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A LIE-ADMISSIBLE METHOD OF INTEGRATION OF FOKKER-PLANCK EQUATIONS WITH NON-LINEAR COEFFICIENTS (EXACT AND NUMERICAL SOLUTIONS)

DOCUMENTS DEFECTUEUX

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A Lagrangian method is introduced for the integration of non-linear Fokker-Planck equations. Examples of exact solutions obtained in this way are given, and also the explicit scheme used for the computation of numerical solutions. The method is, in addition, shown to be of a Lie-admissible type.

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A Lie-admissible method of integration of Fokker-Planck equations with non-linear coefficients (exact and numerical solutions)

I. CONCEPTUAL FRAMEWORK OF THE ARTICLE.

1) Generalities related to our treatment of Fokker-Planck equations.

Let us consider, at any point x_ℓ of $\mathbb{R}^m$ and at any time t, a density of probability $\rho(x_\ell,t)$ which satisfies the Fokker-Planck equation (Ref[1], page 144)

$$\textcircled{1} \qquad \frac{\partial \rho}{\partial t} + \sum_{h=1}^{m} \partial_h(\rho D_h) = \frac{1}{2} \sum_{h=1}^{m} \sum_{k=1}^{m} \partial_h \partial_k (\rho \sigma^2_{hk}) \quad .$$

The deterministic aspect of evolution is represented by the vector D with the components $D_h(x_\ell,t)$, and the diffusion by the symmetrical and positive matrix $[\sigma^2]$ with the general term $\sigma^2_{hk}(x_\ell,t)$.

The first step of the method that we will use consists in associating the following system of coupled equations with ①

$$\textcircled{2} \qquad \begin{cases} \dfrac{dx_h}{dt} = V_h = D_h - \dfrac{1}{2\rho} \displaystyle\sum_{k=1}^{m} \partial_k(\rho \sigma^2_{hk}) & (2\text{-a}) \\[2ex] \dfrac{\partial \rho}{\partial t} + \displaystyle\sum_{h=1}^{m} \partial_h(\rho V_h) = 0 & (2\text{-b}) \end{cases}$$

The choice of the auxiliary system (2) is a priori reasonable, since it is easy to verify that system (2) implies equation (1).

The two equations which make up (2) cannot evidently be dissociated since they are linked by the unknown function ρ. However, when ρ is known (analytically by integration of (1) for example, or numerically due to a preceding step of integration), the relation (2-a) becomes an independent differential system. Let us consider its solution

$$x_h(t) = X_h(t, x_\ell(0); \rho) \qquad (\ell = 1,2,\ldots,m) \tag{3}$$

and the associated Jacobian

$$J = J(t, x_\ell(0); \rho) = \det\left[\frac{\partial X_h}{\partial x_\ell(0)}\right] \tag{4}$$

where $x_\ell(0)$ is the initial value of $x_\ell(t)$.

The second step of our method (Ref[2]) consists in utilizing the fact that the Fokker-Planck equation conserves probability during time evolution, and in writing this law of conservation along the trajectories (3), i.e., denoting as $d\mu(x_\ell)$ the element of volume at point x_ℓ of $\mathbb{R}^m$,

$$\rho(x_\ell(t),t)\, d\mu(x_\ell(t)) = \rho(x_\ell(0),0)\, d\mu(x_\ell(0)) \tag{5}$$

or still, by introducing the Jacobian (4) of the change of variables $x_h(t) \rightsquigarrow x_\ell(0)$ defined by (3),

$$\rho(x_\ell(t),t) = \frac{\rho(x_\ell(0),0)}{J(t, x_\ell(0); \rho)} \tag{6}$$

The third and last step consists in utilizing Liouville's theorem,

in its original form (Ref[3][4][5]), to calculate the Jacobian J :

$$\textcircled{7} \qquad \frac{d}{dt} \text{Log } J = \sum_{h=1}^{m} \partial_h V_h(t, x_\ell(t); \rho)$$

These ideas related to the Fokker-Planck equation and summarized by ②, ⑤ and ⑦ were already presented and used several times (Ref[2][6]...[11]). We will see hereafter that they suggest a new method of numerical integration of this equation.

Let us note that, since we are presenting here a method, the numerical application of which has only begun, starting from I-3, we will consider solely the particular case of one space variable, $x \in \mathbb{R}$. The Fokker-Planck equation will then be studied in the particular case

$$\textcircled{8} \qquad \frac{\partial}{\partial t} \rho(x,t) + \frac{\partial}{\partial x}(\rho(x,t)D(x,t)) = \frac{1}{2} \frac{\partial^2}{\partial x^2}(\rho(x,t)\sigma^2(x,t)) \quad ,$$

with ② , ⑥ and ⑦ being written in the following manner :

$$\textcircled{9} \qquad \begin{cases} \dfrac{dx}{dt} = V = D - \dfrac{1}{2\rho} \dfrac{\partial}{\partial x} (\rho\sigma^2) & (9\text{-a}) \\ \dfrac{\partial \rho}{\partial t} + \dfrac{\partial}{\partial x} (\rho V) = 0 & (9\text{-b}) \end{cases}$$

$$\textcircled{10} \qquad \rho(x(t),t) = \frac{\rho(x(0),0)}{J(t,x(0);\rho)}$$

$$\textcircled{11} \qquad \frac{d}{dt} \text{Log } J = \frac{\partial V}{\partial x} (t, x(t); \rho)$$

2) Our work in the framework of Lie-admissible algebrae (Ref[12],[13],[14],[15] page 261, [20]).

From a purely pragmatic point of view, the generalities of I-1) are sufficient for the understanding of the present article. It is then possible for the reader, if he wants, to go directly to II). However we will take the time here to say some words about the relations existing between our work and that of the theoreticians of Lie-admissible algebrae.

In order to be able to speak in terms of dynamics, let us look at the case when $\mathbb{R}^m$ is a phase space $\mathbb{R}^{2n}$ and, to simplify the notations, limit ourselves to the case where $\mathbb{R}^{2n} = \mathbb{R}^2$, $x_1 = x$, $x_2 = p$, with

$$\text{(12)} \qquad D = \begin{pmatrix} D_1 \\ D_2 \end{pmatrix} = \begin{pmatrix} \partial H/\partial p \\ -\partial H/\partial x + F \end{pmatrix} \quad ; \quad H = H(x,p,t) \quad ; \quad F = F(x,p,t) \quad ;$$

H is the Hamiltonian which describes all the forces derivable from a potential, and F represents all the other deterministic forces (local non-self-adjoint forces according to R.M. Santilli's terminology, Ref[15]). Equation (1) may be then written as

$$\text{(13)} \qquad \frac{\partial \rho}{\partial t} + \{\rho, H\} = -\frac{\partial}{\partial p}(\rho F) + \frac{1}{2} \sum_{h=1}^{2} \sum_{k=1}^{2} \partial_h \partial_k (\rho \sigma^2_{hk})$$

with $$\{\rho, H\} = \frac{\partial \rho}{\partial x}\frac{\partial H}{\partial p} - \frac{\partial \rho}{\partial p}\frac{\partial H}{\partial x} \quad .$$

The non-Hamiltonian effects are concentrated in the right-hand side of the equation. They are represented — remember — by the non-conservative force F and by the diffusion matrix $[\sigma^2]$.

Let us now introduce the following quantity :

$$\mu = \frac{F}{\partial H/\partial p} + \rho \frac{\partial F/\partial p}{\partial \rho/\partial p \; \partial H/\partial p} - \frac{1}{2} \frac{1}{\partial \rho/\partial p \; \partial H/\partial p} \sum_{h=1}^{2} \sum_{k=1}^{2} \rho_{,h} \rho_{,k} (\ldots) \tag{14}$$

which is known when the statistical system is known, i.e., when H, F, ρ, [ ] are determined. All the functions involved are assumed to be infinitely differentiable.

Let us now consider the following product between any two functions A and B (also infinitely differentiable)

$$(A,B) = \partial A/\partial x \quad \partial A/\partial p \begin{pmatrix} 0 & 1 \\ -1 & \mu \end{pmatrix} \begin{pmatrix} \partial B/\partial x \\ \partial B/\partial p \end{pmatrix} \tag{15}$$

which is explicitely known at the same time as μ. It is then easy to verify that (13) reduces to the following :

$$\frac{\partial \rho}{\partial t} + (\rho, H) = 0 \quad , \tag{16}$$

and one notices that, in the particular case $\mu = 0$, relation (16) recovers the traditional form

$$\frac{\partial \rho}{\partial t} + \{\rho, H\} = 0 \quad . \tag{17}$$

It is known that Poisson's brackets, considered as a product, lend a Lie-algebraic structure to the vector space of infinitely differentiable functions defined in phase space. Let us recall that, in the same way, the product (.,.) equips this vector space with an algebraic structure which is called "Lie-admissible". It is indeed easy to verify that

$$(A,B) - (B,A) = 2\{A,B\} = [A,B] \quad , \tag{7}$$

where [.,.] is a Lie product, which is the definition of Lie-admissibility for (.,.) ; (Ref[15] page 68). It may be useful to stress the fact that the Lie-admissible algebra at hand only reduces itself to a Lie algebra when $\nu = 0$, i.e., if the two aspects, dissipative (F) and diffusive $[\sigma^2]$, of evolution are zero or cancel each other.

3) Comparison with the method of characteristics.

Our method of integration of the Fokker-Planck equation consists in replacing the resolution of the second-order partial differential equation (1) by that of the system of first-order equations (2). For equation (8) for example, one makes use of equation (9-b), i.e.,

$$\frac{\partial \rho}{\partial t} + V \frac{\partial \rho}{\partial x} = - \rho \frac{\partial V}{\partial x} \tag{10}$$

which becomes a first-order equation as soon as V has been determined, with sufficient precision, by an auxiliary calculation or by the preceding step of integration. If now, for the following step, the method of characteristics is used, we obtain :

$$dt = \frac{dx}{V} = \frac{d\rho}{- \rho \frac{\partial V}{\partial x}} \tag{11}$$

i.e.,

$$\frac{dx}{dt} = V \tag{12}$$

(22) $$\frac{d\sigma/dt}{\rho} = -\frac{\partial V}{\partial x}$$

Thus one finds again the same results as in I-1) : (21) is the same as (9-a); (22) is (12), taking (10) into account. The difference is only a question of vocabulary. One can, as in I-3), speak in terms of the characteristics of a first-order partial differential equation which is, at each step, an approximation of the second-order equation studied, or, as in I-1), insist on the conservation of probability, and express time evolution, step by step, with the help of the Jacobian J.

II. SOME EXACT SOLUTIONS.

The method developed in I-1) gives us, not only a new numerical approach to the Fokker-Planck equation (cf. III), but also a means of calculating exact solutions in certain cases. Let us note that the application of the method is not limited to equations which are linear with respect to ρ, as is the Fokker-Planck equation, strictly speaking.

Let us consider the example of equation

(23) $$\frac{\partial \rho}{\partial t} = \frac{\partial}{\partial x}\left(\rho^n \frac{\partial \rho}{\partial x}\right) \qquad , \quad n \in \mathbb{N} \quad ,$$

which is said to be the "non-linear heat equation". When $n = 0$, (23) evidently becomes the traditional heat equation. We will assume $n \neq 0$.

Let us look, a priori arbitrarily, for a solution ρ such that the associated differential equation of type (9-a) is a linear equation of the form

(24) $$\frac{dx}{dt} = V = a(t)x + b(t) \quad ,$$

in which the functions a and b will be determined later. It is clear that, if such a solution exists, it will be only a particular solution.

On the other hand, the velocity V associated with (23) is evidently

$$(25) \qquad V = -\frac{1}{n}\frac{\partial}{\partial x}\rho^n \quad .$$

Let us firstly integrate equation (24); the solution may be written as :

$$(26) \qquad x = x(t) = (B(t) + x_0)J(t) \quad , \quad x_0 = x(0) \, ,$$

with

$$(27) \qquad \begin{cases} J = J(t) = \exp\left(\int_0^t a(u)du\right) = \frac{\partial x}{\partial x_0} \text{ such that : } \frac{dJ}{dt} = aJ, \; J(0) = 1 & (27\text{-a}) \\ B = B(t) = \int_0^t (b(u)/J(u))du \text{ such that : } \frac{dB}{dt} = \frac{b}{J}, \; B(0) = 0 & (27\text{-b}) \end{cases}$$

Next, let us integrate $V = a(t)x + b(t)$, i.e., due to (25),

$$(28) \qquad -\frac{1}{n}\frac{\partial}{\partial x}\rho^n = a(t)x + b(t) \quad .$$

It follows :

$$(29) \qquad \rho(x,t) = \left\{-n\left(a(t)\frac{x^2}{2} + b(t)x + c(t)\right)\right\}^{1/n} \quad ,$$

where c, another function of t, will be also determined later.

Let us now utilize the conservation of probability

$$(30) \qquad \rho(x,t) = \frac{\rho(x_0,0)}{J} \quad .$$

Employing (29) and (26), and letting $a_0 = a(0)$, $b_0 = b(0)$, $c_0 = c(0)$,

one then finds :

$$\textcircled{31} \qquad \left\{-n\left(a(t)\frac{x^2}{2}+b(t)x+c(t)\right)\right\}^{1/n} = \frac{1}{J}\left\{-n\left(\frac{a_0}{2}\left(\frac{x}{J}-B\right)^2+b_0\left(\frac{x}{J}-B\right)+c_0\right)\right\}^{1/n}$$

that is :

$$\textcircled{32} \qquad a(t)\frac{x^2}{2}+b(t)x+c(t) = \frac{1}{J^n}\left(\frac{a_0}{2}\left(\frac{x}{J}-B\right)^2+b_0\left(\frac{x}{J}-B\right)+c_0\right) \quad ,$$

from which we obtain :

$$\textcircled{33} \qquad a(t) = \frac{a_0}{J^{n+2}}$$

$$\textcircled{34} \qquad b(t) = \frac{1}{J^{n+1}}\,(b_0-a_0B)$$

$$\textcircled{35} \qquad c(t) = \frac{1}{J^n}\left(\frac{1}{2}a_0B^2-b_0B+c_0\right) \quad .$$

We have here the elements which will allow us to determine the various functions, J, a, B, b and c. From (27-a) and (33), one finds $dJ/dt = aJ = a_0/J^{n+1}$, $J(0)=1$, and then :

$$\textcircled{36} \qquad J(t) = \left(1+(n+2)a_0t\right)^{\frac{1}{n+2}} \quad .$$

Let us recall that a(t) has already been defined in (33) :

$$\textcircled{37} \qquad a(t) = \frac{a_0}{J^{n+2}} \quad .$$

On the other hand, from (27-b) and (34), one obtains :

$$\frac{dB}{dt} = \frac{b}{J} = \frac{b_0 - a_0 B}{J^{n+2}} \quad , \text{ and then } \frac{dB}{b_0 - a_0 B} = \frac{dJ}{a_0 J} \text{ , with } B(0) = 0 \quad ,$$

which gives :

(38) $$B(t) = \frac{b_0}{a_0}\left(1 - \frac{1}{J}\right)$$

and, of course, from (34) and (35),

(39) $$b(t) = \frac{b_0}{J^{n+2}}$$

(40) $$c(t) = \frac{1}{J^n}\left(\frac{b_0^2}{2a_0}\left(\frac{1}{J^2} - 1\right) + c_0\right) \quad .$$

Finally, (29) becomes, as a result of (37), (39), (40),

(41) $$\rho(x,t) = \left\{ - n\left(\frac{1}{2a_0 J^{n+2}}(a_0 x + b_0)^2 + \frac{1}{J^n}\left(c_0 - \frac{b_0^2}{2a_0}\right)\right)\right\}^{1/n} \quad ;$$

$$\text{with } J = J(t) = \left(1 + (n+2)a_0 t\right)^{\frac{1}{n+2}} \quad .$$

The solution (41) was published some years ago by other authors (Ref[16][17]), who had obtained it by applying a method of groups of transformations. Letting $\mu_0 = (n+2)a_0$, equation (41) then becoming

(42) $$\rho(x,t) = \left\{ - \frac{n(n+2)}{2\mu(1+\mu t)}\left(\frac{\mu}{n+2}x + b_0\right)^2 - n(1+\mu t)^{-\frac{n}{n+2}}\left(c_0 - \frac{(n+2)b_0^2}{2\mu}\right)\right\}^{1/n} ,$$

one will recognize (41) - (42) in formula (19) of Ref[17], after the correction of two printing errors in [17], in agreement with [16]. The advantage

of our method is that it does not require any difficult mathematical preliminary, and that its physical interpretation is immediate, in terms of the conservation of probability. One may also notice that our solution contains one more parameter (3 free parameters instead of 2 ; indeed, b_0 is equal to zero in the preceding publications).

As may be understood from the beginning of II), we have no theoretical criteria which would allow us to know a priori whether the preceding technique is applicable or not to such or such an equation. (There is only one evident necessary condition, i.e., the fact that the equation may be written in the form (9-b)). However, it is clear that the utilization of the method is not limited to the non-linear heat equation (23) . For the Fokker-Planck equation (8), for example, in the particular case where D is linear with respect to x, and σ is constant, i.e.,

$$(43) \qquad \frac{\partial \rho}{\partial t} - \lambda \frac{\partial}{\partial x}(\rho x) = \frac{\sigma^2}{2} \frac{\partial^2 \rho}{\partial x^2} \quad , \quad \lambda = \text{constant},$$

one can find, by using the procedure just described and beginning with the same equation (24) , the well-known Gaussian solution :

$$(44) \qquad \rho(x,t) = \frac{K_0}{J} \exp\left\{ - \frac{1}{\sigma^2 J^2} \left(a_0 x^2 + 2 b_0 e^{-\lambda t} x + \frac{b_0^2}{\lambda} (e^{-2\lambda t} - 1) \right) \right\} ,$$

$$\text{with} \quad K_0 = e^{-2 \frac{c_0}{\sigma^2}} \quad , \quad \alpha_0 = a_0 + \lambda \quad ,$$

(a_0, b_0, c_0 having the same meaning as before)

$$J = e^{-\lambda t} \sqrt{1 + \frac{\alpha_0}{\lambda} (e^{2\lambda t} - 1)} \quad ,$$

which is the solution corresponding to the initial condition :

$$\rho_0(x) = K_0 \exp\left\{ - \frac{1}{\sigma^2} (a_0 x^2 + 2 b_0 x) \right\}$$

III. THE NUMERICAL VERSION OF THIS METHOD.

The Fokker-Planck equation (8) is a partial differential equation of parabolic type. The current method of numerical integration consists in considering (8) as an ordinary differential equation with respect to t, the value of x being fixed (Ref[10] page 225). One uses for that a grid of x and t, the mesh of which is fixed, at least for x. When interpreting it from a physical point of view, it can be said that this method of numerical integration reflects an Eulerian approach to the problem (The chosen x are fixed, and one studies the variation of the density at these fixed points).

A priori, the same problem may be considered from a Lagrangian point of view (all the x chosen at the beginning evolve in time, and one calculates ρ along trajectories). It is the core of our method : the grid is not fixed ; all the x and Δx vary. This approach surely complicates the numerical problem, but it allows the grid to adapt itself naturally to the variation of the density ρ. Furthermore, it allows us to obtain, not only the solution $\rho(x,t)$, but also trajectories which contain a piece of information which will be discussed later.

Our aim is to determine numerically a solution $\rho(x,t)$ corresponding to a given initial condition $\rho(x,0) = \rho_0(x)$. At this moment, we are working on regular and integrable functions, and have chosen limits of integration such that the solutions ρ have an almost-zero value on the trajectories of the initial limits. This procedure allows us, at least temporarily, to disregard the general problem of boundary conditions.

In the following, the solution $\rho(x,t)$ that one looks for will be parametrized by t, and then denoted as $\rho_t(x)$. Our purpose is evidently to calculate $\rho_{t_{j+1}}$ knowing ρ_{t_j}, for $t_{j+1} = t_j + \Delta t$, with Δt being sufficiently small. Let us then consider, at a given moment t_j, n points x denoted as x_{i,t_j} $(i = 1,2,\ldots,n)$. During the time interval Δt, the x_i will vary from x_{i,t_j} to $x_{i,t_{j+1}}$, and the function ρ, assumed to be known at time t_j by its values in the n points x_{i,t_j}, will be determined at time t_{j+1} by its values in the n points $x_{i,t_{j+1}}$. The easiest way to express the idea is to make a graph :

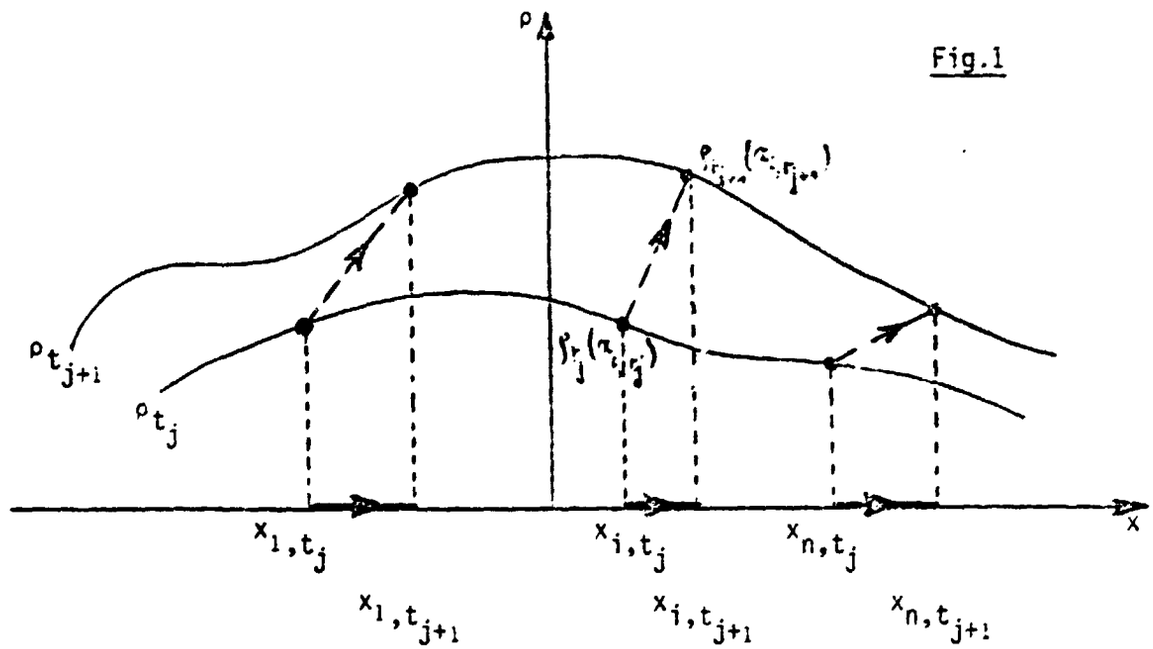

Fig.1

To apply this idea, it suffices to discretize relations (9-a), (10), (11) as follows :

(45) : (9*a) $$x_{i,t_{j+1}} \simeq x_{i,t_j} + V\left(x_{i,t_j}, t_j ; \rho_{t_j}\left(x_{i,t_j}\right)\right) \Delta t$$

(46) : (10*)
$$\rho_{t_{j+1}}\left(x_i,t_{j+1}\right) \simeq \frac{\rho_{t_j}\left(x_i,t_j\right)}{J_{t_j,t_{j+1}}\left(x_i,t_j\right)}$$

(47) : (11*)
$$J_{t_j,t_{j+1}}\left(x_i,t_j\right) \simeq \exp\left\{\int_{t_j}^{t_{j+1}}\left[\frac{\partial}{\partial x}V\left(x,t_j;\rho_{t_j}(x)\right)\right]\left(x_i,t_j\right)dt\right\}$$

$$= \exp\left\{\left[\frac{\partial}{\partial x}V\left(x,t_j;\rho_{t_j}(x)\right)\right]\left(x_i,t_j\right)\Delta t\right\}$$

This explicit scheme has been used to write a program (until now very elementary) which works satisfactorily if one correctly adapts the time integration step Δt to the variation of the space integration step Δx, in order to maintain the convergence of the numerical procedure. Fig.2 presents the results obtained for the Fokker-Planck equation with non-linear coefficients in the case $D = -x^3$, $\sigma = 1$, $\rho_0(x) = \exp\left(-\frac{x^2}{2} - x\right)$. We have taken care to put the two types of information obtained, i.e., the curves $\rho_t(x)$ and the trajectories $x(t)$, which are complementary, face to face.

It is known (Ref[1] for example) that the Fokker-Planck equation (8) controls the time evolution of the density of the Brownian trajectories defined by the stochastic differential equation

(48)
$$dx_B(t) = D(x_B(t),t)\,dt + \sigma(x_B(t),t)\,dW(t) \quad ,$$

in which W is the standard Wiener process (variance = 1), and that the Brownian trajectories $x_B(t)$ are almost everywhere non-differentiable. One obviously then would not assimilate the trajectories $x(t)$ of Fig.2 to the

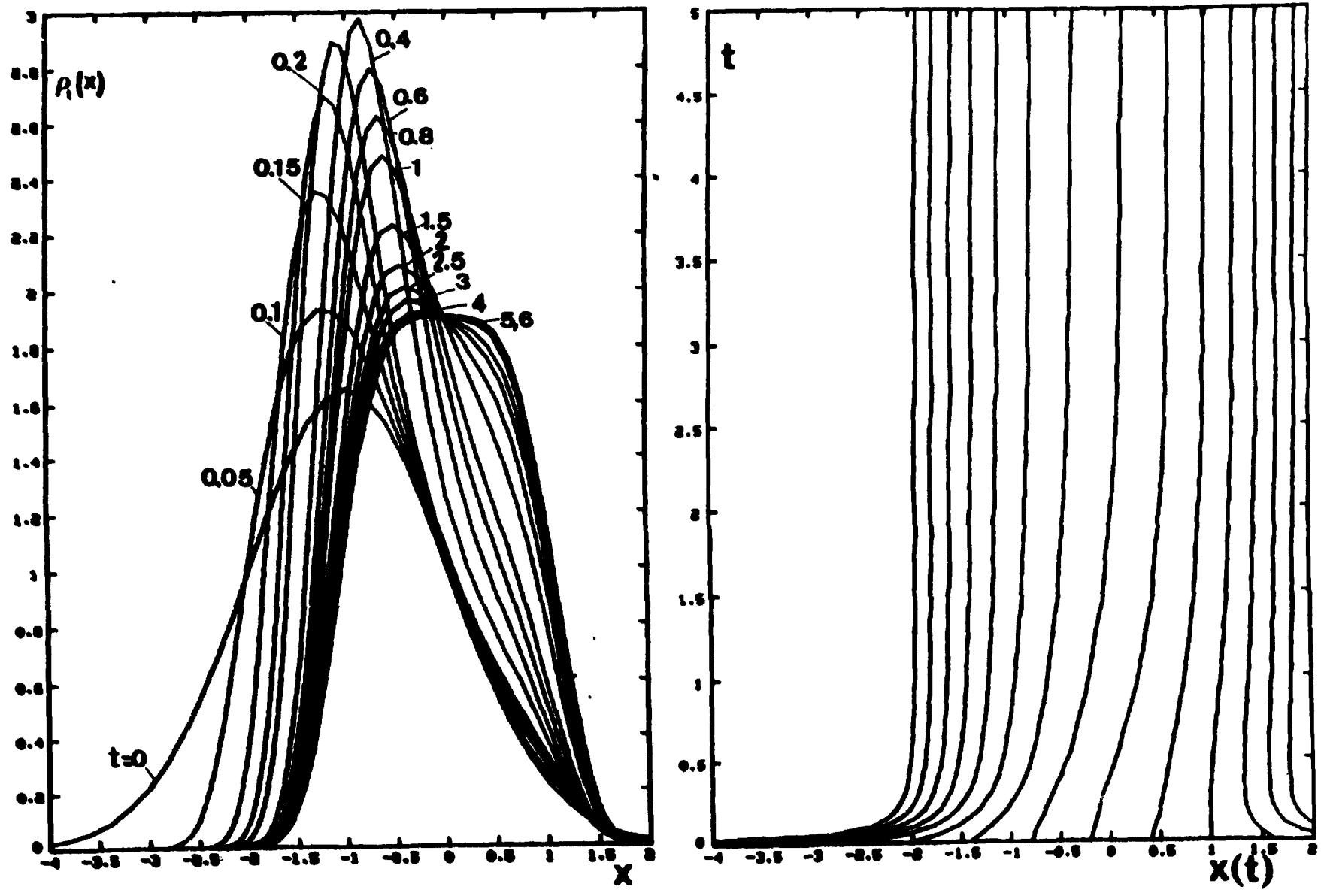

FIG. 2

Brownian trajectories $x_B(t)$. However, due to the way in which they are generated by the Fokker-Planck equation, the trajectories $x(t)$ definitely contain a certain piece of information related to the Brownian phenomenon. In order to stress this double aspect of things (existence of a link with the Brownian motion, and net distinction with the Brownian trajectories), we say that the trajectories $x(t)$ define Brownian "quasi-particles". (Ref [2][8][9][20]). From the point of view of Mathematical Analysis, do not forget that trajectories of quasi-particles are constituted by a sequence of arcs of characteristics, characteristics of a first-order partial differential equation the coefficients of which vary from one integration step to the other (cf. I-3)).

Since fundamental questions of statistical physics remain present-day problems (Ref[19],[20]), we will conclude with a remark of an interpretative nature. It is obvious — and we have already said this in order to justify the utilization of the expression "quasi-particle" — that $x(t)$ does not contain the same information as $x_B(t)$. More precisely, there is a loss of information with respect to the Brownian process $x_B(t)$. To be convinced, one needs only refer to the averaging procedure which allows us to derive the velocity V of (9-a) from the stochastic equation (48) (Ref [21] page 105, [2][8][9]). But, to say that, is not enough. It seems to us, in fact, that the following distinction must be made : if it is really proven experimentally that a phenomenon is of the Brownian type (49), it is irrefutable that the utilization of the trajectories $x(t)$ — even if it is technically profitable - involves a loss of information with respect to reality ; however, if experiments prove only that the phenomenon is governed by a Fokker-Planck equation, equation (8) constituting at a given moment a complete description of reality, there is no reason to speak of a loss of

information concerning quasi-particles ; both $x(t)$ and $x_\beta(t)$ are only two different models compatible with the experimental reality of the moment.

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