Numerical Evaluation of Path Integrals

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A simple path integral formulation of Brownian motions is made on the basis of stochastic differential equations and the fundamental Cameron-Martin-Maruyama theorem. Besides a formal manipulation to relate the mathematical formulation with problems in nonequilibrium statistical physics, a numerical method is proposed to evaluate the path integrals explicitly. Models of linear and nonlinear diffusion processes are used to verify the usefulness of the numerical method.

1. Introduction

The path integral formulation of Brownian motions has been discussed by many authors [1-11]. However, there have been delicate problems in defining the probability measure for the integral.

As will be shown in this paper, it may be the most transparent way to formulate the theory of path integral on the basis of the Cameron-Martin-Maruyama theorem [12-13] on stochastic differential equations. After establishing a path integral theory, we give a numerical method to evaluate path integrals. This is a kind of Monte-Carlo method based on an importance sampling with using an interpolation formula which was devised in solving nonlinear ordinary differential equations [14].

To show the usefulness of our numerical method, we selected two examples, one from statistical physics and the other from theoretical biology. Analytic solutions are known for these examples, so that we can compare our numerical results with the exact solutions.

2. Basic theorem

As the preliminary for our formulation of path integrals, we summarize here mathematical notations and a basic result obtained in the theory of stochastic processes. Consider first a diffusion process

$$\mathrm{d}X(t)=\sigma(X(t))\mathrm{d}B(t)\,, \tag{2.1}$$

where $B(t)$ represents the Brownian motion, i.e. the Winer process. For the process $X(t)$ of (2.1), we have a corresponding equation

$$\frac{\partial}{\partial t}p_t f(x)=\Gamma^{(0)}(x)p_t f(x)\,, \tag{2.2}$$

where

$$\Gamma^{(0)}(x)=\frac{1}{2}\sigma(x)^2\frac{\partial^2}{\partial x^2} \tag{2.3}$$

is the generator of the process. In (2.2), $p_t f(x)$ is given by

$$p_t f(x)=\int p_t(x,\,\mathrm{d}x_t)f(x_t) \tag{2.4a}$$

$$=\int p(x,\,0|x_t,\,t)f(x_t)\mathrm{d}x_t\,, \tag{2.4b}$$

where $p_t(x,\varepsilon)$ is a transition probability to find X in a region ε at a time t with the initial condition $X(0)=x$. The function $p(x,0|x_t,t)$ is the corresponding probability density.

According to the theorem due to Cameron-Martin and Maruyama [12-13], the following equation, a slight generalization of (2.2),

$$\frac{\partial}{\partial t}P_t f(x)=\Gamma(x)P_t f(x) \tag{2.5}$$

with

$$\Gamma(x)=\frac{1}{2}\sigma(x)^2\frac{\partial^2}{\partial x^2}+b(x)\frac{\partial}{\partial x} \tag{2.6}$$

can be solved to give

$$P_t f(x)=E_x\{U(t)f(X(t))\}\,, \tag{2.7}$$

where

$$U(t)=\exp\left[\int_0^t\alpha(X(\tau))\mathrm{d}B(\tau)-\frac{1}{2}\int_0^t\alpha(X(\tau))^2\mathrm{d}\tau\right], \tag{2.8}$$

$\alpha(x)$ being defined by

$$\alpha(x)=\frac{b(x)}{\sigma(x)}\,. \tag{2.9}$$

In (2.7), $E_x\{\cdot\}$ is the symbol to take a conditional average with $X(0)=x$ over the process of (2.1): Namely, the solution of (2.2) is used to represent $E_x\{\cdot\}$ operation.

3. Formulation

(i) *Case of Ito equation*

According to the basic theorem of the previous section, the solution of an Ito type stochastic differential equation

$$\mathrm{d}X(t)=\sigma(X(t))\mathrm{d}B(t)+b(X(t))\mathrm{d}t\,, \tag{3.1}$$

which is equivalent to (2.5), is given by (2.7). In (2.7) and (2.8), $X(t)$ and $B(t)$ are related with each other through (2.1), and $E_x\{\cdot\}$ is the operation defined within a space spanned by solutions of the equation (2.1).

Our next task is to rewrite (2.7) into a more familiar form. The operation $E_x\{\cdot\}$ can be written in the form of path integral:

$$E_x\{\cdot\}=\lim_{N\to\infty}\prod_{j=1}^{N}\int \mathrm{d}x_j w(x_0, 0\,;\, x_1, t_1\,;\, \cdots\,;\, x_N, t_N)\{\cdot\}$$

$$(x_0=x,\ x_N=x_t,\ t_N=t)\,, \tag{3.2}$$

where $w(x_0, 0\,;\, x_1, t_1\,;\cdots;\, x_N, t_N)$ is the n-point joint probability: We have divided the time interval $(0, t)$ into N pieces with time points $(0, t_1, t_2, \cdots, t_N)$ and corresponding values of X are denoted by $(x_0, x_1, x_2, \cdots, x_N)$.

The n-point joint probability is nothing but the solution of (2.2). With the use of the path integral form of $E_x\{\cdot\}$, and after rewriting its integrand into the Stratonovich integral, we finally obtain

$$P_t f(x)=\int \mathscr{D}x \exp\left[-\int_0^t L_I(\dot{x}_\tau, x_\tau)\mathrm{d}\tau\right] f(x_t)\,, \tag{3.3}$$

where

$$\int \mathscr{D}x\cdot=\lim_{N\to\infty}\prod_{j=1}^{N}\int \frac{\mathrm{d}x_j}{\sqrt{2\pi\sigma(x_j)^2\Delta t_j}}\,. \tag{3.4}$$

and

$$L_I(\dot{x}, x)=\frac{1}{2\sigma(x)^2}\{\dot{x}-h(x)\}^2+\frac{1}{2}\sigma(x)\{h(x)/\sigma(x)\}'\,, \tag{3.5}$$

$h(x)$ being given by

$$h(x)=b(x)-\frac{1}{2}\sigma'(x)\sigma(x)\,. \tag{3.6}$$

The transition probability density is obtained from (3.3) by putting $f(x_t)$ to be a delta function:

$$P(x_0, 0|x_t, t)=\int \mathscr{D}'x \exp\left[-\int_0^t L_I(\dot{x}_\tau, x_\tau)\mathrm{d}\tau\right], \tag{3.7}$$

where

$$\int \mathscr{D}'x\cdot=\lim_{N\to\infty}\frac{1}{\sqrt{2\pi\sigma(x_N)^2\Delta t_N}}\prod_{j=1}^{N-1}\int \frac{\mathrm{d}x_j}{\sqrt{2\pi\sigma(x_j)^2\Delta t_j}}\cdot\,. \tag{3.8}$$

(ii) *Case of Stratonovich equation*

A Stratonovich type stochastic differential equation

$$\mathrm{d}X(t)=\sigma(X(t))\circ\mathrm{d}B(t)+b(X(t))\mathrm{d}t \tag{3.9}$$

is transformed into an Ito type equation

$$\mathrm{d}X(t)=\sigma(X(t))\mathrm{d}B(t)+\left\{b(X(t))+\frac{1}{2}\sigma'(X(t))\sigma(X(t))\right\}\mathrm{d}t\,. \tag{3.10}$$

The latter is equivalent to an equation of the form

$$\frac{\partial}{\partial t}P_t f(x)=\Gamma(x)P_t f(x) \tag{3.11}$$

where

$$\Gamma(x)=\frac{1}{2}\sigma(x)^2\frac{\partial^2}{\partial x^2}+\left\{b(x)+\frac{1}{2}\sigma'(x)\sigma(x)\right\}\frac{\partial}{\partial x}\,. \tag{3.12}$$

Thus we can obtain a solution of (3.11) from (3.3)~(3.5) by a simple substitution of

$$b(x)\longrightarrow b(x)+\frac{1}{2}\sigma'(x)\sigma(x)\,.$$

The result is as follows:

$$P_t f(x)=\int\mathcal{D}x\,\exp\left[-\int_0^t L_S(\dot{x}_\tau, x_\tau)\mathrm{d}\tau\right]f(x_t) \tag{3.13}$$

and

$$P(x, 0|x_t, t)=\int\mathcal{D}'x\,\exp\left[-\int_0^t L_S(\dot{x}_\tau, x_\tau)\mathrm{d}\tau\right], \tag{3.14}$$

where

$$L_S(\dot{x}, x)=\frac{1}{2\sigma(x)^2}\left\{\dot{x}-b(x)\right\}^2+\frac{1}{2}\sigma(x)\{b(x)/\sigma(x)\}'\,. \tag{3.15}$$

4. Numerical evaluation of path integrals

We have formulated a path integral theory in the previous sections. However, it is difficult to perform the path integrals explicitly. Usual treatments of the path integrals are, therefore, more or less approximate: Most of them are confined to the so-called extremum approximation where various possible paths are replaced by a single most probable path. This is a sort of mean field theory.

Instead, we propose here a numerical method to evaluate path integrals precisely. As is seen in the following examples, our method gives satisfactory results. Although the following procedure is equally applicable to the quantity $P_t f(x)$, we shall give explicit formulae for the probability density $P(x_0, 0|x_t, t)$.

It is convenient to transform the variable x into z such that

$$\mathrm{d}z=\mathrm{d}x/\sigma(x)\,. \tag{4.1}$$

Then we choose the probability density corresponding to an unperturbed part as

$$\frac{\partial}{\partial t} q(z, t) = \frac{1}{2} \frac{\partial^2}{\partial z^2} q(z, t) . \tag{4.2}$$

(i) *Case of Ito equation*

For the generator Γ, (2.6), of the Ito equation we have

$$\frac{\partial}{\partial t} Q(z, t) = \left\{ \frac{1}{2} \frac{\partial^2}{\partial z^2} + c_I(z) \frac{\partial}{\partial z} \right\} Q(z, t) , \tag{4.3}$$

where

$$c_I(z) \equiv h(x)/\sigma(x) , \tag{4.4}$$

$h(x)$ being defined by (3.6).

The quantities $P(x, 0|x_t, t)$ and $Q(z, 0|z_t, t)$ are related with each other through the relation:

$$\sigma(x_t) P(x, 0|x_t, t) = Q(z, 0|z_t, t) . \tag{4.5}$$

According to the theorem in section 2, (4.3) has a solution of the form

$$\begin{aligned} Q(z_0, 0|z_t, t) = &\lim_{N\to\infty} \int dz_1 \int dz_2 \cdots \int dz_{N-1} \\ &\times q(z_0, 0|z_1, t_1) \cdots q(z_{N-1}, t_{N-1}|z_N, t_N) \\ &\times \exp\left[\sum_{j=1}^{N} c_I(z_{j-1})(z_j - z_{j-1}) - \frac{1}{2} \sum_{j=1}^{N} c_I(z_{j-1})^2 (t_j - t_{j-1}) \right] , \end{aligned} \tag{4.6}$$

where we have put

$$z_N = z_t , \quad t_N = t \tag{4.7}$$

and

$$q(z_{j-1}, t_{j-1}|z_j, t_j) = \frac{1}{\sqrt{2\pi \Delta t_j}} \exp\left[-(z_j - z_{j-1})^2/(2\Delta t_j) \right] \tag{4.8}$$

is a solution of (4.2) and Δt_j is given by

$$\Delta t_j = t_j - t_{j-1} . \tag{4.9}$$

These relations, (4.6)~(4.8), provide a convenient basis for the numerical evaluation.

(ii) *Case of Stratonovich equation*

The probability density corresponding to (3.11) evolves in time according to

$$\frac{\partial}{\partial t} Q(z, t) = \left\{ \frac{1}{2} \frac{\partial^2}{\partial z^2} + c_S(z) \frac{\partial}{\partial z} \right\} Q(z, t) , \tag{4.10}$$

where

$$c_S(z) \equiv b(x)/\sigma(x) . \tag{4.11}$$

Similarly, we have a basic expression for the numerical evaluation in case of the Stratonovich equation (3.9):

$$Q(z_0, 0|z_t, t)=\lim_{N\to\infty}\int dz_1\int dz_2 \cdots \int dz_{N-1}$$
$$\times q(z_0, 0|z_1, t_1)\cdots q(z_{N-1}, t_{N-1}|z_N, t_N)$$
$$\times\exp\left[\sum_{j=1}^{N} c_S(z_{j-1})(z_j-z_{j-1})-\frac{1}{2}\sum_{j=1}^{N} c_S(z_{j-1})^2(t_j-t_{j-1})\right]. \quad (4.12)$$

If we can evaluate either (4.6) or (4.12) depending on the type of a stochastic differential equation, we find the probability density of the relevant variable X, namely, $P(x_0, 0|x_t, t)$ with the aid of (4.5).

In the following, a method to evaluate the basic formulas (4.6) and/or (4.12) is given:
In these expressions, (4.6) and (4.12), we find a product of transition probabilities $\{q(z_{j-1}, t_{j-1}|z_j, t_j)\}$ each of which has a Gaussian distribution (4.8).. Thus it seems at first that we have only to generate the Gaussian random numbers to produce random paths. However, this is an ineffective procedure because the final point (t, x_t) is fixed as well as the initial point $(0, x_0)$. Therefore, a desired random path must have the Gaussian property in each step and moreover must reach the final point.

These requirements are satisfied by adopting the following interpolation formula, which was used in solving nonlinear ordinary differential equations [14]:

$$z_j=\frac{z_{j-1}(t_N-t_j)+z_N(t_j-t_{j-1})}{t_N-t_{j-1}}+\xi\left[\frac{(t_N-t_j)(t_j-t_{j-1})}{t_N-t_{j-1}}\right]^{1/2} \quad (4.13a)$$

$$=\frac{z_{j-1}(N-j)+z_N}{N-(j-1)}+\xi\left[\frac{\Delta t(N-j)}{N-(j-1)}\right]^{1/2}, \quad (4.13b)$$

where ξ is a Gaussian random number of zero mean with $\langle\xi^2\rangle=1$. It is seen from (4.13a) that the point (t_j, z_j) is determined by the previous point (t_{j-1}, z_{j-1}) and the final point $(t_N, z_N)\equiv(t, z_t)$ in the following way: The first term of r.h.s. of (4.13) determines an average position $\langle\bar{z}_j\rangle$ on a line connecting (t_{j-1}, z_{j-1}) and (t_N, z_N). Fluctuations around $\langle\bar{z}_j\rangle$ is represented by the second term of (4.13) which is of the order $(\Delta t)^{1/2}$.

The true probability density should be given by (4.8), whereas the path represented by (4.13) is generated by the random number ξ assumed to have Gaussian distribution:

$$\frac{1}{\sqrt{2\pi}}e^{-\xi^2/2}.$$

In order to obtain the correct weight for a path, we must multiply the following correction factor for each step of the path:

$$\exp[-(z_j-z_{j-1})^2/(2\Delta t)]/\exp(-\xi^2/2).$$

Thus we can evaluate the transition probability density as

$$Q(z_0, 0|z_t, t)=\lim_{M\to\infty}\lim_{N\to\infty}\frac{1}{M}\sum_{k=1}^{M}\prod_{j=1}^{N}\exp[V(z_j{}^{(k)}, z_{j-1}{}^{(k)})], \tag{4.14}$$

where

$$V(z_j, z_{j-1})=\exp\Bigg[\alpha(z_{j-1})(z_j-z_{j-1})-\frac{1}{2}\alpha(z_{j-1})^2\Delta t - \frac{1}{2\Delta t}\left\{\frac{z_N-z_{j-1}}{N-(j-1)}\right\}^2-\frac{z_N-z_{j-1}}{\Delta t}\cdot\xi\left\{\frac{\Delta t(N-j)}{N-(j-1)}\right\}^{1/2} + \frac{\xi^2}{2(N-(j-1))}\Bigg]. \tag{4.15}$$

In (4.14), M is the total number of generated paths. In principle, this is a correct procedure. But in practice, we have to confine ourselves to finite values of M and N, so that it is better to normalize further by a quantity thus obtained

$$\int Q(z_0, 0|z_t, t)\mathrm{d}z_t.$$

The final result for $P(x_0, 0|x_t, t)$ is derived from (4.5).

Once the probability density is obtained, it is straightforward to find such a quantity like the time correlation functions.

5. Examples

It is instructive to apply the method of the path integral to physical and biological problems.

5-1. *Quasi-fixation model of genes*

We give here, as the first example, a model of the quasi-fixation of genes in the theory of genetics [15]. This is expressed by the following equation:

$$\mathrm{d}X(t)=\sqrt{V}X(t)[1-X(t)]\mathrm{d}B(t), \tag{5.1}$$

where X represents the relative frequency of a relevant gene; (5.1) is equivalent to the following forward equation

$$\frac{\partial}{\partial t}P(t)=\frac{V}{2}\frac{\partial^2}{\partial x^2}x^2(1-x)^2P(t), \tag{5.2}$$

which can be solved to give

$$P(x_0, 0|x_t, t)=\frac{1}{\sqrt{2\pi Vt}}\frac{\{x_0(1-x_0)\}^{1/2}}{\{x_t(1-x_t)\}^{3/2}}\exp\left[-\frac{Vt}{8}-\frac{L^2}{2Vt}\right], \tag{5.3}$$

where

$$L=\ln\frac{x_t(1-x_0)}{x_0(1-x_t)}. \tag{5.4}$$

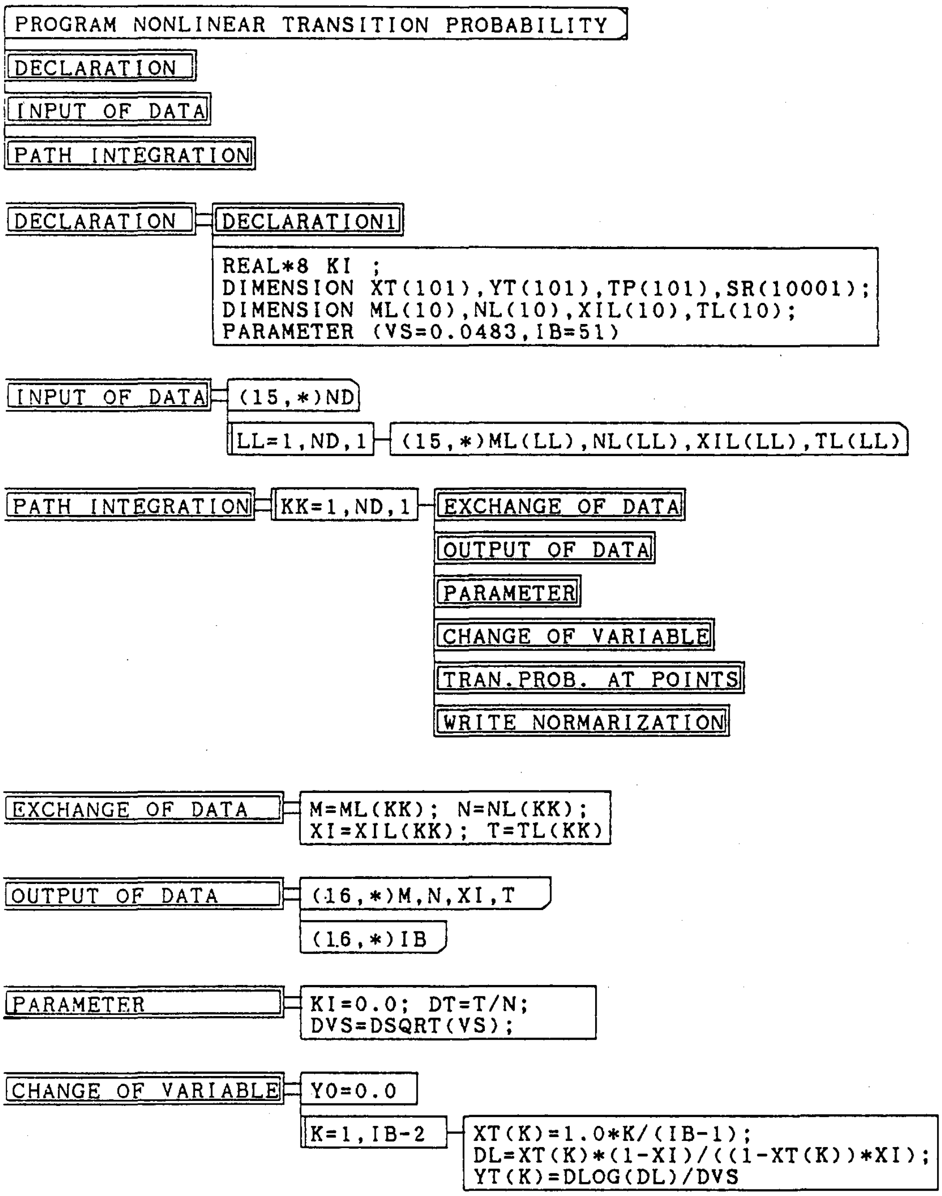

Fig. 1 PAD diagram for the quasi-fixation model of genes.

We compare the analytic solution (5.3) with our numerical path integral solution. Details of the numerical method are found in Fig. 1, where PAD (Problem Analysis Design) diagram is shown, and we list the FORTRAN source program below:

```
TRAN.PROB. AT POINTS ─ II=1,IB-2 ─ (*,*)' II= ',II
                                   TP(II)=0.0
                                   I=1,M,1 ─ BY=Y0;P=1.0
                                             GAUSS(SR,N)
                                             J=1,N,1 ─ PATH
                                                       WEIGHT
                                                       P=P*DEXP(V);
                                                       BY=Y
                                             TP(II)=TP(II)+P
                                   YA=DVS*XT(II)*(1-XT(II));
                                   TP(II)=TP(II)/YA;
                                   KI=KI+TP(II)/(IB-1)

                                   PATH ─ JJ=N-J;
                                          W=SR(J)*DSQRT(DT*JJ/(JJ+1));
                                          DYY=(YT(II)-BY)/(JJ+1);
                                          DY=DYY+W;   Y=BY+DY
                                   WEIGHT ─ V1=DR(BY)*DY;
                                            V2=-DR(BY)*DR(BY)*DT/2;
                                            V3=-DYY*DYY/(2*DT);
                                            V4=-W*DYY/DT;
                                            V5=SR(J)*SR(J)/(2*(JJ+1));
                                            V=V1+V2+V3+V4+V5

WRITE NORMARIZATION ─ K=1,IB-2,1 ─ TP(K)=TP(K)/KI
                                   (16,*)XT(K),TP(K)

DOUBLE PRECISION FUNCTION DR(Y)
DECLARATION1
RUN1
RETURN

DECLARATION1 ─ IMPLICIT REAL*8 (A-H,O-Z);
               OMMON  XI,DVS

RUN1 ─ EY=Y*DVS;
       DRR=XI*DEXP(EY);
       DR=DVS*(XI-1.0+DRR)/(2.0*(1.0-XI+DRR))
```

Fig. 1 (continued 1)

```
SUBROUTINE GAUSS(SR,N)
DECLARATION2
RUN2
RETURN

DECLARATION2 ─ IMPLICIT REAL*8 (A-H,O-Z);
               DIMENSION X(15),SR(10001),SR2(10001);
               SE=80629.0

RUN2 ─ L=1,N,1 ─ UNTIL(GG<1.0) ─ DURAND(SE,3,X)
                                 G1=2.0*X(1)-1.0;
                                 G2=2.0*X(2)-1.0;
                                 GG=G1*G1+G2*G2;
                                 SE=SE+50
                 SR(L)=G1*DSQRT(-2.0*DLOG(GG)/GG);
                 SR2(L)=SR(L)*G2/G1
```

Fig. 1 (continued 2)

Program list for quasi-fixation model

```
**************TRANSITION PROBABILITY IBM*****************
*       GAUSSIAN RANDOM NUMBER BY SHIBUYA METHOD        *
*        UNIFORM RANDOM NUMBER BY IBM LIBRARY           *
*********************************************************
        IMPLICIT REAL*8 (A-H,O-Z)
        REAL*8 KI
        DIMENSION XT(1001),YT(1001),TP(101),SR(10001)
        DIMENSION ML(10),NL(10),XIL(10),TL(10)
        PARAMETER (VS=0.0483)
        COMMON XI,DVS
        READ(15,*) ND
        READ(15,*) IB
        DO 12 LL=1,ND
         READ (15,*) ML(LL),NL(LL),XIL(LL),TL(LL)
12      CONTINUE
        DO 14 KK=1,ND
        M=ML(KK)
        N=NL(KK)
        XI=XIL(KK)
        T=TL(KK)
        WRITE(16,*) M,N,XI,T
        WRITE(16,*) IB
        KI=0.0
        DT=T/N
        DVS=DSQRT(VS)
        DO 30 K=1,IB-2
          XT(K)=1.0*K/(IB-1)
          DL=XT(K)*(1.0-XI)/((1.0-XT(K))*XI)
          YT(K)=DLOG(DL)/DVS
30      CONTINUE
        Y0=0.0
        DO 40 II=1,IB-2
          WRITE(*,*) ' II= ',II
          TP(II)=0.0
          DO 20 I=1,M
            BY=Y0
            P=1.0
            CALL GAUSS(SR,N)
            DO 10 J=1,N
                JJ=N-J
                W=SR(J)*DSQRT(DT*JJ/(JJ+1))
                DYY=(YT(II)-BY)/(JJ+1)
                DY=DYY+W
                Y=BY+DY
                V1=DR(BY)*DY
                V2=-DR(BY)*DR(BY)*DT/2
                V3=-DYY*DYY/(2*DT)
                V4=-W*DYY/DT
                V5=SR(J)*SR(J)/(2*(JJ+1))
                V=V1+V2+V3+V4+V5
                P=P*DEXP(V)
                BY=Y
10          CONTINUE
```

```
          TP(II)=TP(II)+P
20      CONTINUE
        YA=DVS*XT(II)*(1.0-XT(II))
        TP(II)=TP(II)/YA
        KI=KI+TP(II)/(IB-1)
40    CONTINUE
      DO 50 K=1,IB-2
        TP(K)=TP(K)/KI
        WRITE(16,*) XT(K),TP(K)
50    CONTINUE
14    CONTINUE
      STOP
      END
C
C************ DRIFT ***************************************

      REAL FUNCTION DR*8(Y)
      IMPLICIT REAL*8 (A-H,O-Z)
      COMMON XI,DVS
      EY=Y*DVS
      DRR=XI*DEXP(EY)
      DR=DVS*(XI-1.0+DRR)/(2.0*(1.0-XI+DRR))
      RETURN
      END
C
C************ GAUSSIAN RANDOM NUMBER BY SHIBUYA **********
C*            UNIFORM RANDOM NUMBER BY IBM               *
C*********************************************************
      SUBROUTINE GAUSS(SR,N)
      IMPLICIT REAL*8 (A-H,O-Z)
      DIMENSION X(15),SR(10001),SR2(10001)
      SE=80629.0
      DO 10 L=1,N
5      CALL DURAND(SE,2,X)
       G1=2.0*X(1)-1.0
       G2=2.0*X(2)-1.0
       GG=G1*G1+G2*G2
       IF(GG.GE.1.0) GO TO 5
       SR(L)=G1*DSQRT(-2.0*DLOG(GG)/GG)
       SR2(L)=SR(L)*G2/G1
       SE=SE+50.0
10     CONTINUE
       RETURN
       END
```

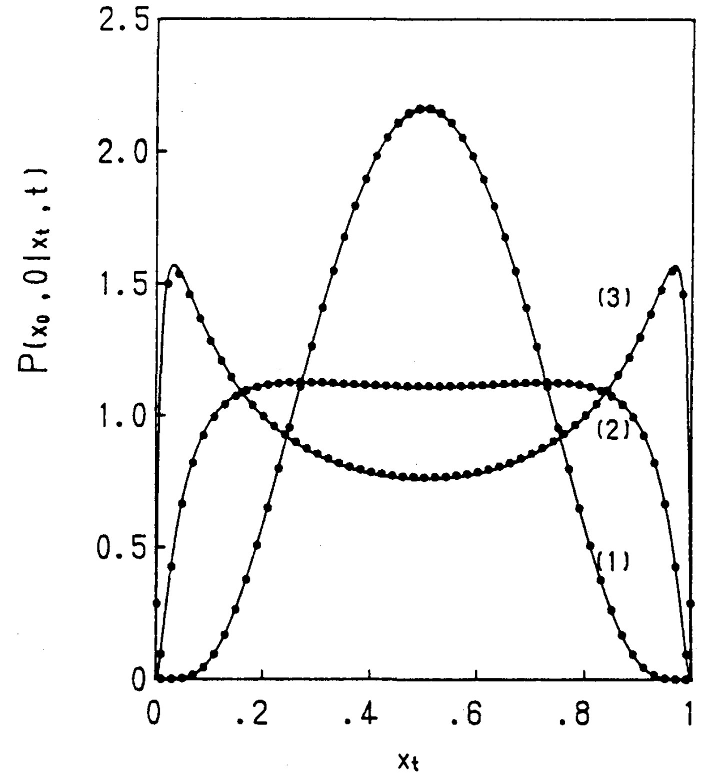

Fig. 2 Probability density in the case of example (i) ; $V=0.0483$, $x_0=0.5$. (1) : $t=10$, (2) : $t=30$, (3) : $t=50$ for $M=50$ and $N=100$ where M is the number of paths.

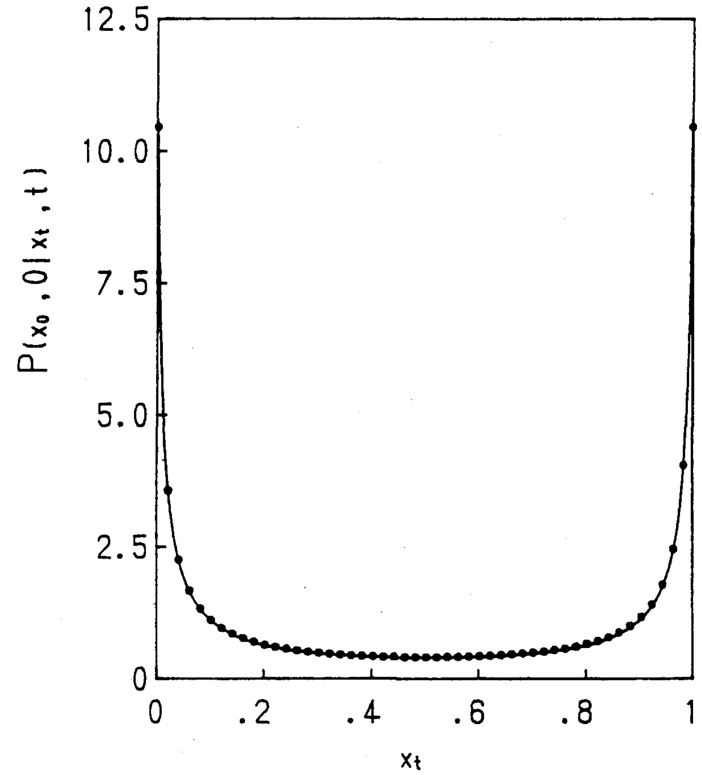

Fig. 3 The same graph as in Fig. 2 for $t=100$.

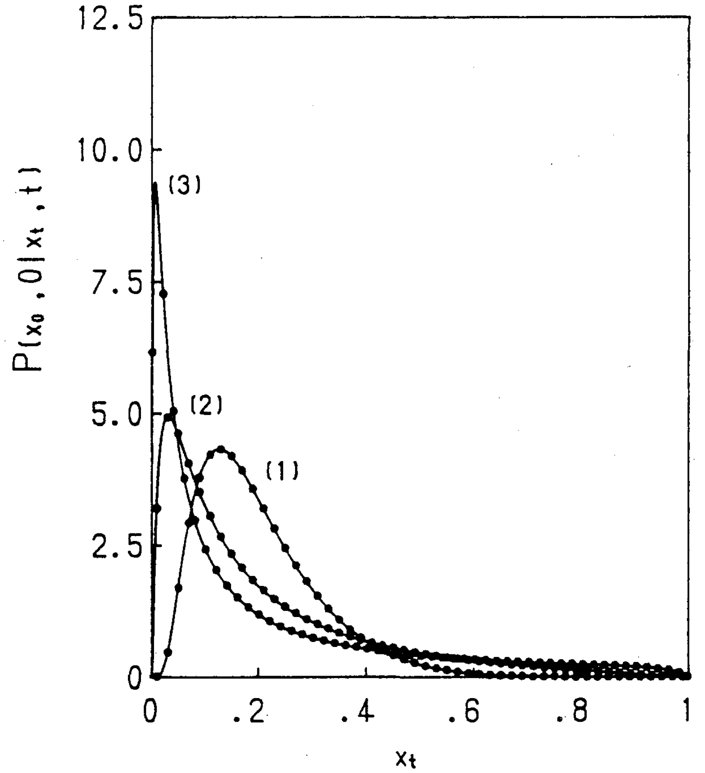

Fig. 4 Probability density in the case of example (i) ; $V=0.0483$, $x_0=0.2$. (1) : $t=10$, (2) : $t=30$, (3) : $t=50$ for $M=50$ and $N=100$.

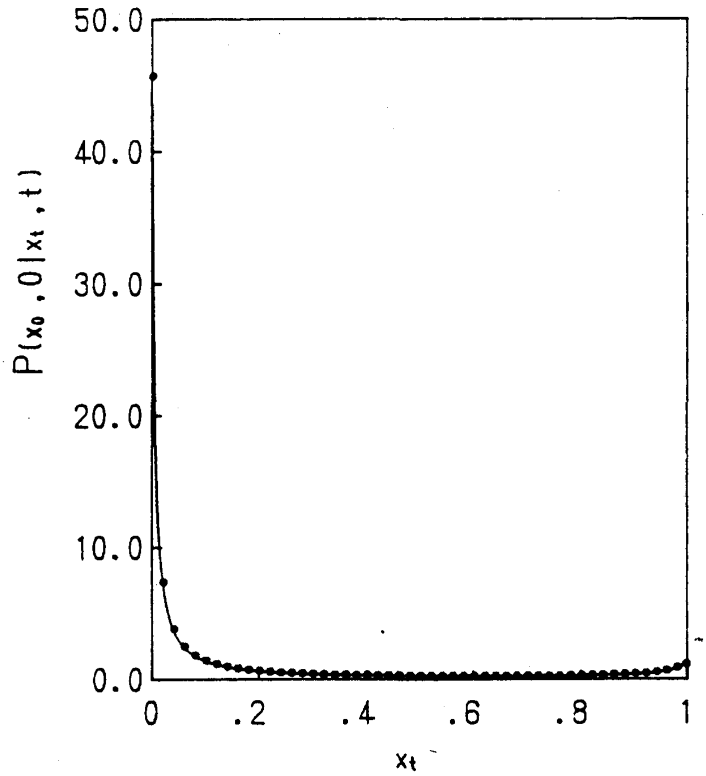

Fig. 5 The same graph as in Fig. 4 for $t=100$.

In figures 2~5, we show results of evaluations: the solid lines represent the analytic solution (5.3), whereas the dots are obtained by our method of numerical path integral, which gives excellent agreement with the former.

5-2. *Linear relaxation model*

The second example is afforded by a linear stochastic differential equation:

$$\mathrm{d}X(t)=\sqrt{2D}\,\mathrm{d}B(t)-\gamma X(t)\mathrm{d}t\,, \tag{5.5}$$

which has a solution of the form [4]:

$$P(x_0, 0|x_t, t)=\frac{1}{\sqrt{2\pi\rho(t)^2}}\exp\left[-\frac{(x_t-x_0e(t))^2}{2\rho(t)^2}\right], \tag{5.6}$$

where

$$e(t)=e^{-\gamma t} \tag{5.7}$$

and

$$\rho(t)=(D/\gamma)\{1-e(t)^2\}\,. \tag{5.8}$$

In figures 6 and 7, the solid lines represent the result from the analytic solution (5.6), while the dots are obtained by our numerical method of path integral. Irrespective of the initial conditions, our method gives satisfactory agreement with the analytic solution.

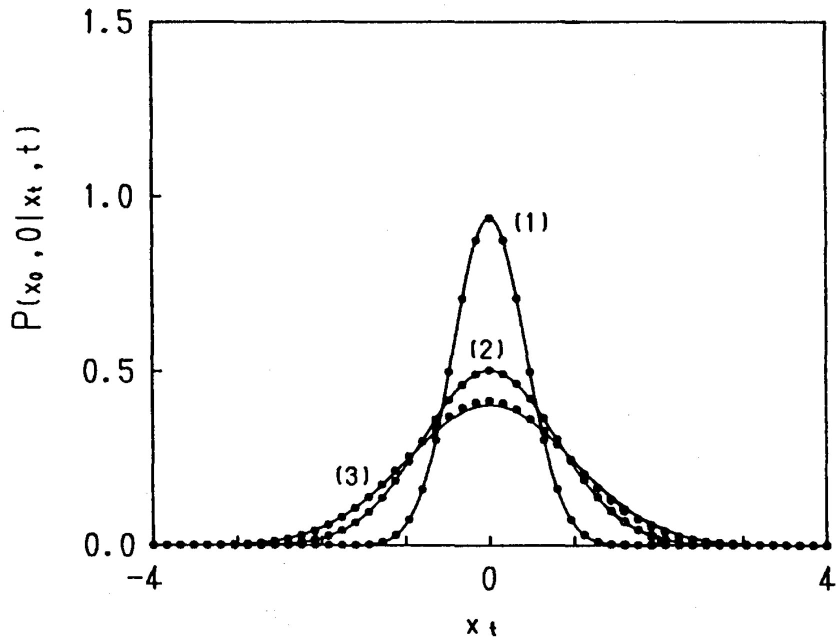

Fig. 6 Probability density in the case of example (ii) ; $\gamma=1$, $D=1$ and $x_0=0$. (1) : $t=0.1$ for $M=10$ and $N=100$. (2) : $t=0.5$ for $M=10$ and $N=100$. (3) : $t=2.0$ for $M=10$ and $N=500$.

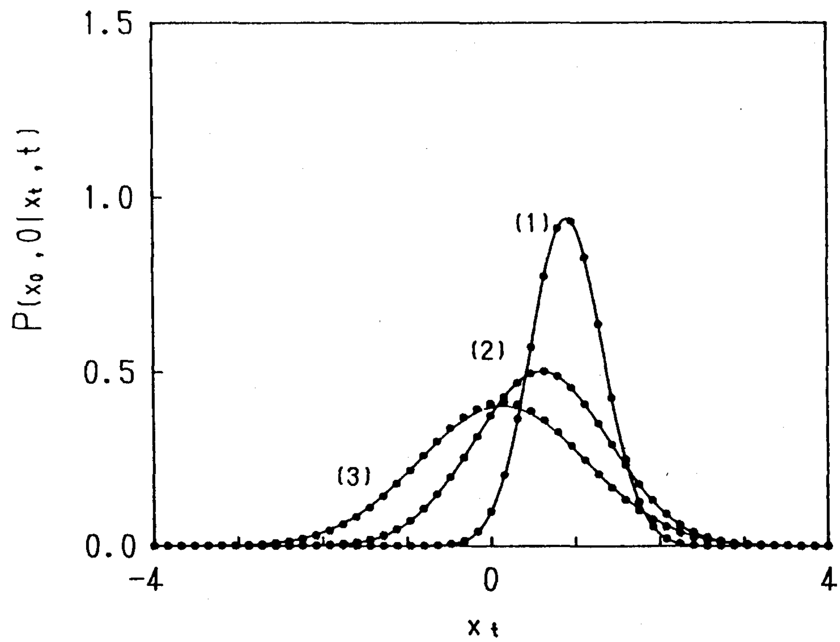

Fig. 7 Probability density in the case of example (ii) ; $\gamma=1$, $D=1$ and $x_0=1$. (1) : $t=0.1$, (2) : $t=0.5$, (3) : $t=2.0$ for $M=10$ and $N=100$.

We also gives a program list of the model as follows:

Program list for linear relaxation model.

```
********TRANSITION PROBABILITY IBM*********
         IMPLICIT REAL*8 (A-H,O-Z)
         REAL*8 KI
         DIMENSION XT(1001),YT(1001),TP(101),SR(10001)
         DIMENSION ML(10),NL(10),XIL(10),TL(10),IBL(10)
         PARAMETER (TAU=1.0,DP=1.0)
         READ(15,*) ND
         DO 12 LL=1,ND
          READ (15,*) ML(LL),NL(LL),XIL(LL),TL(LL)
          READ (15,*) IBL(LL)
12       CONTINUE
         DO 14 KK=1,ND
         M=ML(KK)
         N=NL(KK)
         XI=XIL(KK)
         T=TL(KK)
         IB=IBL(KK)
         WRITE(16,*) M,N,XI,T
         WRITE(16,*) IB
         KI=0.0
         DT=T/N
         DDP=DSQRT(DP)
         YA=DSQRT(2*DP)
         YO=XI/YA
         IB2=INT(0.5*(IB-1))
         DYT=4.0*DDP/IB2
         DO 40 II=1,IB
           WRITE(*,*) ' II= ',II
           YT(II)=DYT*(II-IB2-1)/YA+X0
           TP(II)=0.0
           DO 20 I=1,M
             BY=Y0
             P=1.0
             CALL GAUSS(SR,N)
             DO 10 J=1,N
                 JJ=N-J
                 W=SR(J)*DSQRT(DT*JJ/(JJ+1))
                 DYY=(YT(II)-BY)/(JJ+1)
                 DY=DYY+W
                 Y=BY+DY
                 S1=-BY*DY/TAU
                 S2=-BY*BY*DT/(2*TAU*TAU)
                 S3=-DYY*DYY/(2*DT)
                 S4=-W*DYY/DT
                 S5=SR(J)*SR(J)/(2*(JJ+1))
                 S=S1+S2+S3+S4+S5
                 P=P*DEXP(S)
                 BY=Y
10           CONTINUE
             TP(II)=TP(II)+P
20         CONTINUE
```

```
          TP(II)=TP(II)/YA
          KI=KI+TP(II)*DYT
40      CONTINUE
        DO 50 K=1,IB
          TP(K)=TP(K)/KI
          XT(K)=YT(K)*YA
          WRITE(16,*) XT(K),TP(K)
50      CONTINUE
14      CONTINUE
        STOP
        END
C************ GAUSSIAN RANDOM NUMBER BY SHIBUYA **********
C*               UNIFORM RANDOM NUMBER BY IBM             *
C*********************************************************
        SUBROUTINE GAUSS(SR,N)
        IMPLICIT REAL*8 (A-H,O-Z)
        DIMENSION X(15),SR(10001),SR2(10001)
        SE=80629.0
        DO 10 L=1,N
5        CALL DURAND(SE,3,X)
         G1=2.0*X(1)-1.0
         G2=2.0*X(2)-1.0
         GG=G1*G1+G2*G2
         IF(GG.GE.1.0) GO TO 5
         SR(L)=G1*DSQRT(-2.0*DLOG(GG)/GG)
         SR2(L)=SR(L)*G2/G1
C        SE=SE+50.0
10       CONTINUE
         RETURN
         END
```

6. Summary and conclusion

We have formulated a path integral theory on the basis of a mathematical theorem. We have presented not only the formalism but also the practical method of numerical evaluation of path integrals.

As was explicitly shown, our method gives satisfactory results for a nonlinear diffusion process as well as for a linear relaxation process. Usefulness of our theory will be further clarified when we apply the method to unsolved problems in statistical physics and other area of researches (for instance, the communication theory or the theoretical biology). These are left for our future study.

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