Natural Science Report, Ochanomizu University, Vol. 43, No. 1, 1992 25
お茶の水女子大学 自然科学報告 第43巻 第1号

Path Integral Theory of Brownian Motion

Fumiaki Shibata, Harumi Kawasaki*) and Miki Watabe)**

Department of Physics, Faculty of Science,
Ochanomizu University, Bunkyo-ku, Tokyo 112, Japan

(Received April 10, 1992)

On the basis of a mathematical theorem of stochastic processes, a path integral theory of Brownian motion is formulated. The abstract mathematical formula is transformed into a tractable path integral form. Besides formal manipulation, a practical method of evaluating the path integrals is presented and applied to linear and nonlinear problems of irreversible processes including Brownian motion of spins. Results are shown to be satisfactory.

1. Introduction

Many years ago the concept of path probability was introduced in the theoy of irreversible processes[1~3]. There have been a large literature on the subject[4~14]. We give here a systematic method of path integrals on the basis of a mathematical theorem. This may be the simplest and transparent way to formulate a path integral theory of Brownian motion.

In the first part of the paper (sections 2～3), we summarize rather formal aspects of the theory which lead to a "Lagrangian" formalism of the Brownian motion, some of which are already known. In the second part (sections 4～7), we propose a practical method of evaluating the path integrals and apply the method to linear and nonlinear problems of the irreversible processes including Brownian motion of spins.

A preliminary report[15] and numerical examples[16] have already been given.

2. Preliminaries

As the preliminary of path integrals, we summarize here mathematical notations and basic results in the theory of stochastic processes[17].

We consider a stochastic differential equation of Ito type:

$$dX(t)=\sigma(X(t))dB(t)+b(X(t))dt \tag{2.1}$$

*) Present address: Research and Development Center RICOH COMPANY, LTD. 16-1 Shinei-cho, Kohoku-ku, Yokohama, 223 Japan

**) Present address: Software Division RICOH COMPANY, LTD. 1-17, Koishikawa, 1-Chome, Tomin-Bldg 7F Bunkyo-ku, Tokyo, 112, Japan

where $\{B(t)\,;\ t\geqq 0\}$ is the Brownian motion, i.e., the Wiener process. This is equivalent to the following equation (backward equation):

$$\frac{\partial}{\partial t}P_t f(x)=\Gamma(x)P_t f(x) \tag{2.2}$$

where the generator $\Gamma(x)$ is given by

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

and

$$\begin{aligned} P_t f(x) &\equiv \int P_t(x, dx_t)f(x_t) \\ &= \int P(x,0|x_t,t)f(x_t)dx_t \\ &= \boldsymbol{E}_x(f(X(t)))\,. \end{aligned} \tag{2.4}$$

In (2.4), $P_t(x,\varepsilon)$ is the transition probability and $P(x,0|x_t,t)$ the corresponding probability density. The last expression of (2.4) represents the conditional average of an arbitrary function $f(X(t))$.

A quantity $\tilde{\Gamma}$ conjugate to Γ satisfying

$$\int(\tilde{\Gamma}(x)f(x))g(x)dx=\int f(x)(\Gamma(x)g(x))dx \tag{2.5}$$

is given by

$$\tilde{\Gamma}(x)\cdot=\left\{\frac{\partial^2}{\partial x^2}\frac{1}{2}\sigma(x)^2-\frac{\partial}{\partial x}b(x)\right\}. \tag{2.6}$$

We note that the Fokker-Planck type equation (forward equation) is written in the form

$$\frac{\partial}{\partial t}P(x_t,t)=\tilde{\Gamma}(x_t)P(x_t,t)\,. \tag{2.7}$$

Thus it is equivalent to solve (2.2) in stead of the Fokker-Planck type equation (2.7) as far as the probability density exists.

To solve (2.2) or (2.7), the following theorem (Cameron-Martin[18], Maruyama[19], Girsanov[20]) plays an essential role:

A formal solution of (2.2) is given by

$$P_t f(x)=\boldsymbol{E}_x(Z_t f(X(t))) \tag{2.8}$$

where

$$Z_t=\exp\left[\int_0^t\gamma(X(\tau))dB(\tau)-\frac{1}{2}\int_9^t\gamma(X(\tau))^2d\tau\right] \tag{2.9}$$

with

$$\gamma(x)=\sigma(x)^{-1}b(x)\,. \tag{2.10}$$

A symbol $\boldsymbol{E}_x$ represents an average over a stochastic procss having the following generator :

$$\Gamma^{(0)}(x)\cdot=\frac{1}{2}\sigma(x)^2\frac{\partial^2}{\partial x^2}\cdot \tag{2.11}$$

These are generalized to multi-dimensional systems. For a stochastic differential equation

$$d\boldsymbol{X}(t)\underline{\sigma}(\boldsymbol{X}(t))d\boldsymbol{B}(t)+\boldsymbol{b}(\boldsymbol{X}(t))dt \tag{2.12}$$

we have

$$\frac{\partial}{\partial t}P_t f(\boldsymbol{x})=\Gamma(\boldsymbol{x})P_t f(\boldsymbol{x}) \tag{2.13}$$

where $\boldsymbol{X}(t), \boldsymbol{B}(t), \boldsymbol{b}(\boldsymbol{X}(t))$ and $\boldsymbol{x}$ are vectors and $\underline{\sigma}(\boldsymbol{X}(t))$ is a tensor. The generator in (2.13) is giveu by

$$\Gamma(\boldsymbol{x})=\sum_{i,j}D(\boldsymbol{x})_{ij}\frac{\partial^2}{\partial x_i\partial x_j}+\sum_i b(\boldsymbol{x})_i\frac{\partial}{\partial x_i} \tag{2.14}$$

where the diffusion "constant" is given by

$$D(\boldsymbol{x})_{ij}=\frac{1}{2}\sum_k\underline{\sigma}(\boldsymbol{x})_{ik}\underline{\sigma}(\boldsymbol{x})_{jk} \tag{2.15}$$

Then the theorem states that (2.13) is solved to give

$$P_t(\boldsymbol{x})=\boldsymbol{E}_x(Z_t f(\boldsymbol{X}(t))) \tag{2.16}$$

where

$$Z_t=\exp\left[\int_0^t\sum_i\gamma(\boldsymbol{X}(\tau))_i dB(\tau)_i-\frac{1}{2}\int_0^t\sum_i\gamma(\boldsymbol{X}(\tau))_i{}^2 d\tau\right] \tag{2.17}$$

and

$$\gamma(\boldsymbol{X}(t))=\underline{\sigma}(\boldsymbol{X}(t))^{-1}\boldsymbol{b}(\boldsymbol{X}(t))\,. \tag{2.18}$$

The symbol $\boldsymbol{E}_x$ represents a stochastic average over a process with the generator

$$\Gamma^{(0)}(\boldsymbol{x})=\sum_{i,j}D(\boldsymbol{x})_{ij}\frac{\partial^2}{\partial x_i\partial x_j}\,. \tag{2·19}$$

These results will play important roles in our subsequent development.

3. Path Integrals

The backward equation (2.2) and (2.14) are solved in the form of (2.8) and (2.16), respectively. However, these are rather formal and therefore are of little practical use. In the following we transform the formulas of section 2 into more tractable ones, namely, into the form of path integrals.

As was shown in the previous section, a stochastic differential equation

$$dX(t)=\sigma(X(t))dB(t)+b(X(t))dt \tag{3.1}$$

has a corresponding generator $\Gamma(x)$, (2.3), and is equivalent to the Fokker-Planck equation

$$\frac{\partial}{\partial t}P(x_t, t)=\tilde{\Gamma}(x_t)P(x_t, t), \tag{3.2}$$

$\tilde{\Gamma}(z)$ being given by (2.6).

By a change of variable[21)]

$$dy=\sigma(x)^{-1}dx \tag{3.3}$$

we can transform (3.2) into

$$\frac{\partial}{\partial t}Q(y, t)=\tilde{A}(y)Q(y, t) \tag{3.4}$$

where

$$Q(y, t)=\sigma(x)P(x, t) \tag{3.5}$$

and

$$\tilde{A}(y)\equiv\frac{1}{2}\frac{\partial^2}{\partial y^2}-\frac{\partial}{\partial y}c_I(y) \tag{3.6}$$

with

$$c_I(y)=\sigma(x)^{-1}\left[b(x)-\frac{1}{2}\sigma(x)'\sigma(x)\right], \tag{3.7}$$

Thus we find a generator of the form

$$A(y)=\frac{1}{2}\frac{\partial^2}{\partial y^2}+c_I(y)\frac{\partial}{\partial y} \tag{3.8}$$

and a corresponding stochastic differential equation

$$dY(t)=dB(t)+c_I(Y(t))dt. \tag{3.9}$$

Applying the theorem (2.8) to the system of (3.8)~(3.9), we have

$$\begin{aligned} Q_t f(y)&=\boldsymbol{E}_y(Z_t f(Y(t))) \\ &=\int Q(y, 0|y_t, t) f(y_t)dy_t \end{aligned} \tag{3.10}$$

where

$$Z_t=\exp\left[\int_0^t c_I(Y(\tau))dB(\tau)-\frac{1}{2}\int_0^t c_I(Y(\tau))^2 d\tau\right]. \tag{3.11}$$

Consequently the probability density is found to be

$$\begin{aligned} Q(y, 0|y_t, t)=\lim_{N\to\infty}\prod_{j=1}^{N-1}\int dy_j Q^{(0)}(y_{j-1}, t_{j-1}|y_j, t_j)\times Q^{(0)}(y_{N-1}, t_{N-1}|y_N, t_N) \\ \times\exp\left[\int_0^t c_I(Y(\tau))dB(\tau)-\frac{1}{2}\int_0^t c_I(Y(\tau))^2 d\tau\right], \end{aligned} \tag{3.12}$$

where $y_0=y$ and $y_N=y_t$. In (3.12), $Q^{(0)}$ is a solution of the equation with the generator

$$A^{(0)}(y)=\frac{1}{2}\frac{\partial^2}{\partial y^2} \tag{3.13}$$

that is, $Q^{(0)}$ is given by

$$Q^{(0)}(y_{j-1}, t_{j-1}|y_j, t_j)=\frac{1}{\sqrt{2\pi\Delta t_j}}\exp[-(y_j-y_{j-1})^2/(2\Delta t_j)] \tag{3.14}$$

which determines the conditional average $\boldsymbol{E}_y(\cdot)$.

We further transform (3.12) into more familiar form. First we rewrite the conditional average $\boldsymbol{E}_y$ as

$$\boldsymbol{E}_y(\cdot)=\int \boldsymbol{D}y_\tau \exp\left[-\frac{1}{2}\int_9^t \dot{y}_\tau{}^2 d\tau\right] \tag{3.15}$$

where

$$\int \boldsymbol{D}y_\tau\cdot=\lim_{N\to\infty}\prod_{j=1}^{N}\int\frac{1}{\sqrt{2\pi\Delta t_j}}dy_j\cdot \tag{3.16}$$

and use has been made of

$$\lim_{N\to\infty}\sum_{j=1}^{N}\exp[(y_j-y_{j-1})/\Delta t_j]^2\Delta t_j=\int_0^t \dot{y}_\tau{}^2 d\tau\,. \tag{3.17}$$

The first Ito integral in the exponential function of (3.12) is written in terms of the usual (Stratonovich) integral by the formula:

$$\int_0^t \Phi(X(\tau))\circ dB(\tau)=\int_0^t \Phi(X(\tau))dB(\tau)+\frac{1}{2}\int_0^t \sigma(X(\tau))\Phi'(X(\tau))d\tau$$

Thus we have

$$Q_t f(y)=\int \boldsymbol{D}y_\tau \exp\left[-\int_0^t L_I(y_\tau, \dot{y}_\tau)d\tau\right]f(y_t) \tag{3.18}$$

and

$$Q(y_0, 0|y_t, t)=\int \boldsymbol{D}'y_\tau \exp\left[-\int_0^t L_I(y_\tau, \dot{y}_\tau)d\tau\right] \tag{3.19}$$

where

$$L_I(y, \dot{y})=\frac{1}{2}\{\dot{y}-c_I(y)\}^2+\frac{1}{2}c'_I(y) \tag{3.20}$$

and

$$\int \boldsymbol{D}'y_\tau\cdot=\lim_{N\to\infty}\frac{1}{\sqrt{2\pi\Delta t_N}}\prod_{j=1}^{N-1}\int\frac{1}{\sqrt{2\pi\Delta t_j}}dy_j\cdot\,. \tag{3.21}$$

In terms of the original variable x, the path integral solutions are given by

$$P_t f(x)=\int \boldsymbol{D}x_\tau \exp\left[-\int_0^t L_I(x_\tau, \dot{x}_\tau)d\tau\right]f(x_t) \tag{3.22}$$

and

$$P(x_0, 0|x_t, t)=\int \boldsymbol{D}'x_\tau \exp\left[-\int_0^t L_I(x_\tau, \dot{x}_\tau)d\tau\right] \tag{3.23}$$

where

$$L_I(x, \dot{x})=\frac{1}{2\sigma(x)^2}\{\dot{x}-h(x)\}^2+\frac{1}{2}\sigma(x)\left\{\frac{h(x)}{\sigma(x)}\right\}' \tag{3.24}$$

with

$$h(x)=b(x)-\frac{1}{2}\sigma'(x)\sigma(x)\,. \tag{3.25}$$

This is a known result[5].

In these expressions the path integrals are of the form

$$\int \boldsymbol{D}x_\tau\cdot=\lim_{N\to\infty}\prod_{j=1}^{N}\int\frac{1}{\sqrt{2\pi\sigma(x_j)^2\Delta t_j}}dx_j\cdot \tag{3.26}$$

and

$$\int \boldsymbol{D}'x_\tau\cdot=\lim_{N\to\infty}\frac{1}{\sqrt{2\pi\sigma(x_N)^2\Delta t_N}}\prod_{j=1}^{N-1}\int\frac{1}{\sqrt{2\pi\sigma(x_j)^2\Delta t_j}}dx_j\cdot\,. \tag{3.27}$$

In deriving these results we used (3.3) and (3.5).

The Stratonovich stochastic differential equation

$$dX(t)=\sigma(X(t))^\circ dB(t)+b(X(t))dt \tag{3.28}$$

is equivalent to the following Ito equation:

$$dX(t)=\sigma(X(t))dB(t)+\left\{b(X(t))+\frac{1}{2}\sigma'((X(t))\sigma((X(t))\right\}dt \tag{3.29}$$

and therefore we have only to make a replacement

$$b(X(t)) \longrightarrow b(X(t))+\frac{1}{2}\sigma'(X(t))\sigma(X(t)) \tag{3.30}$$

in the preceding results.

We have thus

$$P(x_0, 0|x_t, t)=\int \boldsymbol{D}'x_\tau \exp\left[-\int_0^t L_S(x_\tau, \dot{x}_\tau)d\tau\right] \tag{3.31}$$

and so on. In (3.31), L_S is given by

$$L_S(x, \dot{x})=\frac{1}{2\sigma(x)^2}\{\dot{x}-b(x)\}^2+\frac{1}{2}\sigma(x)\left\{\frac{b(x)}{\sigma(x)}\right\}'\,. \tag{3.32}$$

For the multi-dimensional Ito equation

$$d\boldsymbol{X}(t)=\sigma(\boldsymbol{X}(t))d\boldsymbol{B}(t)+b(\boldsymbol{X}(t))dt \tag{3.33}$$

we have

$$P(\boldsymbol{x}_0, 0|\boldsymbol{x}_t, t)=\int \boldsymbol{D}'\boldsymbol{x}_\tau \exp\left[-\int_0^t L_I(\boldsymbol{x}_\tau, \dot{\boldsymbol{x}}_\tau)d\tau\right] \tag{3.34}$$

where

$$L_I(\boldsymbol{x}, \dot{\boldsymbol{x}}) = \frac{1}{2}(\dot{\boldsymbol{x}} - \boldsymbol{h}(\boldsymbol{x})) \cdot (2D(\boldsymbol{x}))^{-1} \cdot (\dot{\boldsymbol{x}} - \boldsymbol{h}(\boldsymbol{x}))$$

$$+ \frac{1}{2}\sum_{k,l}\sigma(\boldsymbol{x})_{kl}\frac{\partial}{\partial x_l}\sum_m(\sigma(\boldsymbol{x})^{-1})_{km}h(\boldsymbol{x})_m \tag{3.35}$$

and

$$h(\boldsymbol{x})_i = b(\boldsymbol{x})_i - \frac{1}{2}\sum_{j,k}\frac{\partial\sigma(\boldsymbol{x})_{ik}}{\partial x_j}\sigma(\boldsymbol{x})_{jk} \tag{3.36}$$

with

$$D(\boldsymbol{x}) = \frac{1}{2}\sigma(\boldsymbol{x})\sigma(\boldsymbol{x})^T \tag{3.37}$$

Similarly, for the Stratonovich equation

$$d\boldsymbol{X}(t) = \sigma(\boldsymbol{X}(t))^{\circ}d\boldsymbol{B}(t) + \boldsymbol{b}(\boldsymbol{X}(t))dt \tag{3.38}$$

we find

$$P(\boldsymbol{x}_0, 0|\boldsymbol{x}_t, t) = \int \boldsymbol{D}'\boldsymbol{x}_\tau \exp\left[-\int_0^t L_S(\boldsymbol{x}_\tau, \dot{\boldsymbol{x}}_\tau)d\tau\right] \tag{3.39}$$

where

$$L_S(\boldsymbol{x}, \dot{\boldsymbol{x}}) = \frac{1}{2}(\dot{\boldsymbol{x}} - \boldsymbol{b}(\boldsymbol{x})) \cdot (2D(\boldsymbol{x}))^{-1} \cdot (\dot{\boldsymbol{x}} - \boldsymbol{b}(\boldsymbol{x}))$$

$$+ \frac{1}{2}\sum_{k,l}\sigma(\boldsymbol{x})_{kl}\frac{\partial}{\partial x_l}\sum_m(\sigma(\boldsymbol{x})^{-1})_{km}b(\boldsymbol{x})_m\,. \tag{3.40}$$

These are the straightforward generalizations of the single variable results.

4. Method of Numerical Evaluation of Path Integrals

Although the results of section 3 are rather formal, they have own right in connection with the long historical development in irreversible statistical mechanics since the pioneering work of Onsager-Machlup[1] and Hashitsume[2].

Besides this, we give here a practical numerical method of evaluating the path integrals which is quite useful when we treat nonlinear problems in Brownian motion.

For this puppose it is convenient to use (3.12) in the following form

$$Q(y, 0|y_t, t) = \lim_{N\to\infty}\prod_{j=1}^{N-1}\int dy_j Q^{(0)}(y_{j-1}, t_{j-1}|y_j, t_j) \times Q^{(0)}(y_{N-1}, t_{N-1}|y_N, t_N)$$

$$\times \exp\left[\sum_{j=1}^{N}\left\{c_I(y_{j-1})(y_j - y_{j-1}) - \frac{1}{2}c_I(y_{j-1})^2(t_j - t_{j-1})\right\}\right] \tag{4.1}$$

where$Q^{(0)}$ has been given by (3.14).

We must calculate (4.1) by fixing y and y_t during time interval $[0, t]$. It is useful in practical calculations to take advantage of an interpolation method[22] which was originally devised in solving ordinary differential equations :

$$y_j=\frac{y_{j-1}(t_N-t_j)+y_N(t_j-t_{j-1})}{t_N-t_{j-1}}+\xi\left[\frac{(t_N-t_j)(t_j-t_{j-1})}{t_N-t_{j-1}}\right]^{1/2}$$

$$=\frac{y_{j-1}(N-j)+y_N}{N-(j-1)}+\xi\left[\frac{\Delta t(N-j)}{N-(j-1)}\right]^{1/2} \tag{4.2}$$

where ξ is a Gaussian random number with zero mean and variance of unity. In the original expression (4.1), the path is generated with the probability density

$$\frac{1}{\sqrt{2\pi\Delta t}}\exp[-(y_j-y_{j-1})^2/(2\Delta t)] \tag{4.3}$$

whereas the path is weighted by

$$\frac{1}{\sqrt{2\pi\Delta t}}\exp[-(\xi\Delta t)^2/(2\Delta t)] \tag{4.4}$$

when (4.2) is used. Thus we must multiply the ratio of (4.3) and (4.4) in each time step.

Then (4.1) becomes

$$Q(y,0|y_t,t)=\lim_{M\to\infty}\lim_{N\to\infty}\frac{1}{M}\sum_{m=1}^{M}\prod_{j=1}^{N}\exp[V(y_j^{(m)},y_{j-1}^{(m)})] \tag{4.5}$$

where

$$V(y_j,y_{j-1})=c_I(y_{j-1})(y_j-y_{j-1})-c_I(y_{j-1})^2\Delta t/2$$
$$-\left(\frac{y_N-y_{j-1}}{N-(j-1)}\right)^2\Big/(2\Delta t)-\frac{y_N-y_{j-1}}{\Delta t(N-(j-1))}\cdot\xi\left\{\frac{\Delta t(N-j)}{N-(j-1)}\right\}^{1/2}$$
$$+\frac{\xi^2}{2(N-(j-1))} \tag{4.6}$$

and the superscript (m) on y_j specifies M different paths.

We finally obtain the desired probability density (3.3):

$$\sigma(x_t)P(x,0|x_t,t)=Q(y,0|y_t,t)\,. \tag{4.7}$$

In actual calculations, we normalize P by

$$\int P(x,0|x_t,t)dx_t\,, \tag{4.8}$$

because M is finite.

For the Stratonovich equation, we have only to make a substitution:

$$c_I(y_{j-1})\longrightarrow c_S(y_{j-1}) \tag{4.9}$$

where c_I has been defined by (3.7) and

$$c_S(y)=b(x)/\sigma(x)\,. \tag{4.10}$$

Generalization of (4.5) to the multi-dimensional system is straightforward:

$$Q(\boldsymbol{y},0|\boldsymbol{y}_t,t)=\lim_{M\to\infty}\lim_{N\to\infty}\frac{1}{M}\sum_{m=1}^{M}\prod_{j=1}^{N}\exp\left[\sum_{k=1}^{d}V(\boldsymbol{y}_j{}^{(m)},\boldsymbol{y}_{j-1}{}^{(m)})_k\right] \tag{4.11}$$

where

$$\begin{aligned}V(\boldsymbol{y}_j,\boldsymbol{y}_{j-1})_k=&c_I(\boldsymbol{y}_{j-1})_k(\boldsymbol{y}_j-\boldsymbol{y}_{j-1})_k-c_I(\boldsymbol{y}_{j-1})_k{}^2\Delta t/2\\&-\left(\frac{(\boldsymbol{y}_N-\boldsymbol{y}_{j-1})_k}{N-(j-1)}\right)^2\Big/(2\Delta t)-\frac{(\boldsymbol{y}_N-\boldsymbol{y}_{j-1})_k}{\Delta t(N-(j-1))}\cdot\xi\left\{\frac{\Delta t(N-j)}{N-(j-1)}\right\}^{1/2}\\&+\frac{\xi^2}{2(N-(j-1))}\,,\end{aligned} \tag{4.12}$$

and

$$|\sigma(\boldsymbol{x}_t)|P(\boldsymbol{x},0|\boldsymbol{x}_t,t)=Q(\boldsymbol{y},0|\boldsymbol{y}_t,t)\,. \tag{4.13}$$

For the multi-dimensional Stratonovich equation, we should make a substitution:

$$\boldsymbol{c}_I(\boldsymbol{y}_{j-1})\longrightarrow\boldsymbol{c}_S(\boldsymbol{y}_{j-1}) \tag{4.14}$$

where

$$\boldsymbol{c}_S(\boldsymbol{y})=\sigma(\boldsymbol{x})^{-1}\boldsymbol{b}(\boldsymbol{x})\,. \tag{4.15}$$

We have thus given a numerical method in evaluating path integrals.

5. Linear Relaxation

A simple nevertheless non-trivial model of relaxation is represented by a stochastic differential equation,

$$dX(t)=\sqrt{2D}\,dB(t)-\gamma X(t)dt\,. \tag{5.1}$$

We can solve (5.1) analytically with the use of (3.23) or (3.31) together with the following formula.

$$\begin{aligned}&\prod_{j=1}^{N-1}\int dx_j\exp[-(x_{j-1}-bx_j)^2/(2a)]\exp[-(x_{N-1}-bx_N)^2/(2a)]\\&=(\sqrt{2\pi a})^{N-1}\frac{1}{c}\cdot\exp[-(x_0-b^Nx_N)^2/(2ac^2)]\end{aligned} \tag{5.2}$$

where

$$c=\sqrt{\frac{1-b^{2N}}{1-b}}\,. \tag{5.3}$$

The solution is well-known:

$$P(x_0,0|x_t,t)=\frac{1}{\sqrt{2\pi\rho(t)^2}}\exp\left[-\frac{(x_t-x_0e(t))^2}{2\rho(t)^2}\right] \tag{5.4}$$

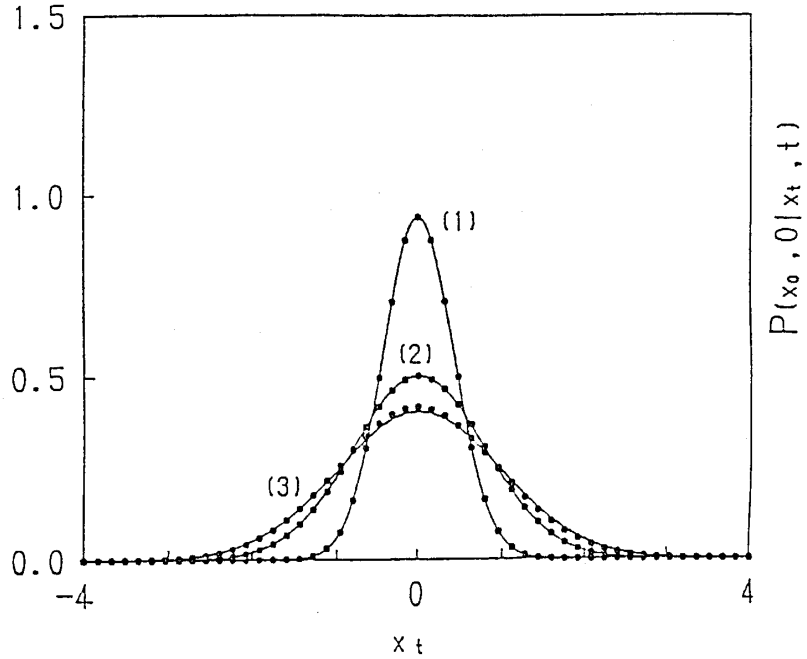


Fig. 1. Probability density: $\gamma=1$, $D=1$ and $x_0=0$.
(1): $t=0.1$ for $M=10$ and $N=100$.
(2): $t=0.5$ for $M=10$ and $N=100$.
(3): $t=2.0$ for $M=10$ and $N=500$.

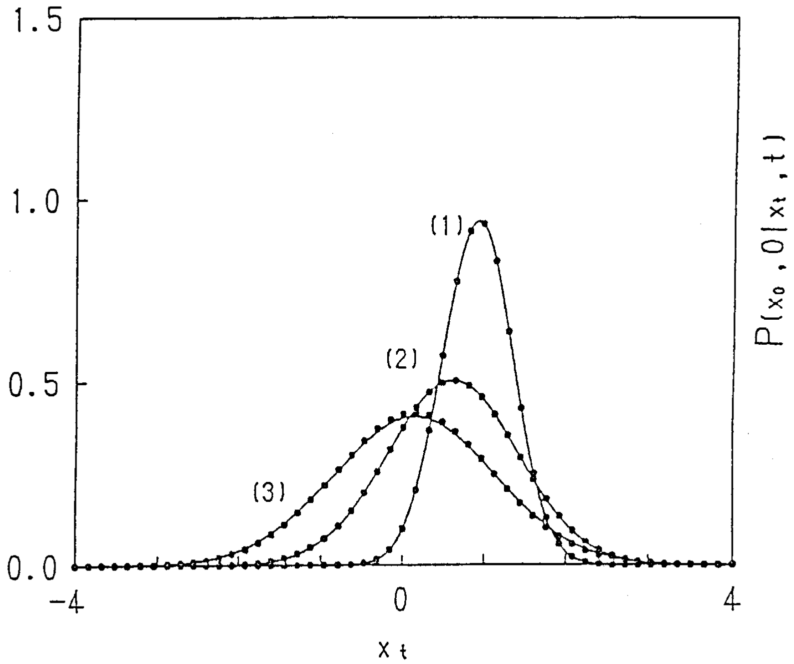


Fig. 2. Probability density: $\gamma=1$, $D=1$ and $x_0=1$.
(1): $t=0.1$, (2): $t=0.5$,
(3): $t=2.0$ for $M=10$ and $N=100$.

where

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

and

$$\rho(t)^2 = (D/\gamma)\{1 - e(t)^2\}. \tag{5.5}$$

We have calculated the probability density by the method of section 4 and compared with (5.4). This is shown in figures 1~2 where excellent agreement is found.

6. Relaxing Angular Velocity

For a three-dimensional rotator, time evolution of angular velocity is determined by[23)]

$$\dot{\omega}_i = \lambda_i \omega_j \omega_k - \beta_i \omega_i + R_i(t) \tag{6.1}$$

where i, j, k represent a cyclic permutation of 1, 2, 3; λ_i is the ratio of the

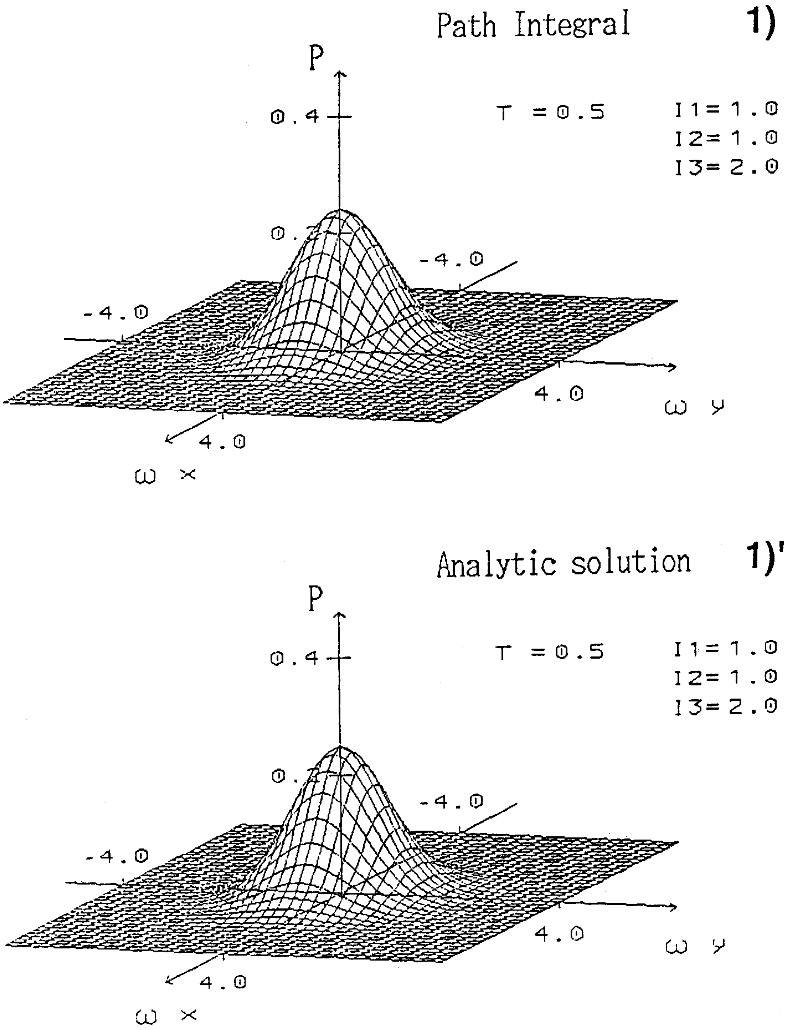


Fig. 3. 1), 1)′ in $\omega_x - \omega_y$ plane.

principal moment of inertia:

$$\lambda_i \equiv (I_j - I_k)/I_i\,. \tag{6.2}$$

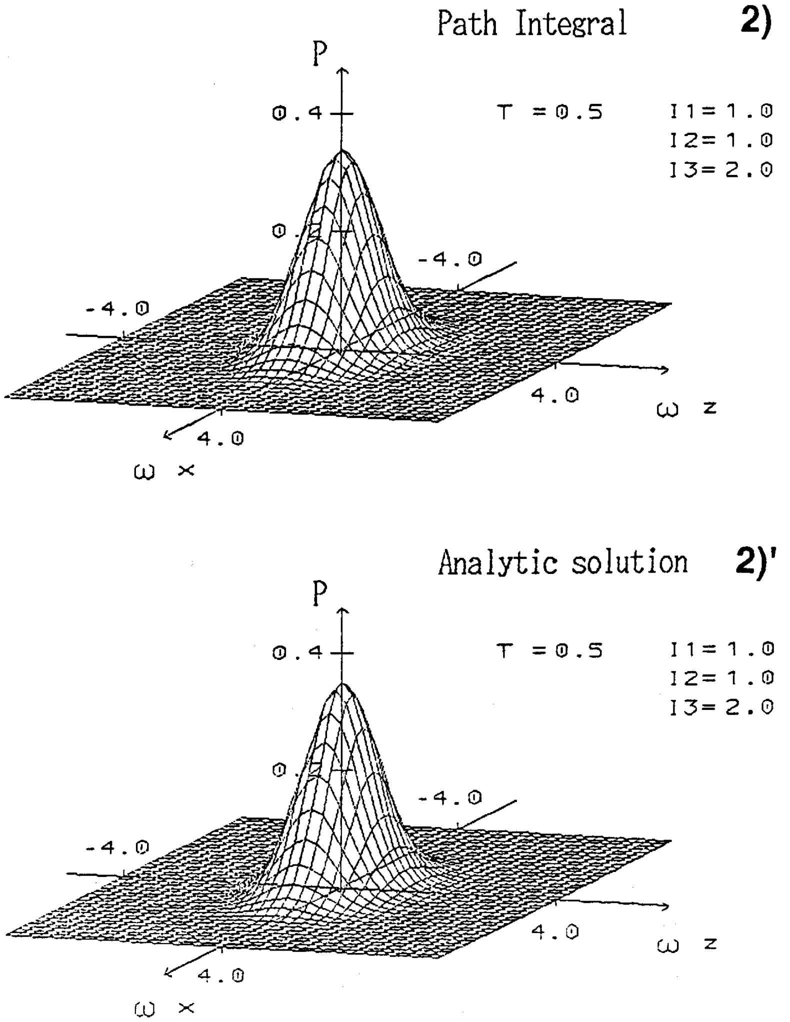
In (6.1) the damping term, $-\beta_i\omega_i(t)$, is related with $R_i(t)$ which is due to random torque. We assume that $R_i(t)$ has a white spectrum. Thus the Langevin type equation (6.2) is equivalent to the following stochastic differential equation:

$$\begin{pmatrix} d\omega_1 \\ d\omega_2 \\ d\omega_3 \end{pmatrix} = \begin{pmatrix} \sigma_1 & & \\ & \sigma_2 & \\ & & \sigma_3 \end{pmatrix} \begin{pmatrix} dB_1 \\ dB_2 \\ dB_3 \end{pmatrix} + \begin{pmatrix} \lambda_1\omega_2\omega_3 - \beta_1\omega_1 \\ \lambda_2\omega_3\omega_1 - \beta_2\omega_2 \\ \lambda_3\omega_1\omega_2 - \beta_3\omega_3 \end{pmatrix} dt \tag{6.3}$$

or

$$d\boldsymbol{\omega}(t) = \underline{\sigma} d\boldsymbol{B}(t) + \boldsymbol{b}(\boldsymbol{\omega}(t))dt\,. \tag{6.4}$$

The elements of $\underline{\sigma}$ is determined by the fluctuation-dissipation theorem:



2), 2)′ in $\omega_x - \omega_z$ plane.

Fig. 3. Probability density $P(\omega_0, 0|\omega, t)$: $I_1 = I_2 = 1.0$, $I_3 = 2.0$, $\omega_0 = 0$, $t = 0.5$.

$$\sigma_i^2 = 2k_B T/(I_i \beta_i) \tag{6.5}$$

where T is the temperature.

A set of equation (6.4) can be solved by a direct application of the method of section 4. Our results should be compared with an analytic solution for a symmetric top $(I_1 = I_2 \neq I_3)$:

$$P(\boldsymbol{\omega}_0, 0|\boldsymbol{\omega}_t, t) = \frac{1}{2\pi\rho_1^2} \exp\left[-\frac{(\omega_1 - \omega_{01}e^{-\beta_1 t})^2 + (\omega_2 - \omega_{02}e^{-\beta_2 t})^2}{(2\rho_1^2)}\right]$$
$$\times \frac{1}{\sqrt{2\pi\rho_3^2}} \exp\left[-\frac{(\omega_3 - \omega_{03}e^{-\beta_3 t})^2}{(2\sigma_3^2)}\right] \tag{6.6}$$

where

$$\rho_i^2 = (k_B T/I_i)(1 - e^{-2\beta_i t}) \tag{6.7}$$

Both solutions are shown in fig. 3~4. Our path integral calculations give satisfactory results.

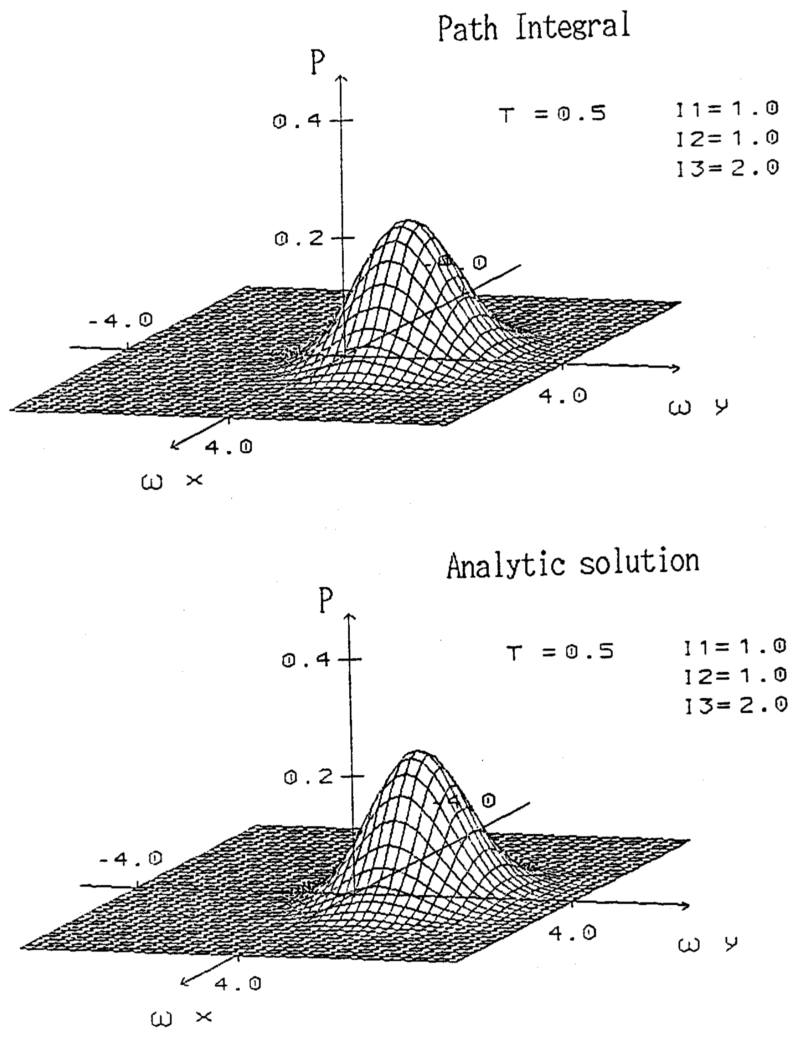


Fig. 4. Probability density $P(\omega_0, 0|\omega, t)$ with $\omega_0 = (0, 2.0, 0)$: The other conditions are the same as in Fig. 3.

7. Relaxing Spins

When a fluctuating field in a condensed phase exerts its influence upon spins, orientational "random walks" are observed: This is called Brownian motion of spins[24].

Let the magnetization be $\boldsymbol{M}(t)$. Then we have a torque equation with the Landau-Lifshitz term:

$$\frac{d}{dt}\boldsymbol{M}(t)=\gamma'\boldsymbol{H}(t)\times\boldsymbol{M}(t)-\eta[\boldsymbol{H}(t)\times\boldsymbol{M}(t)]\times\boldsymbol{M}(t) \tag{7.1}$$

where γ' is the gyromagnetic ratio and the magnetic field is of the form

$$\boldsymbol{H}(t)=\boldsymbol{H}_0+\boldsymbol{H}'(t)\,. \tag{7.2}$$

In the above expressions η is determined by a requirement of the fluctuation-dissipation theorem:

$$\eta=1/(2\tau_1 k_B T) \tag{7.3}$$

where τ_1 is a measure of the longitudinal relaxation time. The magnetic field is composed of the static field $\boldsymbol{H}_0$ and the fluctuation field $\boldsymbol{H}'(t)$. When the narrowing and high temperature conditions are satisfied, $\boldsymbol{H}(t)$ in the second term of the right hand side of (7.1) can be replaced by $\boldsymbol{H}_0$.

A probability density $W(\boldsymbol{M},t)$ to find $\boldsymbol{M}$ at time t is determined by the stochastic Liouville equation:

$$\frac{\partial}{\partial t}W(\boldsymbol{M},t)=-\frac{\partial}{\partial\boldsymbol{M}}\cdot(\dot{\boldsymbol{M}}W(\boldsymbol{M},t)) \tag{7.4}$$

which is written in the form

$$\frac{\partial}{\partial t}W(\boldsymbol{M},t)=-i\mathfrak{L}(t)W(\boldsymbol{M},t) \tag{7.5}$$

where

$$\mathfrak{L}(t)=\mathfrak{L}_0+\mathfrak{L}'(t)\,. \tag{7.6}$$

In (7.6) we have put

$$\mathfrak{L}_0=\omega_0 L_z+\eta H_0(\boldsymbol{L}\times\boldsymbol{M})_z\,, \tag{7.7}$$

$$\mathfrak{L}'(t)=\gamma'\boldsymbol{H}'(t)\cdot\boldsymbol{L} \tag{7.8}$$

where

$$\boldsymbol{L}=-i\boldsymbol{M}\times\frac{\partial}{\partial\boldsymbol{M}} \tag{7.9}$$

and

$$\omega_0=\gamma' H_0 \tag{7.10}$$

for $\boldsymbol{H}_0=(0,0,H_0)$.

In an interaction representation defined by

$$\hat{W}(t)=e^{i\mathfrak{L}_0 t}W(t) \tag{7.11}$$

(7.5) becomes

$$\frac{\partial}{\partial t}\hat{W}(t)=-i\hat{\mathfrak{L}}'(t)\hat{W}(t) \tag{7.12}$$

where

$$\hat{\mathfrak{L}}'(t)=e^{i\mathfrak{L}_0 t}\mathfrak{L}'(t)e^{-i\mathfrak{L}_0 t}\,. \tag{7.13}$$

Now we take a stochastic average over the process of the fluctuating field. This procedure denoted by $\langle\cdots\rangle_B$ is conveniently performed by the time-convolutionless projection operator method[25]. Up to the lowest non-trivial order, it is explicitly given by

$$\frac{\partial}{\partial t}\langle\hat{W}(\boldsymbol{M},t)\rangle_B=\Big\{-i\langle\hat{\mathfrak{L}}'(t)\rangle_B$$

$$+(-i)^2\int_0^t d\tau\langle\hat{\mathfrak{L}}'(t)\hat{\mathfrak{L}}'(\tau)\rangle_{B,o.c.}\Big\}\langle\hat{W}(\boldsymbol{M},t)\rangle_B \tag{7.14}$$

where

$$\hat{P}(\boldsymbol{M},t)=\langle\hat{W}(\boldsymbol{M},t)\rangle_B \tag{7.15}$$

and $\langle\cdots\rangle_{B,o.c.}$ is the ordered cumulant defined by

$$\langle AB\rangle_{B,o.c.}=\langle AB\rangle-\langle A\rangle\langle B\rangle\,. \tag{7.16}$$

After some algebra, we finally obtain

$$\Big\{\frac{\partial}{\partial t}+i\gamma'(1+\delta)\boldsymbol{H}_0\cdot\boldsymbol{L}-(i\boldsymbol{L}\cdot\underline{D}\cdot i\boldsymbol{L})\Big\}\langle\hat{W}(\boldsymbol{M},t)\rangle_B=0 \tag{7.17}$$

where

$$\underline{D}=D_1\Big(1-\frac{\boldsymbol{H}_0\boldsymbol{H}_0}{H_0^2}\Big)+D_0\frac{\boldsymbol{H}_0\boldsymbol{H}_0}{H_0^2} \tag{7.18}$$

and

$$D_1=\frac{1}{2\tau_1}=\int_0^\infty\varphi_\perp(t)\cos(\omega_0 t)dt\,,$$

$$D_0=\frac{1}{2\tau_0}=\int_0^\infty\varphi_\parallel(t)dt\,. \tag{7.19}$$

In these expressions we used the narrowing condition and put

$$\varphi_\perp(\tau)=\gamma'^2\langle H'_x(t)H'_x(t-\tau)\rangle_B$$

$$=\gamma'^2\langle H'_y(t)H'_y(t-\tau)\rangle_B\,, \tag{7.20}$$

$$\varphi_\parallel(\tau)=\gamma'^2\langle H'_z(t)H'_z(t-\tau)\rangle_B\,, \tag{7.21}$$

and

$$\delta=(1/\omega_0)\int_0^\infty d\tau\varphi_\perp(\tau)\sin(\omega_0\tau)\,. \tag{7.22}$$

For later application, it is convenient to express (7.17) in a polar coordinate rotating with an angular velocity $\omega_0' = \omega_0 + \delta\omega_0$.

That is, for

$$\hat{P}(\boldsymbol{M}, t) = e^{\omega'_0 t(\partial/\partial\phi)} \langle \hat{W}(\boldsymbol{M}, t) \rangle_B \tag{7.23}$$

we have

$$\frac{\partial}{\partial t}(\hat{P}(\boldsymbol{M}, t)\sin\theta) = \left\{\frac{\partial^2}{\partial\theta^2}D_1 + \frac{\partial^2}{\partial\phi^2}(D_0 + D_1\cot^2\theta) - \frac{\partial}{\partial\theta}D_1(\cot\theta - \eta'\sin\theta)\right\}(\hat{P}(\boldsymbol{M}, t)\sin\theta)$$
$$= \tilde{\Gamma}(\theta, \phi)(\hat{P}(\boldsymbol{M}, t)\sin\theta) \tag{7.24}$$

where

$$\boldsymbol{M} = (M\sin\theta\cos\phi, M\sin\theta\sin\phi, M\cos\theta) \tag{7.25}$$

and

$$\eta' = H_0 M / k_B T\,. \tag{7.26}$$

Thus the corresponding generator is found to be

$$\Gamma(\theta, \phi)\cdot = \left\{D_1\frac{\partial^2}{\partial\theta^2} + (D_0 + D_1\cot^2\theta)\frac{\partial^2}{\partial\phi^2} + D_1(\cot\theta - \eta'\sin\theta)\frac{\partial}{\partial\theta}\right\}\cdot\,. \tag{7.27}$$

Extension of (7.17) to quantum spin system has already been done[26]. Then the stochastic differential equations are obtained as

$$\begin{pmatrix} d\theta \\ d\phi \end{pmatrix} = \begin{pmatrix} \sqrt{2D_1} & 0 \\ 0 & \sqrt{2(D_0 + D_1\cot^2\theta)} \end{pmatrix}\begin{pmatrix} dB_1 \\ dB_2 \end{pmatrix} + \begin{pmatrix} D_1(\cot\theta - \eta'\sin\theta) \\ 0 \end{pmatrix}dt\,. \tag{7.28}$$

Transforming (θ, ϕ) into (Y_1, Y_2):

$$d\boldsymbol{Y} = \begin{pmatrix} dY_1 \\ dY_2 \end{pmatrix} = \underline{\sigma}^{-1}\begin{pmatrix} d\theta \\ d\phi \end{pmatrix}, \tag{7.29}$$

we find

$$d\boldsymbol{Y} = d\boldsymbol{B} + \begin{pmatrix} \sqrt{D_1/2}\,(\cot\theta - \eta'\sin\theta) \\ 0 \end{pmatrix}dt \tag{7.30}$$

and the method of sectiod 4 can be applied.

Time evolution of the probability density

$$\hat{P}(\theta_0, \phi_0, 0 | \theta, \phi, t)$$

is shown in fig. 5: the upper diagram represents a distribution in the Northern hemisphere whereas the lower for the Southern hemisphere both of which are viewed from the North.

It is clearly seen that the initially localized spins at (θ_0, ϕ_0) move toward the equilibrium: The static magnetic field $\boldsymbol{H}_0$ is applied along z-axis.

Averages of spin $\boldsymbol{S}$ (proportional to $\boldsymbol{M}$) are obtained by the following formulas ($d\Omega = \sin\theta d\theta d\phi$):

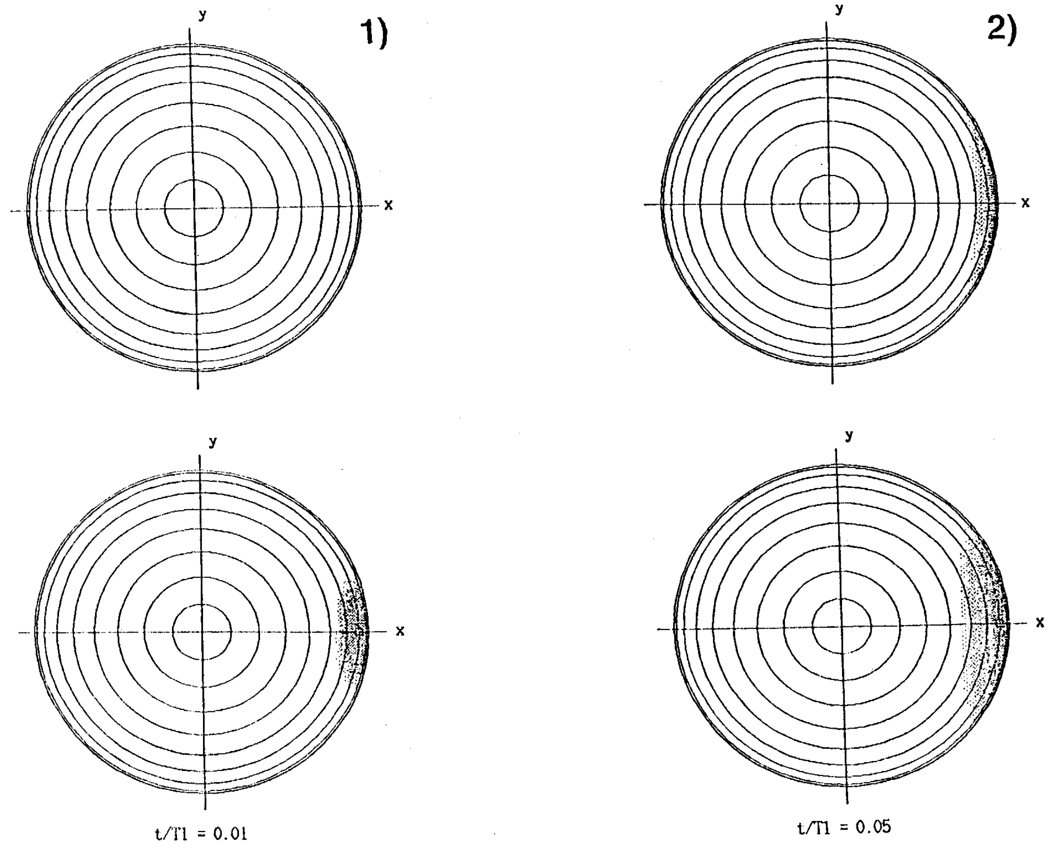


Fig. 5.

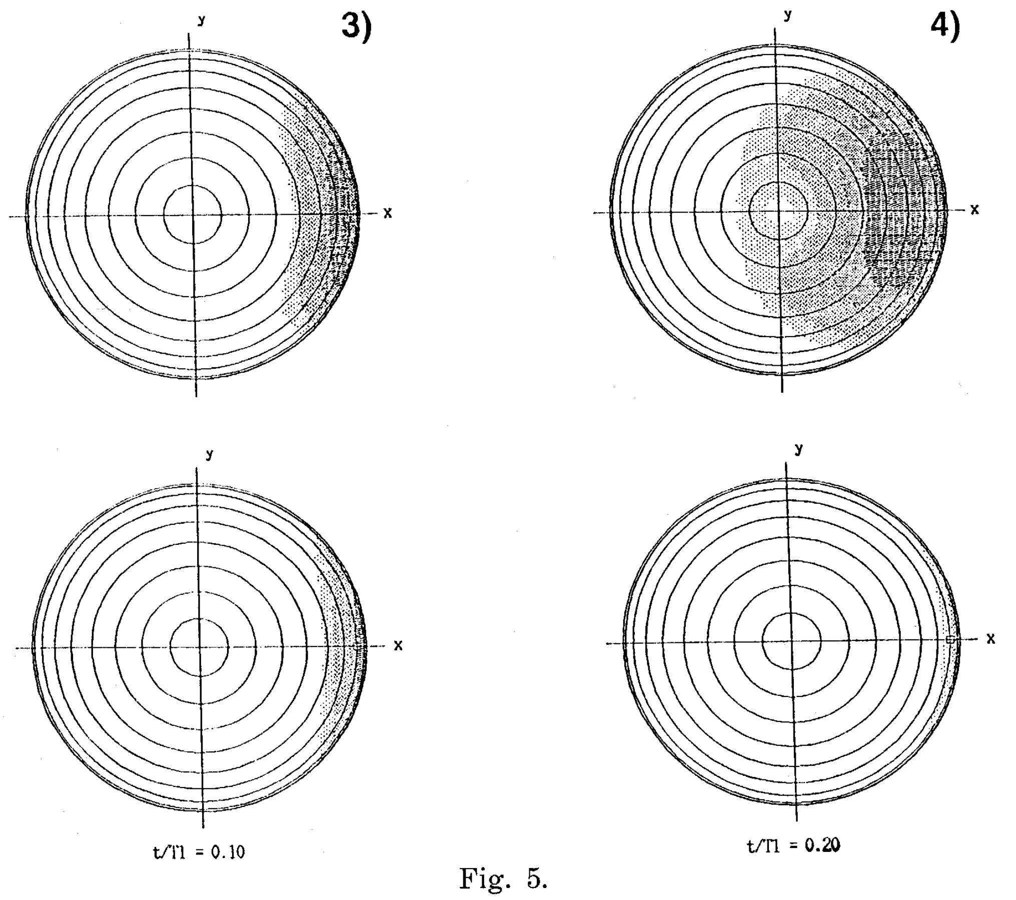


Fig. 5.

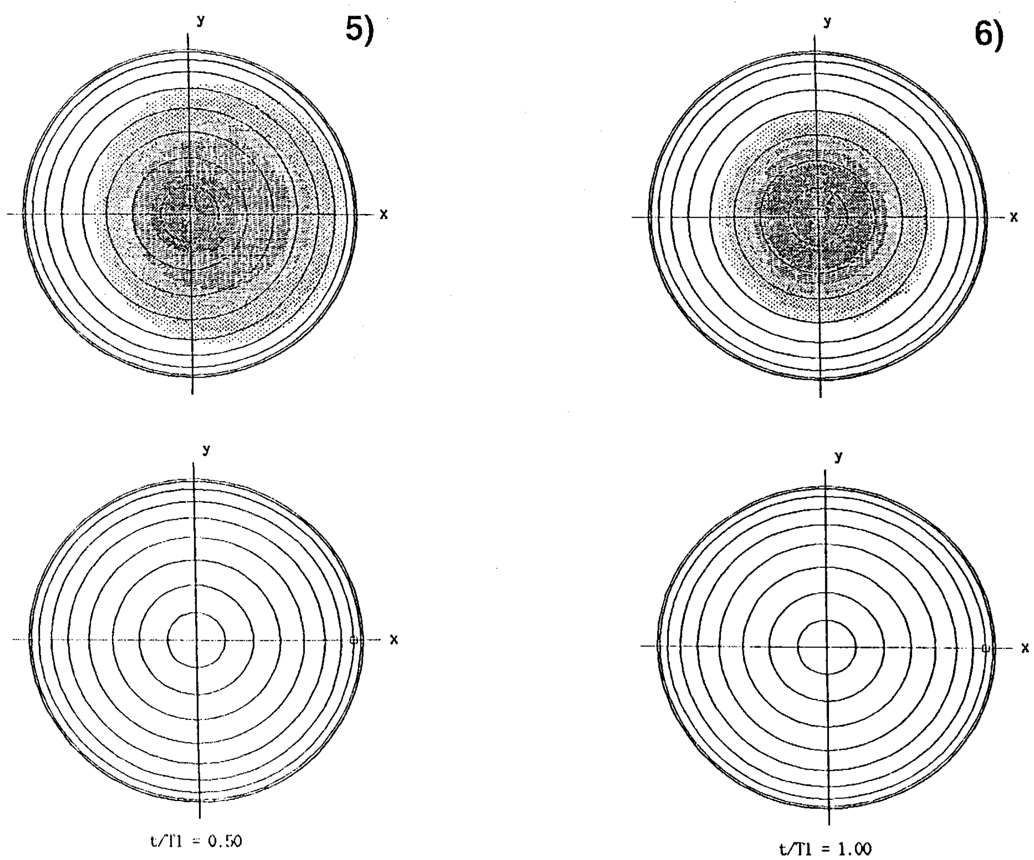


Fig. 5. Time-evolution of probability density $P(\theta_0, \phi_0, 0 | \theta, \phi, t)$: $\eta'=10$, $\hat{D}=D_0/D_1=1$, $(\theta_0, \theta_0)=(110°, 0°)$; $\hat{t}=t/T_1=0.01$ [for 1)], 0.05 [for 2)], 0.1 [for 3)], 0.2 [for 4)], 0.5 [for 5)], 1.0 [for 6)].

$$\langle S_x \rangle_t = S\int d\Omega \sin\theta \cos\phi \hat{P} \Big/ \int d\Omega \hat{P}, \tag{7.31}$$

$$\langle S_y \rangle_t = S\int d\Omega \sin\theta \sin\phi \hat{P} \Big/ \int d\Omega \hat{P}, \tag{7.32}$$

$$\langle S_z^2 \rangle_{c,t} = \langle S_z^2 \rangle_t - \langle S_z \rangle_t^2 \tag{7.33}$$

and so on.

We show in fig. 6 these quantities, where $\langle S_z \rangle_t$ tends to the correct equilibrium value:

$$\langle S_z \rangle_{eq} = SL(\eta') \tag{7.34}$$

where

$$L(x) = \cot(x) - (1/x) \tag{7.35}$$

is the Langevin function.

The problem of Brownian motion of spins (nonlinear spin relaxation) has been solved completely.

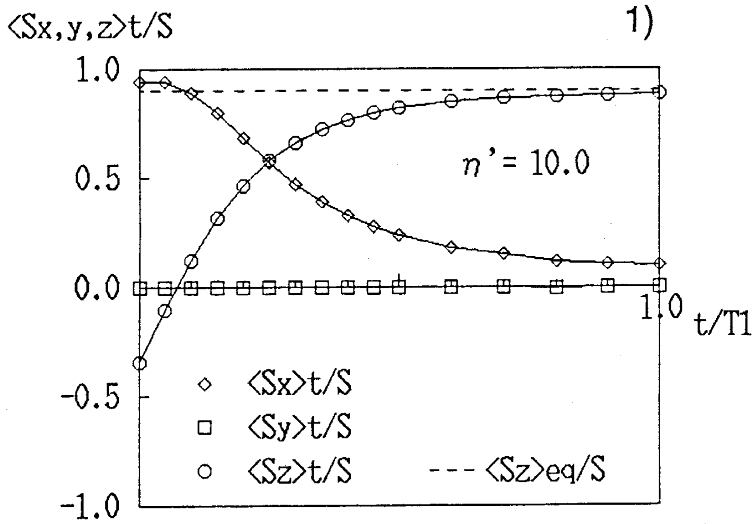


Fig. 6-1) $\langle S_\mu \rangle_t / S$ as a function of $\hat{t}=t/T_1$. The parameters are the same as in Fig. 5.

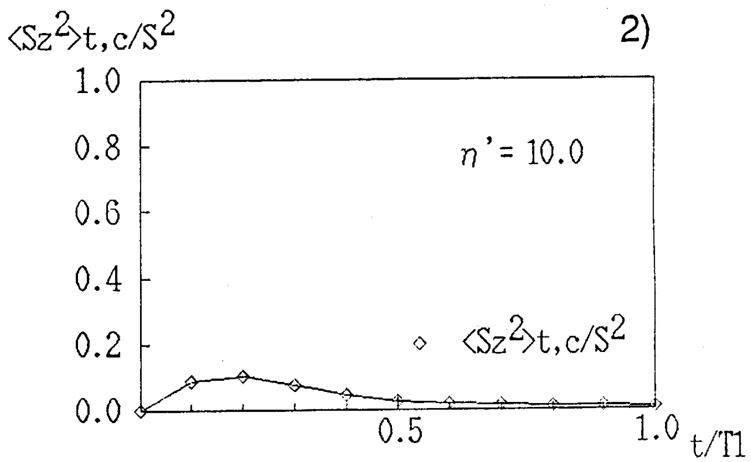


Fig. 6-2) $\langle S_z^2 \rangle_{t,c} / S^2$ as a function of $\hat{t}$. The parameters are the same as in Fig. 5.

8. Summary

We have formulated a path integral theory of Brownian motion. This is based on a mathematical theorem of the stochastic process. Besides formal manipulation which leads to the "Lagrangian" path integral formulas of section 3, we have given a practical method of numerical evaluation of path integrals. Indeed the method is applied to the solvable models of relaxation in sections 5~6 meeting with good agreement with the exact solutions.

Our formulation is further applied to the problem of Brownian motion of spins. An approach to the correct equilibrium is guaranteed by the nonlinear Landau-Lifshitz term and hence the nonlinearity plays an essential role in this problem. Our theory has been proved to be successful in section 7 even for this kind of nonlinearities.

Acknowledgement

The authors are grateful to Professor N. Hashitsume for his valuable suggestions during this work.

References

[1] L. Onsager and S. Machlup: Phys. Rev. **91** (1953) 1505, 1512.
[2] N. Hashitsume: Proc. Int. Conf. Theor. Phys. (1953) 495.
[3] N. Hashitsume: Progr. Theor. Phys. 8 (1952) 461; ibid **15** (1956) 369.
[4] L. Tisza and J. Manning: Phys. Rev. **105** (1957) 1695.
[5] W. Horsthemke and A. Bach: Z. Phys. **B22** (1975) 189; A. Bach, D. Dürr and B. Stawicki, Z. Phys. **B26** (1977) 191.
[6] H. Hasegawa: Progr. Theor. Phys. **57** (1977) 1523, **58** (1977) 128.
[7] R. Graham: Z. Phys. **B26** (1977) 281; ibid 397.
[8] B. Chan Eu: Physica **90A** (1978) 288.
[9] *Path Integrals and Their Applications in Quantum, Statistical, and Solid State Physics,* ed. G.J. Papadopoulos and J.T. Devreese (Plenum Press, New York and London, 1978).
[10] K.L.C. Hunt and J. Ross: J. Chem. Phys. **75** (1981) 976.
[11] H. Dekker: Phys. Rev. **A24** (1981) 3182.
[12] R.P. Feynman and A.R. Hibbs: *Quantum Mechanics and Path Integrals* (McGraw-Hill Inc., New York and London 1965).
[13] L.S. Schulman: *Techniques and Applications of Path Integration* (John Wiley & Sons Inc., New York and Toronto, 1981).
[14] H. Kleinert: *Path Integrals in Quantum Mechanics, Statistics, and Polymer Physics* (World Scientific, Singapore, New Jersey, London, 1990).
[15] M. Watabe and F. Shibata: J. Phys. Soc. Jpn. **59** (1990) 1905.
[16] F. Shibata, M. Watabe, H. Kawasaki and N. Hashitsume: Nat. Sci. Rep. Ochanomizu Univ. **40** (1989) 57.
[17] See for instance, N. Ikeda and S. Watanabe: *Stochastic Differential Equations and Diffusion Processes,* second edition (North-Holland, Amsterdam, and Kodansha Ltd, Tokyo, 1989).
[18] R.H. Cameron and W.T. Martin: Trans. Amer. Math. Soc. **66** (1949) 253.
[19] G. Maruyama: Rend. Circolo Math. Palermo **4** (1955) 48; Nat. Sci. Rep. Ochanomizu Univ. **5** (1954) 10.
[20] I.V. Girsanov: Theor. Probability and Appl. **5** (1960) 285.
[21] See for instance, H. Tomita, A. Ito and H. Kidachi: Progr. Theor. Phys. **56** (1976) 789.
[22] T. Tsuda, K. Ichida and T. Kiyono: Numeriche Mathematik **10** (1967) 110.
[23] P.S. Hubbard: Phys. Rev. **A15** (1977) 329.
[24] R. Kubo and N. Hashitsume: Suppl. Proqr. Theor. Phys. No. 46 (1970) 210.
[25] F. Shibata and T. Arimitsu: J. Phys. Soc. Jpn. **49** (1980) 891 and references cited therein.
[26] Y. Takahashi and F. Shibata: J. Phys. Soc. Jpn. **38** (1975) 656; F. Shibata, ibid **49** (1980) 15.