

Solution of Fokker–Planck Equation Using Trotter’s Formula

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Solution of Fokker–Planck equation using Trotter’s formula is discussed. The method is illustrated on the linear Fokker–Planck equation and the Ornstein–Uhlenbeck solution is obtained. For the case of a general nonlinear Fokker–Planck equation the method yields an integral representation amenable to approximations. In the lowest order approximation Suzuki’s scaling result emerges. Physical interpretation and limitations of the approximations are also discussed.

KEY WORDS: Langevin equation; Fokker–Planck equation; Trotter’s formula; path integral formulation; scaling theory.

1. INTRODUCTION

In the Langevin approach to problems in irreversible statistical mechanics, the deterministic equation of motion is made stochastic by addition of a random noise term. Alternately one can model the problem by an equivalent Fokker–Planck equation (FPE)⁽¹⁾ for the probability density of the solution process. Both these equations are in general nonlinear and are not amenable to closed form solutions. Approximate procedures have become imperative. For physical systems that have a unique single steady state, the fluctuations rapidly relax to the equilibrium values which are small. These small fluctuations can be amply represented as corrections to the mean path and the approximations like the system size expansion^(2,3) and the generalized statistical linearization^(4,5) yield satisfactory results during the entire time domain. Even for systems with multiple steady states, these

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approximations perform fairly well,^(4,5) if the evolution is from the extensive regime. However, for the passage from unstable steady states, since the solution process is far from Gaussian, these “linear” approximations break down. For such problems, the scaling theory^(6,7) of Suzuki, WKB method⁽⁸⁾ of Caroli *et al.* and the integral transform method⁽⁹⁾ of Haake prove to be very useful. It should be pointed out, however, that these methods do not correctly predict the asymptotic fluctuations.

There have been attempts to solve the FPE exactly, and noteworthy amongst these are the eigenfunction method⁽¹⁰⁾ and the path integral formulation.^(11,12) The eigenfunction method, for its application, demands the knowledge of the complete eigen spectrum of the FPE set in its self adjoint form, which is rather difficult to obtain. The path integral formulation, though formal, is easily amenable for subsequent approximations.

Our recent investigations in this problem revealed that Trotter’s formula,⁽¹³⁾ widely used in perturbation theory,⁽¹⁴⁾ can be profitably exploited to study nonlinear FPE. We first apply Trotter’s formula on a linear FPE and derive the well known Ornstein–Uhlenbeck solution.⁽¹⁾ We then apply it to a general nonlinear FPE and obtain a formal integral representation of the solution process which is equivalent to the path integral result. Then we show that Suzuki’s scaling result⁽⁷⁾ emerges naturally as the lowest-order approximation to our general formulation.

The plan of the note is as follows. In Section 2 we formulate the method and illustrate it with the simple example of a linear FPE. Section 3 contains the result for the general nonlinear FPE. Section 4 is devoted for the approximate solution. The physical interpretation and limitations of the approximation are also discussed. Conclusions are brought out in Section 5.

2. THE METHOD AND ITS ILLUSTRATION ON A SIMPLE EXAMPLE

We consider a FPE given by

$$\frac{\partial}{\partial t} P(x, t) = LP(x, t) \quad (1a)$$

where

$$L = -\gamma \frac{\partial}{\partial x} C(x) + \epsilon \frac{\partial^2}{\partial x^2} \quad (1b)$$

The formal solution of the above partial differential equation is

$$P(x, t) = e^{tL}P(x, 0) \quad (2)$$

Since L is a sum of two non commuting operators, the exponential operator

e^{tL} cannot be expressed in terms of simple products of functions involving each of these. Nevertheless the solution of Eq. (2) can be obtained by using the Trotter’s product formula which reads as

$$e^{A+B} = \lim_{n \rightarrow \infty} (e^{A/n} e^{B/n})^n \tag{3}$$

where A and B are two arbitrary operators. The solution can be formally expressed as

$$P(x, t) = \lim_{n \rightarrow \infty} \left\{ \exp \left[-b \frac{d}{dx} C(x) \right] \exp \left(a \frac{d^2}{dx^2} \right) \right\}^n P(x, 0) \tag{4a}$$

where

$$a = \epsilon t/n \quad \text{and} \quad b = \gamma t/n \tag{4b}$$

In the remaining part of this section we illustrate the use of Eq. (4) on a linear Langevin equation for which

$$C(x) = -x \tag{5a}$$

with the initial condition

$$P(x, 0) = \delta(x - y) \tag{5b}$$

For convenience of algebraic manipulations we use the integral representation of the delta function and write the solution as

$$P(x, t) = \lim_{n \rightarrow \infty} \Theta^n \frac{1}{2\pi} \int_{-\infty}^{\infty} dk e^{-ikx} e^{iky} \tag{6a}$$

where

$$\Theta = \exp \left(b \frac{d}{dx} x \right) \exp \left(a \frac{d^2}{dx^2} \right) \tag{6b}$$

It is easy to show that

$$e^{ad^2/dx^2} e^{-ikx} = e^{-ak^2 - ikx} \tag{7a}$$

and

$$\exp \left(b \frac{d}{dx} x \right) \exp(-ikx) = e^b \exp(-ike^b x) \tag{7b}$$

Therefore

$$\Theta^n e^{-ikx} = \exp \{ -ak^2 [1 + e^{2b} + \dots + e^{2(n-1)b}] \} e^{nb} e^{-ike^{nb} x}$$

Summing the geometric series in the above, we get

$$\Theta^n e^{-ikx} = \exp \{ -a [e^{2nb} - 1] k^2 / (e^{2b} - 1) \} e^{-ike^{nb} x} \tag{8}$$

Applying the limit of $n \rightarrow \infty$ in Eq. (8) and using the fact that

$$\lim_{n \rightarrow \infty} \frac{a}{e^{2b} - 1} = \frac{\epsilon}{2\gamma}$$

we get

$$\lim_{n \rightarrow \infty} \Theta^n e^{-ikx} = \exp\left[-\frac{\epsilon}{2\gamma} (e^{2\gamma t} - 1)k^2\right] e^{\gamma t} e^{-ike^{\gamma t}x} \quad (9)$$

Substituting Eq. (9) in Eq. (6a) and interchanging order of integration and operation of Θ we get

$$\begin{aligned} P(x, t) &= \frac{1}{2\pi} \int_{-\infty}^{\infty} dk e^{\gamma t} \exp\left[-\frac{\epsilon}{2\gamma} (e^{2\gamma t} - 1)k^2\right] \exp\{-ik[xe^{\gamma t} - y]\} \\ &= \left[2\pi \frac{\epsilon}{\gamma} (1 - e^{-2\gamma t})\right]^{-1/2} \exp\left[-(x - ye^{-\gamma t})^2 / \frac{2\epsilon}{\gamma} (1 - e^{-2\gamma t})\right] \end{aligned} \quad (10)$$

which is the same as the Ornstein-Uhlenbeck solution.⁽¹⁾

It is trivial to extend the solution for an initial Gaussian density given by

$$P(x, 0) = [2\pi\sigma_0^2]^{-1/2} \exp[-(x - y)^2/2\sigma_0^2] \quad (11a)$$

Again using the integral representation of $P(x, 0)$ as

$$P(x, 0) = \frac{1}{2\pi} \int_{-\infty}^{\infty} dk \exp(-ikx - k^2\sigma_0^2/2 +iky) \quad (11b)$$

and interchanging the order of integration and operation of Θ we get

$$\begin{aligned} P(x, t) &= \frac{1}{2\pi} \int_{-\infty}^{\infty} dk e^{\gamma t} \exp\left\{-k^2\left[\frac{\epsilon}{2\gamma} (e^{2\gamma t} - 1) + \frac{\sigma_0^2}{2}\right] + ik(y - xe^{\gamma t})\right\} \\ &= \left\{2\pi\left[\sigma_0^2 e^{-2\gamma t} + \frac{\epsilon}{\gamma} (1 - e^{-2\gamma t})\right]\right\}^{-1/2} \\ &\quad \times \exp\left\{-(x - ye^{-\gamma t})^2/2\left[\sigma_0^2 e^{-2\gamma t} + \frac{\epsilon}{\gamma} (1 - e^{-2\gamma t})\right]\right\} \end{aligned} \quad (12)$$

In deriving the above result (which is the same as the Ornstein-Uhlenbeck solution⁽¹⁾) we have utilized Eq. (9).

3. SOLUTION FOR THE GENERAL PROBLEM

Now we consider the solution for general $C(x)$ with the initial condition given by Eq. (5b). Further generalization for arbitrary initial condition

is straightforward. We proceed along the same line as in the previous section.

It is easily seen that

$$\begin{aligned} \exp\left[-b \frac{d}{dx} C(x)\right] f(x) &= \frac{1}{C(x)} \exp\left[-bC(x) \frac{d}{dx}\right] C(x) f(x) \\ &= \frac{C[G(x)]}{C[x]} f[G(x)] \end{aligned} \tag{13}$$

where

$$G(x) = \xi = F^{-1}(F(x)e^{-b}) \tag{14a}$$

In the above the nonlinear function $F(x)$ is given by

$$F(x) = \exp\left[\int^x dx' / C(x')\right] \tag{14b}$$

Therefore we get

$$\Theta e^{-ikx} = \frac{C[G(x)]}{C[x]} \exp[-ak^2 - ikG(x)] = H(k, x) \tag{15}$$

Subsequent application of the operator Θ on Eq. (15) is not obvious. The trick we employ is to perform Fourier transform and inverse transform on Eq. (15) and write

$$\Theta e^{-ikx} = \frac{1}{2\pi} \int_{-\infty}^{\infty} dk_1 e^{-ik_1x} \int dx_1 e^{ik_1x_1} H(k, x_1) \tag{16}$$

In the above equation the limits of x_1 integral is to be chosen such that $G(x)$ is real. Now we can operate Θ in Eq. (16). This process can thus be done n number of times. Thus we get the expression for $P(x, t)$ as

$$\begin{aligned} P(x, t) &= \lim_{n \rightarrow \infty} \frac{1}{(2\pi)^n} \int \cdots \int dk_{n-1} \cdots dk_1 dk dx_{n-1} \cdots dx_1 \\ &\quad \times \exp\{i[k_{n-1}x_{n-1} + \cdots + k_1x_1 + ky]\} \\ &\quad \times H(k_{n-1}, x) \cdots H(k, x_1) \end{aligned} \tag{17}$$

Starting from Eq. (14) it is easy to show that

$$\frac{dG(x)}{dx} = \frac{\partial \xi}{\partial x} = \frac{C[G(x)]}{C[x]} \tag{18}$$

Working with the transformed variable ξ and using the fact that

$$P(\xi, t) d\xi = P(x, t) dx \tag{19}$$

we get

$$\begin{aligned}
 P(\xi, t) = & \lim_{n \rightarrow \infty} \frac{1}{(2\pi)^n} \int_{-\infty}^{\infty} \cdots \int_{-\infty}^{\infty} dk_{n-1} \cdots dk_1 dk d\xi_{n-1} \cdots d\xi_1 \\
 & \times \exp\{i[k_{n-1}G^{-1}(\xi_{n-1}) + \cdots + k_1G^{-1}(\xi_1) + ky]\} \\
 & \times \exp\{-a[k_{n-1}^2 + \cdots + k^2]\} \\
 & \times \exp\{-i[k_{n-1}\xi + \cdots + k\xi_1]\} \tag{20}
 \end{aligned}$$

Performing $\{k\}$ integrations, we get

$$\begin{aligned}
 P(\xi, t) = & \lim_{n \rightarrow \infty} \frac{1}{(4\pi a)^{n/2}} \int_{-\infty}^{\infty} \cdots \int_{-\infty}^{\infty} d\xi_{n-1} \cdots d\xi_1 \\
 & \times \exp\left(-\frac{1}{4a} \left\{ [\xi - G^{-1}(\xi_{n-1})]^2 \right. \right. \\
 & \left. \left. + [\xi_{n-1} - G^{-1}(\xi_{n-2})]^2 + \cdots + (\xi_1 - y)^2 \right\}\right) \tag{21}
 \end{aligned}$$

These are the main results of this paper. They are equivalent to the ones obtained via path integral formulation^(11,12) of the problem.

4. APPROXIMATE SOLUTION AND DISCUSSIONS

Equations (20) and (21) are the formal integral representations of the solution process. For evaluating these integrals approximations on the function G^{-1} is required. For the purpose of illustration we take a specific example widely studied in the context of passage from an unstable point, given by

$$C(x) = x - \frac{g}{\gamma} x^3 \tag{22}$$

For this case the nonlinear transformation $\xi = G(x)$ reads as

$$\xi = xe^{-b} / \left[1 - \frac{g}{\gamma} x^2(1 - e^{-2b}) \right]^{1/2} \tag{23a}$$

and

$$G^{-1}(\xi) = \xi e^b / \left[1 + \frac{g}{\gamma} \xi^2(e^{2b} - 1) \right]^{1/2} \tag{23b}$$

To a first order approximation in ξ , Eq. (23b) reduces to

$$G^{-1}(\xi) \simeq \xi e^b \tag{24}$$

Suzuki⁽⁷⁾ has demonstrated this approximation to be valid in the scaling limit (i.e., $\epsilon \rightarrow 0$ and b fixed). This result is true for any $C(x)$ with x as the

leading term.⁽⁷⁾ It is expedient to apply this approximation to Eq. (20). For this choice, the $\{\xi\}$ integrals turn out to be delta functions in $\{k\}$ which can be trivially handled. Carrying out the $\{k\}$ integrations of this expression and changing the argument of ξ to the actual time of interest γt , we get

$$P(\xi(\gamma t), t) = \left[2\pi \frac{\epsilon}{\gamma} (1 - e^{-2\gamma t}) \right]^{-1/2} \exp \left[-(\xi - y)^2 / \frac{2\epsilon}{\gamma} (1 - e^{-2\gamma t}) \right] \tag{25}$$

This result is the same as the scaling solution⁽⁷⁾ of Suzuki. Here also it is the presence of the small diffusion constant ϵ that permits us to arrive at this approximate solution. The connections between the scaling solution and the path integral result has already been established by Suzuki.⁽⁷⁾ Another remark we would like to make is that we do not throw away terms of order b^2 or higher. Though it may simplify algebra, we believe it will lead to erroneous results as can be easily seen with the example of the Ornstein–Uhlenbeck solution.

Suzuki obtains the above solution by a different approach. The essential idea there is that the transition from the unstable state is largely dictated by the initial fluctuations (since fluctuations are essential for the evolution of the system from the unstable steady state). However, in the intermediate time fluctuations are unimportant and the nonlinearity of the system “completely” determines the evolution. Suzuki’s idea is to go over from the original nonlinear Langevin equation to an equivalent linear equation (obtained via a nonlinear transformation to be discussed later) in which we have a multiplicative noise. The noise term is approximated in such a manner that the initial fluctuations are correctly taken care of. By this procedure the time evolution in the initial and intermediate time domain is fairly well represented.

Consider the nonlinear Langevin equation

$$\frac{dx}{dt} = \gamma C(x) + \eta(t) \tag{26}$$

where $\eta(t)$ is Gaussian and white. Let us now make a nonlinear transformation $G(x, t)$. Then

$$\frac{dG(x, t)}{dt} = \left[\gamma C(x) \frac{\partial G}{\partial x} + \frac{\partial G}{\partial t} \right] + \frac{\partial G}{\partial x} \eta(t) \tag{27}$$

We now demand the quantity in parentheses to be equal to zero

$$\gamma C(x) \frac{\partial G}{\partial x} + \frac{\partial G}{\partial t} = 0 \tag{28a}$$

The general solution of this partial differential equation is

$$G(x, t) = \phi(F(x) e^{-\gamma t}) \tag{28b}$$

where

$$F(x) = \exp \left[\int_{\beta}^x dx' / C(x') \right] \quad (28c)$$

The particular solutions for the initial condition $G(x, 0) = x$ is

$$G(x, t) = F^{-1}(F(x)e^{-\gamma t})$$

As shown by Suzuki,

$$\frac{\partial G}{\partial x} = e^{-\gamma t} + \text{higher order}$$

and hence it may be sufficient to truncate it to $e^{-\gamma t}$. In this case the resulting equation

$$\frac{dG}{dt} = e^{-\gamma t} \eta(t) \quad (29)$$

can be trivially solved and we get the so-called scaling solution. Here we have correctly incorporated the nonlinearity and initial fluctuations. This in turn guarantees satisfactory results in the initial and intermediate time domains. However, the fluctuations are absent asymptotically [see Eq. (29)] and hence it fails in that limit. At this stage it is worthwhile looking at the exact asymptotic solution

$$P(x, \infty) = \text{const} \times \exp \left[\frac{\gamma}{\epsilon} \int^x C(x') dx' \right] \quad (30)$$

Notice that the diffusion constant ϵ occurs in a nonanalytic fashion in Eq. (30). Thus it is clear that no finite-order perturbation theory can correctly represent the asymptotic solution. In this context it is pertinent that in principle we may make use of the two parameters in determining $G(x)$ which is the solution of a first-order partial differential equation in two variables [see Eq. (28a)]. For the particular choice of $G(x, 0) = x$, the function is independent of β . It may be interesting to investigate whether there exists a function G dependent on β so that we can impose the condition of correct asymptotic solution also, on the choice of β .

5. CONCLUSIONS

We have shown in this note that the application of Trotter's product formula leads to a straightforward derivation of the Ornstein-Uhlenbeck solution for a linear FPE. The method, when applied to the general nonlinear FPE, yields an integral representation, equivalent to that obtained via path integral formulation. This representation is amenable to approximation. In the lowest order approximation Suzuki's scaling result emerges. Physical interpretation and limitations of the approximation are discussed.

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