}\left(\gamma + \frac{\partial \gamma}{\partial x}qV^{\beta} + \ldots\right)\right) \tag{9}$$

where $h = \sum_k \omega_k \left(v_k^+ - v_k^-\right)$ is the drift term which will appears in the Fokker-Planck equation,

$\gamma = \sum_k \omega_k \left(v_k^+ + v_k^-\right)\omega_k^T$ is the diffusion term in the Fokker-Planck equation.

It is convenient at this point to perform some simplification: first, we will neglect all terms in the Kramers-Moyal expansion (9) up to the second order due to their smallness; second, we will study the one-dimensional case only. In view of the preceding statements, it follows that:

$$\frac{\partial P_{(q,t)}}{\partial t} = -\frac{\partial}{\partial q}\left(P\left(\frac{\partial h}{\partial x}q + \frac{1}{2!}\frac{\partial^2 h}{\partial x \partial x^T}V^{\beta}qq^T + \ldots\right)\right) + \\ + \frac{1}{2}\frac{\partial^2}{\partial q \partial q^T}\left(P\left(V^{-1-2\beta}\gamma + \frac{\partial \gamma}{\partial x}qV^{-1-\beta} + \ldots\right)\right) \tag{10}$$

Finally, it may be noted that it is more convenient to integrate Fokker-Planck equation (10) after the following change of variable : $\tau = tV^{\beta}$. As a consequance, equation (10) becomes:

$$\frac{\partial P}{\partial \tau} = \frac{\partial}{\partial q}\left(\frac{P}{i!}\frac{\partial^i h}{\partial x^i}q^i\right) + \frac{1}{2!}\frac{\partial^2 (P\gamma)}{\partial q \partial q^T} \tag{11}$$

which have the general solution:

$$P(q) = \frac{i+1}{2}\left(\frac{2}{(i+1)!}\frac{\partial^i h}{\partial x^i}\right)^{\frac{1}{i+1}} \frac{1}{\Gamma\left(\frac{1}{i+1}\right)} \exp\left(-\frac{2}{(i+1)!}\frac{\partial^i h}{\partial x^i}q^{i+1}\right) \tag{12}$$

The Kramers-Moyal expansion was used [1,2,3,4] to study the behavior of the fluctuation around the critical points. But, what all authors above mentionated do not explain is why it is necessary to rescal the Fokker-Planck equation and, furthermore, how we can choose the scaling parameter β.

Our main result concerns both these problems . First, in (9) we must consider the drift and diffusion terms to have the same power of V, which allows us to determine the scaling constant β. Also, if the system is in a steady state then $\partial h/\partial t <> 0$ and (9) becomes:

$$\frac{\partial P}{\partial \tau} = -\frac{\partial}{\partial q}\left(Pq \frac{\partial h}{\partial x} \right) + \frac{1}{2!}\frac{\partial^2 (P\gamma)}{\partial q \partial q^T} \quad (13)$$

whose solution is:

$$P(q) = \left(\frac{2}{\gamma}\frac{\partial h}{\partial x} \right)^{\frac{1}{2}} \frac{1}{\Gamma\left(\frac{1}{2}\right)} \exp\left(-\frac{2}{\gamma}\frac{\partial h}{\partial x} q^2 \right) \quad (14)$$

As it can be seen from this equation, we have a Gaussian-like fluctuation around the stady state and a scaling factor $\beta=1/2$. If the system is near a critical point then $\partial h/\partial t <> 0$ and (9) becomes:

$$\frac{\partial P}{\partial \tau} = -\frac{\partial}{\partial q}\left(\frac{Pq^2}{2!}\frac{\partial^2 h}{\partial x^2} q^i \right) + \frac{1}{2!}\frac{\partial^2 (P\gamma)}{\partial q \partial q^T} \quad (15)$$

whose solution has the following form:

$$P(q) = \frac{3}{2}\left(\frac{2}{\gamma}\frac{\partial^2 h}{\partial x^2} \right)^{\frac{1}{3}} \frac{1}{\Gamma\left(\frac{1}{3}\right)} \exp\left(-\frac{2q^3}{3\gamma}\frac{\partial^2 h}{\partial x^2} \right) \quad (16)$$

This result indicate that near a critical point the fluctuations are not Gaussian and this behavior will characterize all critical points.

3. CONCLUSIONS

We have shown, within the framework of the stochastic canonical theory, that there is a unitary approach to the scaling problem of the Fokker-Planck solutions. The scaling factor results from realistic condition imposed to the drift and diffusion terms in the Kramers-Moyal expanded equation.

REFERENCES

1. Fox R.F.,Uhlenbeck G. E., – Contribution to Nonequilibrium Thermodynamics, Phys. Fluids, **13**, (1970).
2. Keizer J.,– *Statistical Thermodynamics of Nonequilibrium Processes* , Springer-Verlag, New-York, (1987).
3. Ma S. K., – *Modern Theory of Critical Phenomena*, Massachusetts, Benjamin-Cummings,1077.
4. Oppenheimer I. , Shuler K. E. ,Weiss G. H., – *Stochastic processes in Chemical Physics*, MIT Press, Cambridge, (1977).
5. Stratonovich R. L., – *Topics in the Theory of Random Nois*, Gordon-Breach, New-York, (1963).