Journal of Statistical Physics, Vol. 15, No. 2, 1976

On the Path Integral Representation of Stochastic Processes

Kazuo Kitahara[1] and Horia Metiu[2]

Received November 25, 1976

We derive the path integral representation of the conditional probability for a Markovian process starting from the master equation. Existing derivations require both the variable and the transition probability to be extensive. We show that this requirement may be relaxed if Langer's formula for the transition probability is used. We prove that different path integral representations appearing in the literature are in fact equivalent and correspond to various choices of an arbitrary parameter.

KEY WORDS: Path integral; Markovian process; Langevin equation.

1. INTRODUCTION

Recently, Kubo, Matsuo, and Kitahara[1] (KMK) showed that in a thermodynamic system whose nonequilibrium evolution can be described by a Markovian master equation, the conditional probability $G(nt|n_0t_0)$ that an *extensive* thermodynamic variable has the value n at time t when starting at $t = t_0$ from the initial value n_0 can be written as a path integral,

$$G(nt|n_0t_0) = \int \mathcal{D}(n) \exp\left[\int_{t_0}^{t} ds\, L(n(s), \dot{n}(s))\right] \tag{1}$$

Here $\int \mathcal{D}(n)$ represents the path integration and $L(n, \dot{n})$ is a function of n and $\dot{n}$, which we shall call in what follows the Lagrangian. Such a representation of the conditional probability is useful; first, it is similar to the expression of the partition function in the renormalization group theory[2] and this similarity can be exploited to study the dynamics of critical phenomena.[3,4]

This work was supported in part by the National Science Foundation and the Office of Naval Research (Project SQUID).

[1] Department of Chemistry, Massachusetts Institute of Technology, Cambridge, Massachusetts.

[2] James Franck Institute, The University of Chicago, Chicago, Illinois.

© 1976 Plenum Publishing Corporation, 227 West 17th Street, New York, N.Y. 10011. No part of this publication may be reproduced, stored in a retrieval system, or transmitted, in any form or by any means, electronic, mechanical, photocopying, microfilming, recording, or otherwise, without written permission of the publisher.

Second, by maximizing the exponent $\int_{t_0}^{t} ds\, L(n, \dot{n})$, one can derive an equation for the most probable evolution of $n(t)$ in time.[5]

The representation (1) is based on the assumption that the transition probability in the master equation can be written as[1,6]

$$W(n \to n + a) = \Omega w(n/\Omega; a) \tag{2}$$

where the jump a, the scaled quantity n/Ω, and the function w are independent of the size Ω of the system. There are, however, situations in which this assumption is not valid; for example, in the case of a cluster growth in homogeneous nucleation,[5] the number of molecules in the cluster and the rate W are independent of the size Ω. Other such examples are various nonuniform systems for which the variables of interest are the densities (or some order parameter) at each point of the system.

The purpose of this paper is twofold. First we show that the path integral representation is possible when the assumption of Eq. (2) is not valid if W is given by[3]

$$W(n \to n + a) = \frac{\exp(-a^2/2\Delta)}{(2\pi\Delta)^{1/2}} \exp\{-\beta[F(n + a) - F(n)]/2\} \tag{3}$$

Here F is the free energy of the system, $\beta = 1/kT$, and Δ is a constant.

Second, we show that various existing path integral representations of G,[3,4,9] though derived from different starting points and looking quite different, are in fact equivalent with the one given here. This allows the use of the simplest among them and eliminates a potential cause of confusion.

Throughout this paper we restrict ourselves to the case of one variable. The infinite-variable case, describing nonuniform systems, can be discussed in a similar manner.[10]

2. PATH INTEGRAL REPRESENTATION OF THE CONDITIONAL PROBABILITY

We derive here the path integral representation of the conditional probability and show that if Δ in Eq. (3) is a small parameter, then the representation (1) is possible. To do this, we obtain the conditional probability $G(n, t + \Delta t | n_0, t)$ for a very short Δt. The result is given by Eq. (14). The smallness of Δ is used to ensure the convergence of various expansions. The conditional probability for arbitrary times can be computed from that at short times by using Eq. (15). This leads to the path integral representation [Eqs. (16)–(17) which has the desired form [Eq. (1)].

[3] The proof of the statement can be made if it is required that $W(n \to n + a)$ be a sharply peaked function of a. We prefer to use the specific Gaussian form Eq. (3) since it has been found useful in applications (see Refs. 3–5, 7, and 8).

We start with the master equation[1]

$$\tau\, \partial P(n, t)/\partial t = -H(n, \partial/\partial n)P(n, t) \tag{4}$$

with $H(n, \partial/\partial n)$ defined by

$$\begin{aligned} H(n, \partial/\partial n) &= \sum_a (1 - e^{-a\partial/\partial n})W(n \to n + a) \\ &= \sum_{m=1}^{\infty} (-1)^{m+1}(1/m!)(\partial/\partial n)^m \sum_a a^m W(n \to n + a) \end{aligned} \tag{5}$$

For small time intervals Δt, the change of the probability is

$$P(n, t + \Delta t) = \{1 - (\Delta t/\tau)H(n, \partial/\partial n)\}P(n, t) + O(\Delta t/\tau)^2 \tag{6}$$

Up to the order $O(\Delta t/\tau)$, Eq. (6) is equivalent to

$$\begin{aligned} P(n, t + \Delta t) = \{1 &- \mu(\Delta t/\tau)H(n, \partial/\partial n)\} \\ &\times \{1 - (1 - \mu)(\Delta t/\tau)H(n, \partial/\partial n)\}P(n, t) \\ &+ O(\Delta t/\tau)^2 \end{aligned} \tag{7}$$

For purposes of comparison with previous work, we have introduced an arbitrary parameter μ by adding and subtracting the same quantity. Assuming that $(\partial^k/\partial n^k)W(n \to n + a)P(n, t)$ vanishes sufficiently fast for large $|n|$ and for all k, we take the Fourier transform,

$$\begin{aligned} &\int_{-\infty}^{\infty} dn\, e^{-ikn}\{1 - (1 - \mu)(\Delta t/\tau)H(n, \partial/\partial n)\}P(n, t) \\ &\quad = \int_{-\infty}^{\infty} dn\, e^{-ikn}\{1 - (1 - \mu)(\Delta t/\tau)H(n, ik)\}P(n, t) \end{aligned} \tag{8}$$

Taking the inverse transform of Eq. (8) and putting it into Eq. (6) we obtain

$$\begin{aligned} P(n, t + \Delta t) = \{1 &- \mu(\Delta t/\tau)H(n, \partial/\partial n)\} \\ &\times (1/2\pi)\int_{-\infty}^{\infty} dk \int_{-\infty}^{\infty} dn_0\, e^{ik(n - n_0)}\{1 - (1 - \mu)(\Delta t/\tau)H(n_0, ik)\} \\ &\times P(n_0, t) + O(\Delta t/\tau)^2 \end{aligned} \tag{9}$$

For small $\Delta t/\tau$ we can approximate $1 - \alpha\, \Delta t/\tau \approx e^{-\alpha \Delta t/\tau}$ and, using Eq. (5), we have

$$\begin{aligned} P(n, t + \Delta t) = \int_{-\infty}^{\infty} dn_0 \Big\{ &(1/2\pi)\int_{-\infty}^{\infty} dk \exp[ik(n - n_0) - \mu(\Delta t/\tau) \\ &\times \sum_a \{W(n \to n + a) - [\exp(-ika)]W(n - a \to n)\} \\ &-(1 - \mu)(\Delta t/\tau)\sum_a [1 - \exp(-ika)]W(n_0 \to n_0 + a)]\Big\} \\ &\times P(n_0, t) + O(\Delta t/\tau)^2 \end{aligned} \tag{10}$$

So far we have not used the form (3) for the transition probability. For this choice of the transition probability we can compute

$$\sum_a (1 - e^{-ika}) W(n \to n + a)$$
$$= -(\langle a^2 \rangle / 2)[\beta ikF'(n) - k^2] + O(\langle a^4 \rangle) \tag{11}$$
$$\sum_a \{W(n \to n + a) - e^{-ika} W(n - a \to n)\}$$
$$= -(\langle a_2 \rangle / 2)[\beta F''(n) + \beta ikF'(n) - k^2] + O(\langle a^4 \rangle) \tag{12}$$

Inserting these functions into Eq. (10) and integrating over k, we obtain for the short-time evolution of the probability

$$P(n, t + \Delta t) = \int_{-\infty}^{\infty} dn_0 \, G(n, t + \Delta t | n_0, t) P(n_0, t) + O(\Delta t/\tau)^2 \tag{13}$$

where the kernel

$$G(n, t + \Delta t | n_0, t)$$
$$= \exp\left\{ - \frac{\tau}{2\langle a^2 \rangle} \Delta t \left[\frac{n - n_0}{\Delta t} + \frac{\langle a^2 \rangle}{2\tau} \beta F'(n_0)(1 - \mu) + \frac{\langle a^2 \rangle}{2\tau} \beta F'(n) \mu \right]^2 \right.$$
$$\left. + \frac{\langle a^2 \rangle}{2\tau} \Delta t \, \mu \beta F''(n) \right\} \tag{14}$$

is the conditional probability for the short time interval Δt.

For finite time intervals, we partition the time axis $t_0 < t_1 < \cdots < t_N = t$ and the conditional probability is

$$G(n, t | n_0, t_0) = \int dn_{N-1} \cdots \int dn_1 \, G(n, t | n_{N-1}, t_{N-1}) \cdots G(n_1, t_1 | n_0, t_0) \tag{15}$$

Using Eq. (14) for the conditional probabilities for small interval $t_j - t_{j-1} = \Delta t$ and taking the limit of $\Delta t \to 0$ (i.e., $N \to \infty$), we obtain

$$G(n, t | n_0, t_0) = \int \mathcal{D}(n) \exp\left[- \frac{\tau}{2\langle a^2 \rangle} \int_{t_0}^{t} ds \left\{ \left[\dot{n}(s) + \frac{\beta \langle a^2 \rangle}{2\tau} F'(n(s)) \right]^2 \right.\right.$$
$$\left.\left. - \left(\frac{\langle a^2 \rangle}{\tau} \right)^2 \mu \beta F''(n(s)) \right\} \right] \tag{16}$$

Thus the Lagrangian in Eq. (1) is

$$L(n, \dot{n}) = -(\tau/2\langle a^2 \rangle)\{[\dot{n} + (\beta \langle a^2 \rangle / 2\tau) F'(n)]^2 - (\langle a^2 \rangle / \tau)^2 \mu \beta F''(n)\} \tag{17}$$

We emphasize that the only difficulty in such calculations is finding a small parameter that ensures the convergence of all the expansions. In KMK the parameter is the Ω^{-1}, the inverse of the size of the system. In the

present case, it is essentially Δ—to be more precise, products of Δ and various derivatives of the free energy. The concrete expressions can be easily derived by analyzing the expansions. Physically, Δ is the largest change in n that has a finite probability [see Eq. (3)]. If the time scale τ in the master equation is small, Δ becomes small. Therefore Eq. (17) is accurate when the time scale is so small that Δ multiplied by the derivatives of the free energy is small.

3. COMPARISON WITH PREVIOUS WORK

The Lagrangian, Eq. (17), is not uniquely determined, because of the presence of the arbitrary parameter μ. We have introduced this parameter in going from Eq. (6) to Eq. (7) in such a manner that the resulting formulas will not depend on μ. All results corresponding to different choices of μ must therefore be equivalent. In what follows we show that different formulas derived in the literature for L correspond to different values of μ in Eq. (17). KMK[1] derived a formula corresponding to $\mu = 0$ [they used Eq. (2) for W]. Yahata[3] started from the Fokker–Planck equation and has derived a formula which, once adapted to our choice of W, corresponds to $\mu = 1$. Graham,[9] starting from a Langevin equation, obtains a formula, which, upon modification to correspond to our choice of W, corresponds to $\mu = 1/2$. The parameter μ, being at our disposal, can be chosen in the most convenient form for a given purpose. For example, if we want to obtain the most probable evolution, it is most convenient to choose $\mu = 0$. Then the Lagrangian (17) is a quadratic form and we see immediately that the most probable path is given by

$$\dot{n} + (\beta\langle a^2\rangle/2\tau)F'(n) = 0 \tag{18}$$

The arbitrariness of the Lagrangian (17) may be illustrated in a different manner for the simple example of a Gaussian process. Let us start from a Langevin equation

$$\dot{n}(t) + (\beta\langle a^2\rangle/2\tau)F'(n(t)) = f(t) \tag{19}$$

obtained from Eq. (18) by adding the Gaussian random force $f(t)$. If we assume that the random force is a Wiener process, we have for each path the weight [9,11]

$$P(f(s)) \prod_{t_0<s<t} df(s) = \exp\left[-(1/2\gamma)\int_{t_0}^{t} ds f^2(s)\right] \prod_{t_0<s<t} \left(\frac{\Delta t}{2\pi}\right)^{1/2} df(s) \tag{20}$$

The constant γ is introduced to give the variance of the random force

$$\langle f(s)f(s')\rangle = \gamma\delta(s - s') \tag{21}$$

The conditional probability of changing from n_0 to n is given by the path integral

$$G(n, t|n_0, t_0) = \int \mathscr{D}(f) \exp\left[-(1/2\gamma)\int_{t_0}^{t} ds f^2(s)\right] \tag{22}$$

In order to derive the equivalent of Eq. (16) for the process (19), we must change the variable of integration from $f(s)$ $(t_0 < s < t)$ to $n(s)$ $(t_0 < s < t)$. To do this, we discretize the time as

$$t_0 < t_1 < \cdots < t_{N-1} < t_N = t$$

and rewrite Eq. (19) as

$$\frac{n_{i+1} - n_i}{\Delta t} + \frac{\beta\langle a^2\rangle}{2\tau}[\mu F'(n_{i+1}) + (1 - \mu)F'(n_i)] = f_{i+1}, \qquad i = 0, 1, \ldots, N - 1 \tag{23}$$

with $n_i \equiv n(t_i)$, $f_i \equiv f(t_i)$, and $\Delta t \equiv t_{i+1} - t_i$. Indeed, for $\Delta t \to 0$, Eq. (23) is equivalent to Eq. (19). Equation (23) is the transformation of variables from f_i $(i = 1, 2, \ldots, N - 1)$ to n_i $(i = 1, 2, \ldots, N - 1)$ and the Jacobian is

$$\frac{\partial(f_1, f_2, \ldots, f_{N-1})}{\partial(n_1, n_2, \ldots, n_{N-1})} = \prod_{i=1}^{N-1} \frac{\partial f_i}{\partial n_i} \simeq \left(\frac{1}{\Delta t}\right)^{N-1} \exp\left[\Delta t \frac{\beta\langle a^2\rangle}{2\tau} \mu \sum_{i=1}^{N-1} F''(n_i)\right] \tag{24}$$

Introducing Eqs. (19) and (24) in Eq. (22), we obtain

$$G(n, t|n_0, t_0) \propto \int \mathscr{D}(n) \exp\left[(\beta\langle a^2\rangle/2\tau)\mu \int_{t_0}^{t} ds\, F''(n(s))\right] \times \exp\left\{-(1/2\gamma)\int_{t_0}^{t} ds[\dot{n}(s) + (\beta\langle a^2\rangle/2\tau)F'(n(s))]^2\right\} \tag{25}$$

This equation is the same as Eq. (16) ($\gamma = \langle a^2\rangle/\tau$) and again the parameter μ is arbitrary. The appearance of μ is due to the fact that there is no unique way of writing the discrete correspondent Eq. (23) of the continuous equation (19).

ACKNOWLEDGMENT

The authors are indebted to Prof. John Ross for stimulating discussions and for a critical reading of the manuscript.

REFERENCES

1. R. Kubo, K. Matsuo, and K. Kitahara, *J. Stat. Phys.* **9**:53 (1973).
2. Sheng Keng Ma, *Rev. Mod. Phys.* **45**:589 (1973); R. Brout, *Phys. Rep.* **10**:1 (1974); K. Wilson and J. Kogut, *Phys. Rep.* **12**:75 (1974).
3. H. Yahata, *Prog. Theor. Phys.* **52**:871 (1974).

4. C. DeDominicis, *Lett. Nuovo Cimento* **12**:567 (1975).
5. K. Kitahara, H. Metiu, and J. Ross, *J. Chem. Phys.* **63**:3156 (1975).
6. N. G. van Kempen, in *Fluctuation Phenomena in Solids*, R. E. Burgess, ed., Academic Press, New York (1965); *Adv. Chem. Phys.* **15**:65 (1969).
7. J. S. Langer, *Ann. Phys.* **54**:258 (1969); **65**:53 (1971).
8. H. Metiu, K. Kitahara, and J. Ross, *J. Chem. Phys.* **64**:292 (1976).
9. R. Graham, *Springer Tracts of Modern Physics, Vol. 66*, Springer, New York (1973), p. 1.
10. H. Metiu, J. Ross, and K. Kitahara, *J. Chem. Phys.*, to be published.
11. J. L. Doob, *Stochastic Processes*, Wiley, New York (1953); M. Kac, *Probability and Related Topics in Physical Sciences*, Interscience, New York (1957); I. M. Gelfand and A. M. Yaglom, *J. Math. Phys.* **1**:48 (1960); M. Lax, *Rev. Mod. Phys.* **38**:541 (1966).