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1992 J. Phys. A: Math. Gen. 25 6733

(http://iopscience.iop.org/0305-4470/25/24/024)

J. Phys. A: Math. Gen. 25 (1992) 6733–6742. Printed in the UK

Method of divergent series summation in the problem of particle diffusion in a bistable potential

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Received 28 August 1991

Abstract. An infinite system for the moments of a particle moving in a potential with two minima under the action of fluctuations is considered. A class of solutions is found for which a divergent series can be summed up to a simple transcendent function. It is shown numerically that the true solution belongs to this class and conditions are set to define the solution uniquely.

Introduction

The present paper analyses the transient behaviour of the moments $\langle x^n(t)\rangle$ for the well known Langevin equation

$$\dot{x} = \mathrm{d}x - x^3 + \eta \tag{1}$$

where η is a white noise with power N (from Stratonovich's viewpoint). This particular equation is, of course, of special importance in fluctuation theory because it has so frequently been used to describe noise-driven motion in a double-well potential, and thus to model a wide range of bistable physical systems. The corresponding Fokker–Planck equation for the transient probability density is

$$\frac{\partial P}{\partial t} = -\frac{\partial}{\partial x}(\mathrm{d}x - x^3)P + \frac{N}{2}\frac{\partial^2}{\partial x^2}P. \tag{2}$$

The number of works devoted to this and related problems is enormous. Nevertheless, an analytic solution of (2) uniformly valid for $t \in (0, \infty)$ has not yet been obtained.

All previously obtained numerous approximate formulae hold, at best, in limited parts of the (d, N) parameter space or only in limited time intervals given by a particular timescale. The aim of the present paper is to report significant progress towards an analytic solution, based on a new approach.

In the present paper we adhere to the viewpoint of Graham and Schenzle [1] and Brenig and Banai [2] who treated the exactly solvable system by the Carleman embedding method, i.e. writing an infinite chain of equations for the moments of the system coordinate. They have shown that in order to obtain correct results the series in the form of which the expressions for the means are written cannot be (truncated) because of their divergence, but must be convolved to finite expressions, i.e. they must be subjected to summation. The above-mentioned works consider a problem whose solutions are known to *a priori*, but it seems that on these lines other problems could be solved too provided that a suitable method of diverging series summation is proposed.

Trying, however, to investigate problem (1) by studying an infinite chain of equations for $\langle x^n \rangle$ we face a serious difficulty—namely that correspondence between (1, 2) and the infinite system is embedding but not equivalence. In other words, the infinite chain of equations for $\langle x^n \rangle$ is a more general object than (2) and it is not enough to set the initial values of the moments $\langle x^n(t_0) \rangle$ in order to determine $\langle x^n(t) \rangle$ uniquely. This is not surprising since, in the form of an infinite chain of equations, this task is nothing but the famous moment problem which, as is very well known, is not resolved uniquely [3] without some additional conjectures about the distribution function.

It is shown explicitly in the present paper that one needs more than initial conditions for the moments. Choosing additional conditions in a special way, it is possible to single out a special class of three-parameter solutions which on the one hand satisfy the infinite system of equations for moments $\langle x^n(t) \rangle$, and on the other hand admits explicit summation to some transcendent function that coincides with the true solution provided the free parameters are properly chosen. An excellent correspondence of the analytical solution to numerical results is demonstrated.

1. Writing formal expressions

Now, we are interested in the time behaviour of conditional moments $\int_{-\infty}^{\infty} P(x, t; x_0, t_0) x^n \, dx = x_n(x_0, t_0)$ (for obtaining unconditional means one should specify the initial distribution $P_0(x_0, t_0)$ and average x_n with this distribution over the initial data). For the subsequent expressions to be less awkward, however, all the calculations will be made only for x_1. For other odd n, all the formulae are analogous. For even n the formulae are slightly different due to the appearance of an inhomogeneous term in the infinite linear system of differential equations. Nevertheless, the proposed approach is suitable for this case as well. It is also interesting to consider the odd moments specifically because the functions must have different limits $\lim_{N\to 0} \lim_{t\to\infty}$ and $\lim_{t\to\infty} \lim_{N\to 0}$. This can easily be seen from the form of the solution for equation (1) when $\eta \equiv 0$

$$x = x_0 \exp\{dt\}[1 + x_0^2(\exp\{2\,dt\} - 1)d^{-1}]^{-1/2} \tag{3}$$

and from the type of the stationary distribution function obtained from (2)

$$P_{st} = \text{const} \cdot \exp\{(dx^2 - x^4/2)/N\}. \tag{4}$$

For $d > 0$ P_{st} has two maxima symmetric about $x = 0$ at points $\pm d^{1/2}$, and all the stationary odd moments ($\lim_{t\to\infty} x_{2n+1}(N, t)$) must, therefore, be equal to zero, and hence $\lim_{N\to 0} \lim_{t\to\infty} x_{2n+1}(N, t) = 0$. In contrast, it follows from formula (3) for $x = \lim_{t\to\infty} x = \lim_{t\to\infty} \lim_{N\to 0} x_1$ that the limit value depends on the sign of the initial position x_0 (for $x_0 > 0$ $x_{st} = d^{1/2}$, at $x_0 < 0$ $x_{st} = -d^{-1/2}$). The numerous approaches proposed for solving this and similar problems have not often yielded correct limit transition.

Multiplying equation (2) by x^{2n+1} ($n = 0, 1, \ldots$), integrating with respect to x, and taking into account the condition that P is zero at infinitely remote boundaries, we obtain a continued infinite system of linear differential equations for odd moments:

$$\begin{pmatrix} \dot{x}_1 \\ \dot{x}_3 \\ \cdots \\ \dot{x}_{2n+1} \\ \cdots \end{pmatrix} = \begin{pmatrix} d & -1 & 0 & & & \\ 3N & 3d & -3 & & & \\ & \cdots & \cdots & \cdots & \cdots & \cdots \\ & 0 & N(2n+1)n & (2n+1)d & -(2n+1) & 0 \\ & \cdots & \cdots & \cdots & \cdots & \cdots \end{pmatrix} \begin{pmatrix} x_1 \\ x_3 \\ \cdots \\ x_{2n+1} \\ \cdots \end{pmatrix}. \tag{5}$$

Since, as mentioned above, we are interested in conditional moments, we choose initial conditions for the form

$$x_{2n+1}(0) = x_0^{2n+1}. \tag{6}$$

By taking the Laplace transforms of both parts of the new system, we obtain an infinite algebraic system of linear equations for the Laplace images:

$$\begin{pmatrix} p-d & 1 & 0 & & & \\ -3N & p-3d & 3 & & & \\ & \cdots & \cdots & \cdots & \cdots & \cdots \\ & 0 & -N(2n+1)n & p-(2n+1)d & (2n+1) & 0 \\ & \cdots & \cdots & \cdots & \cdots & \cdots \end{pmatrix} \begin{pmatrix} \tilde{x}_1(p) \\ \tilde{x}_3(p) \\ \cdots \\ \tilde{x}_{2n+1}(p) \\ \cdots \end{pmatrix} = \hat{A}(p)\tilde{x}(p) = \begin{pmatrix} x_1(0) \\ x_3(0) \\ \cdots \\ x_{2n+1}(0) \\ \cdots \end{pmatrix}. \tag{7}$$

In the case of $N = 0$, Graham and Schenzle [1] and Brenig and Banai [2] have solved system (7) by formally inverting the infinite matrix $\hat{A}$. In the case of $N \neq 0$, inverting infinite matrix is not an obvious operation. It is useful, therefore, to find out what this operation corresponds to from the point of view of the general theory of difference equations. It is well known that the general solution for three-term recurrence relations, infinite system (7) among them, can be expressed as

$$\tilde{x}_{2n+1} = C_1 \tilde{x}^{\text{hom}}_{2n+1,1} + C_2 \tilde{x}^{\text{hom}}_{2n+1,2} + \tilde{x}^{\text{inhom}}_{2n+1} \tag{8}$$

where $x^{\text{hom}}_{2n+1,i}$ ($i = 1, 2$) are linearly independent solutions of the homogeneous recurrence relations and $\tilde{x}^{\text{inhom}}_{2n+1}$ is a particular solution of the inhomogeneous recurrence relations, C_1 and C_2 are constants determined from the initial conditions which, naturally, will depend on the choice of $\tilde{x}^{\text{inhom}}_{2n+1}$. If $\tilde{x}^{\text{inhom}}_{2n+1}$ is chosen such that $(2\pi i)^{-1} \oint \tilde{x}_{2n+1}(p)\,\mathrm{d}p = x_{2n+1}(0)$, i.e. for the initial conditions to be taken into account only by the inhomogeneous term of system (3), we obtain $C_1, C_2 = 0$. We can seek a particular solution for $\tilde{x}^{\text{inhom}}_{2n+1}$ in terms of the Green function

$$\tilde{x}^{\text{inhom}}_{2n+1} = \sum_{k=1}^{\infty} G_{2n+1,k}(p) x_{2k+1}(0) \qquad (k = 0, 1 \ldots) \tag{9}$$

where $G_{2n+1,k}$ is the solution of

$$\hat{A}\begin{pmatrix} \cdots \\ \cdots \\ \cdots \\ G_{2n+1,k} \\ \cdots \\ \cdots \end{pmatrix} = \begin{pmatrix} 0 \\ \cdots \\ 0 \\ 1 \\ 0 \\ \cdots \end{pmatrix} k. \tag{10}$$

In the case of $N=0$, $G_{2n+1,k}$ *may be chosen as follows: when* $n \leqslant k$ $G_{2n+1,k}$ is a solution of the finite-dimensional system

$$\begin{pmatrix} p-d & 1 & 0 & & \\ 0 & p-3d & 3 & & \\ & & & \cdots & (2n-1) \\ & & & 0 & p-(2n+1)d \end{pmatrix}\begin{pmatrix} G_{2n+1,1} \\ \cdots \\ \cdots \\ G_{2n+1,n} \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix} \tag{11}$$

and when $n > k$

$$G_{2n+1,k} \equiv 0. \tag{12}$$

It is easy to verify (see [1, 2]) that the $G_{2n+1,k}$ found in this way are nothing else but columns of the formally inverted infinite matrix $\hat{A}$. It should be stressed once more that (11) and (12) give a particular solution of system (7) which is singled out of the *whole infinite set of solutions of* (7) *by two requirements:*

(1) An inverse Laplace transformation of $\tilde{x}^{\text{inhom}}_{2n+1}(p)$ satisfies the initial data

$$(2\pi i)^{-1} \oint \mathrm{e}^{pt} \tilde{x}^{\text{inhom}}_{2n+1}(p)\, \mathrm{d}p|_{t=0} = x_{2n+1}(0) \tag{13}$$

or

$$(2\pi i)^{-1} \oint \mathrm{e}^{pt} G_{2n+1,k}(p)\, \mathrm{d}p|_{t=0} = \delta_{nk} \tag{13a}$$

and

(2) There are no elements growing with the number n in the column $G_{2n+1,k}$, which will inevitably appear in any other particular solution.

As a result, this solution corresponds to our intuitive notions of inverse of matrices, but it is achieved at high cost-series (9) diverges in the vicinity of an infinite number of points on the complex plane of p (every $G_{2n+1,k}$ has k poles located in the right half). Therefore, we have to either choose $G_{2n+1,k}$ in a different form or subject series (9) to a summation procedure. Graham and Schenzle [1] and Brenig and Banai [2] have chosen the second way and have summed up divergent series (9) in the case of $N=0$. The aim of this work is to clarify what can be achieved by doing this in the case of $N \neq 0$.

Writing out the system (10) for $G_{2n+1,k}$ in an explicit form yields:

$$\begin{aligned}
&(d-p)G_{1,k}-G_{3,k}=0\\
&NG_{1,k}+(d-p/3)G_{3,k}-G_{5,k}=0\\
&\vdots\\
&kNG_{2k-1,k}+(d-p/(2k+1))G_{2k+1,k}-G_{2k+3,k}=-1/(2k+1)\\
&(k+1)NG_{2k+1,k}+(d-p/(2k+3))G_{2k+3,k}-G_{2k+5,k}=0.
\end{aligned} \tag{14}$$

Now it is clear that it is impossible to put all $G_{2i+1,k}=0$ when $i>k$ as in the case $N=0$, because the finite dimensional system remaining for $G_{2i+1,k}$ with $i\leq k$ will have no solution. It is possible, however, to find the following family of particular solutions for $G_{2i+1,k}$ by expressing $G_{2k+3,k}$ as a linear combination of $G_{2i+1,k}(i\leq k)$, i.e.

$$G_{2k+3,k}=-\sum_{n=0}^{k-1} c_n(p)G_{2n+1,k} \tag{15}$$

and substituting this into (14). This ansatz allows (1) the finite system to be solved

$$\begin{aligned}
&(d-p)G_{1,k}-G_{3,k}=0\\
&NG_{1,k}+(d-p/3)G_{3,k}-G_{5,k}=0\\
&\vdots\\
&kNG_{2k-1,k}+(d-p/(2k+1))G_{2k+1,k}+\sum_{n=0}^{k-1} c_n(p)G_{2n+1,k}-1/(2k+1)
\end{aligned} \tag{16}$$

and (2) the infinite system to be solved

$$(i+1)NG_{2i+1,k}+(d-p/(2i+3))G_{2i+3,k}-G_{2i+5,k}=0 \qquad (i>k) \tag{17}$$

uniquely with respect to $G_{2i+1,k}(i>k)$ since (17), being a three-term recurrence relation, needs two constants to be uniquely solved (Jones and Thron [4]).

So, $G_{2i+1,k}$ for $i\leq k$ depend on k arbitrary functions $c_i(p)$ which can naturally depend on Laplace variable p and other parameters of the problem.

It is worthwhile noting the difference between this case and the case of convergent recurrence relations (Risken [5]). In the latter, a solution is achieved by truncating (17) for some large k, which is absolutely impossible in the case of divergence [1, 2]. However, even in cases where truncation is possible this solution is only a particular one which corresponds to some special choice of $c_i(p)$ in (15). This means that other (perhaps formal) solutions of the same three-term recurrence relations exist, since (15) is admissible in all cases.

2. A class of particular solutions

It is obvious that since arbitrary constants $c_i(p)$ in (15) are generic to infinite systems like (14), they should be determined from considerations which do not depend on any information about $G_{2i+1,k}$ which is possible to extract manipulating the system (14). We thus have the following plan. First, show that it is possible to choose arbitrary constants $c_i(p)$ in such a way that

$$x_{2n+1}(t)=(2\pi i)^{-1}\oint e^{pt}\tilde{x}_{2n+1}^{\text{inhom}}(p)\,dp=(2\pi i)^{-1}\oint e^{pt}\sum_{k=0}^{\infty} G_{2n+1,k}(p)x^k(0)\,dp \tag{18}$$

can be summed to a function which belongs to a class which is much narrower than all possible solutions of (14). Next, using numerical simulations, we show that the true solution can be found inside this class for all values of parameters. We obtain in this way a formula which is uniform with respect to $t\in(0,\infty)$ and therefore solve the old problem of combined description of $\langle x_{2n+1}\rangle$ in different time domains. It is worth mentioning here that the scaling approach by Suzuki [5] solves this problem only approximately for a certain set of parameters and only for even moments.

Let us choose c_i for $i<k$ independent of p, and $c_k=c_k^0-c_k^1p$ $(k>1)$ (all c_i are naturally some functions of $\{d, N\}$). Making this choice we have $k+1$ arbitrary constants and can vary them in such a way that all k roots of

$$D_k(p)=\det\begin{pmatrix} p-d & 1 & 0 & \\ -3N & p-3d & 3 & \\ \cdots & \cdots & & \cdots \\ -c_1 & \cdots & -N(2n+1)n-c_{n-1} & (1+c_k^0)p-(2n+1)d-c_k^1 \end{pmatrix}$$

are situated in prescribed places. The possibility to do this follows from the Wiet theorem stating one-to-one connection between roots of a polynomial and its coefficients. Specifying the roots we can find coefficients, which in our case are c_i. Specifically, we are interested in a class of functions where all roots of $D_k(p)$ in (18) are real and positive, the lowest one being λ, and the distance between each pair being equal to $2d^*$.

To make all formulae more concise we make calculations for $G_{1,k}$ forthcoming only. Equations for arbitrary i can be obtained in the same manner.

For the above-mentioned choice of c_i we obtain $G_{1,k}(p)$ of the form

$$G_{1,k}=\frac{(-1)^k(2k-1)!!}{D_{2k+1}(p)}=\frac{(-1)^k(2k-1)!!}{(c_k^1+1)\Pi_{n=0}^{n=k}(p-(\lambda+2nd^*))}. \tag{19}$$

Substituting (19) into (18) and calculating the reverse Laplace tranformation one obtains

$$\begin{aligned}\langle x_1\rangle &=\exp(\lambda t)x_0\sum_{n=0}^{\infty}\frac{(-1)^n(2n)!}{2^{2n}(n!)^2d^*}(\exp(2d^*t)-1)g_xx_0^2\\ &=x_0\exp\{\lambda t\}[1+g_xx_0^2(\exp\{2d^*t\}-1)d^{*-1}]^{-1/2}\end{aligned} \tag{20}$$

$g_x=c_k^1+1$. Thus we have obtained a family of rather simple transcendental functions (20) which satisfy the infinite chain of equations (7) and are dependent on three arbitrary functions of $\{d, N\}-\lambda$, g_x and d^*.

3. Constant specification

There is no guarantee that the true moment $\langle x_1\rangle$ belongs to the family (20). We hope, however, that we can specify λ, g_x and d^* in such a way that it does. In order to do that we need to use information which is independent of (7).

We know from the eigenvalue decomposition [6, 7] of the solution of (2)

$$P=\sum_{n=0}^{\infty}X_n(x)X_n(x_0)\exp\{-\lambda_nt\}/P_{st}(x_0) \tag{21}$$

where $X_n(x)$ are eigenfunctions of the elliptic operator in the right-hand side of (2), $P_{st}(x_0)$ is the stationary probability distribution and λ_n are corresponding eigenvalues

($\lambda_0 = 0$), such that

$$\langle x_1 \rangle_{t\to\infty} \sim \int \mathrm{d}x\, x\, \boldsymbol{X}_1(x)\boldsymbol{X}_1(x_0)\exp\{-\lambda_1 t\}/P_{\mathrm{st}}(x_0). \tag{22}$$

In order for (20) to have the correct behaviour at $t \to \infty$ we have to choose

$$-\lambda + d^* = \lambda_1 \tag{23}$$

and

$$(d^*/g_x)^{1/2} = \int \mathrm{d}x\, x\, \boldsymbol{X}_1(x)\boldsymbol{X}_1(x_0)/P_{\mathrm{st}}(x_0). \tag{24}$$

The third necessary condition one can obtain from the first equation of system (5)

$$\langle \dot{x}_1 \rangle|_{t\to 0} = \mathrm{d}x_0 - x_0^3 = (d^* - \lambda)x_0 - g_x x_0^3 \tag{25}$$

is nothing but the requirement for $\langle x_1 \rangle$ to have correct time behaviour at $t \to 0$. So, parameters λ, g_x and d^* can be expressed through the first eigenvalue and eigenfunction of the correspondent Fokker–Planck equation.

4. Numerical results

We can now address the last and most important question—how close (20) is to the true solution of the moment problem (5)?

We have carried out extensive direct numerical simulations of stochastic equation (1) for a vast variety of parameters: low, medium and high noise intensity, low, medium and high starting position. The numerical algorithm proposed in [9] was used. The most representative results are summarized in figures 1 and 2. For low values of noise

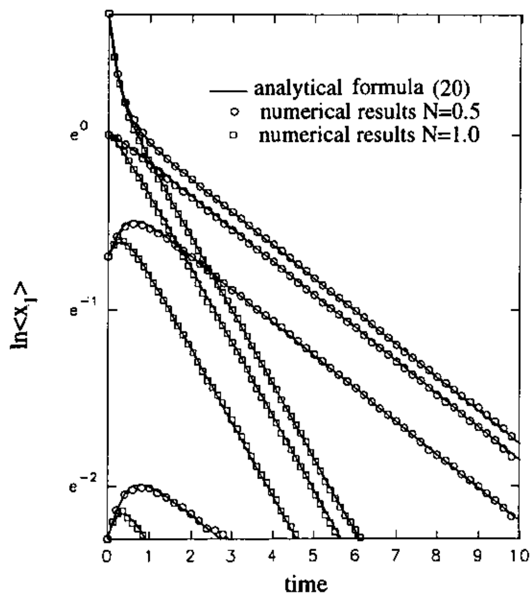

Figure 1. Average position depending on time; high and medium noise intensities. Time step—10^{-2}, number of trajectories—10^{+5}.

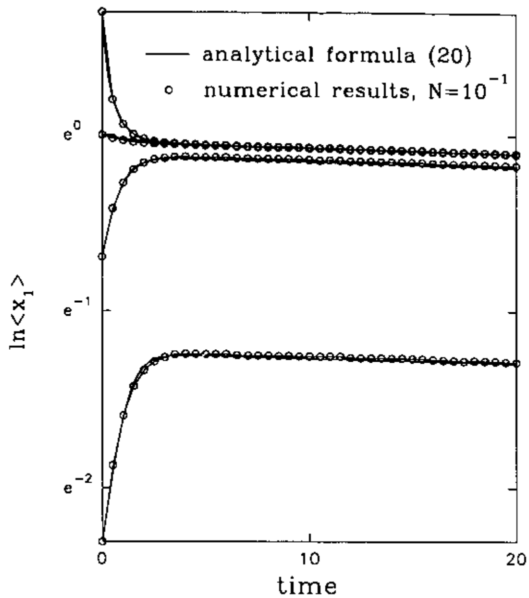

Figure 2. Average position depending on time; low noise intensities. Time step—10^{-1}, number of trajectories—10^{+5}.

intensity ($N \ll 1$) the result

$$\lambda_1 = 2^{1/2}\Pi^{-1} d \exp\{-d^2/2N\}[1-3N/4d^2] \tag{26}$$

of Larson and Kostin [7] was used. For large values of noise intensity no results for λ_1 are known, so, λ, g_x and d^* were treated as fitting parameters. They have a very clear physical meaning. λ, and d^* are responsible for true time asymptotic behaviour at $t \to \infty$ and $t \to 0$, respectively, and g_x for the position of the maximum (for low noises) or the point where the decay constant is changed. We can also regard (20) as a modification of (3)—the formula for x_1 without noise—due to action of fluctuations.

The g_x dependence on starting position x_0 deserves a special comment. As is clear from figures 1 and 2 there must exist a value of $x_0 = x_0^{\lambda_1}$ which gives rise to exact one exponential decay with relaxation constant equal λ_1. It is easy to find this value from (25):

$$x_0^{\lambda_1} = (d + \lambda_1)^{1/2} \tag{27}$$

which is the requirement for $\langle x_1 \rangle$ to have λ_1 as relaxation constant close to $t = 0$. At this point d^* and g_x must be connected by the relation

$$d^* = g_x x_0^2. \tag{28}$$

Returning to equation (20), we see that two combinations of d^* and g_x are possible:

$$d^* = g_x = 0 \tag{29}$$

and

$$d^* = g_x = \infty \tag{30}$$

but of course $d^*/g_x = x_0$.

Numerical calculations show that (29) is realized to the left of $x_0 = x_0^{\lambda_1}$ and (30) to the right.

5. Discussion

Equation (26) for λ_1 states that the lowest non-zero eigenvalue cannot be obtained as a solution of any truncated finite system (18), since the roots of $D_k(p)$ are polynomial functions of N. However, all coefficients in the Taylor expansion of λ_1 (18) are identically zero. This is another manifestation of the arbitrariness in the solution of the infinite chain (5). On the other hand, an excellent agreement between analytical formula (20) and numerical simulations indicates that (20) is very close to an exact solution.

Any deviation from (20) may be found most probable for very low noises or in the vicinity of $x_0^{\lambda_1}$ where special measures should be taken to guarantee high precision. In this case we can improve (20) by choosing c_k as polynomials in p, and defining coefficients of the polynomials in such a way that information about higher eigenvalues (requirement for the right behaviour at infinity) and higher derivatives at $t = 0$ (the right behaviour at short time) would be taken into account.

Figures 1 and 2 show that the dynamics of the moments consists of two distinctively different regions with different relaxation rates. The first part corresponds to the time scale when the non-stochastic behaviour dominates. The second part is determined by λ_1 (figure 5), i.e. mainly by fluctuations.

The values of moments at the instant when one relaxation constant changes for another are strongly dependent on noise intensity and initial position. It is function g_x that is responsible for the correct position of this point. It is evident from figures 3 and 4 that the most dramatic changes in the deterministic dynamics caused by the noise take place for starting positions near the top of the potential (low values of x_0). It is quite interesting to point out that, starting from the barrier, the system never

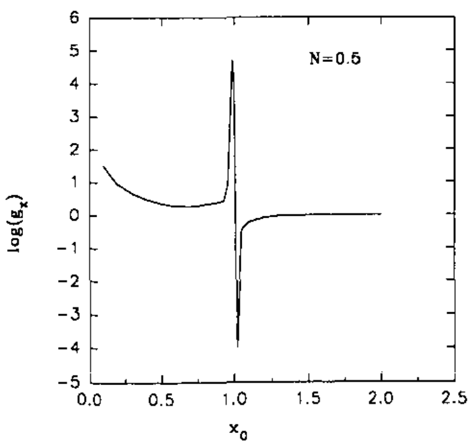

Figure 3. Typical g_x dependence on starting position.

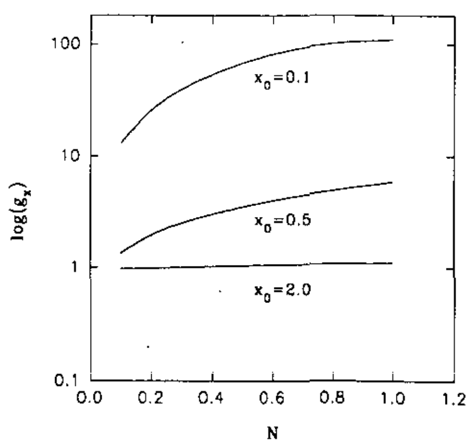

Figure 4. g_x dependence on noise intensity.

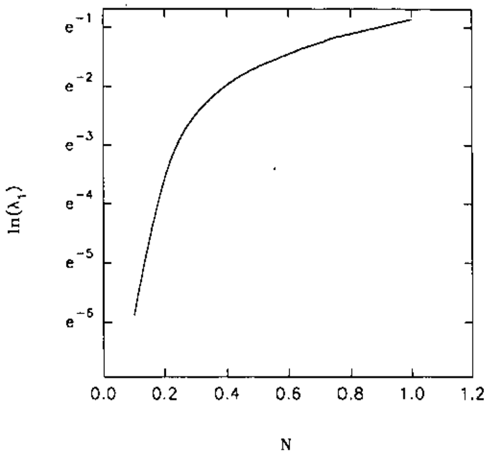

Figure 5. Dependence of the first eigenvalue on noise intensity.

forgets initial conditions—lines in figures 1 and 2 are parallel to infinity. This is the peculiarity of systems prepared in some unstable state.

This approach allows the construction of time-uniform solutions for the moments of more general nonlinear systems in multistable situations (infinite chains of equations which normally lead to divergent series) provided additional (besides initial conditions) information about the system is known.

Acknowledgments

The author is grateful to Dr R Mannella and Professor P V E McClintock for consultations and helpful discussions.

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