Journal of Mathematical Chemistry Vol. 31, No. 1, January 2002 (© 2002)

The mathematical theory of Ito diffusions on hypersurfaces, with applications to NMR relaxation problems *

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Received 27 August 2001

A mathematical framework for translational Brownian motion on hypersurfaces is presented, using an imbedding of the surface and Ito diffusions in the ambient space. This includes a survey of Ito calculus and differential geometry. Computational methods for time correlation functions relevant to spin relaxation studies on curved interfaces are given, and explicit calculations of time correlation functions and order parameters for a "Rippled" surface are presented.

KEY WORDS: Ito diffusion, Brownian motion, hypersurface, relaxation theory, correlation function

1. Introduction

This paper presents a mathematical framework for translational diffusion processes on hypersurfaces, in particular, two-dimensional surfaces imbedded in three-dimensional space. The framework is needed in studies of molecular diffusion at interfaces and spin relaxation studies using NMR or EPR. Molecular translational diffusion along curved interfaces may be studied using spin relaxation since the curvature of the interface introduces a time-modulation of a spin-lattice Hamiltonian and, thus, becomes a relaxation mechanism. In spin relaxation studies of heavy water or deuterated lipids the quadrupole interaction is the dominant relaxation mechanism and is, thus, modulated by translational diffusion along curved interfaces in the strong narrowing regime of BWR theory, cf. [1]. The time correlation function is the relevant quantity we need in order to describe spin relaxation rates and line shapes. Translational diffusion of a particle moving along a curved two-dimensional surface is described by a set of stochastic differential equations which can be simulated numerically to obtain the relevant time correlation functions. We formulate diffusion problems on hypersurfaces of arbitrary dimension $\geqslant 2$. We use

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0259-9791/02/0100-0065/0

the method of imbedding to construct Ito diffusions on hypersurfaces, similar to [2], where Brownian motion on hypersurfaces is considered. Our construction for general Ito diffusions is outlined as a remark in [3, p. 253], but to our knowledge, no one has presented a detailed account of the method. The first account of the Ito integral as well as stochastic differential equations on manifolds are due to Kiyosi Ito [4,5]. There is an extensive literature on diffusions on manifolds, we refer to the monographs [3,6–9].

The paper is organized as follows. We start with a short review of Brownian motion in section 2. We show that Brownian motion is a Markov process (2), and that it is a martingale (4). We note that it has a multinormal distribution and compute its covariance matrix (6). An important scaling property is stated in (8), and we define standard Brownian motion in (9). Finally, we give a short account for the Wiener measure.

In section 3 the Ito integral is defined, which is the fundamental tool in Ito's stochastic calculus. We give a simple example of an Ito integral in example 1.

In section 4, a special case of Ito's formula for transformations of Ito integrals (17) is given. This leads to the informal basic rules (19) of Ito's calculus.

The tranformation rules in (16) lead naturally to the definition of a larger class of stochastic processes described by Ito integrals (20), the *Ito processes*, considered in section 5.

Analogously to the transformation of Brownian motion in section 4, we consider transformations of Ito processes in section 6. The basic result is that the transformation of an Ito process is again an Ito process, and the transformation of coefficients in the corresponding Ito integral (21) is given by the general Ito's formula (25)–(27). Moreover, in case the transformation is a diffeomorphism, we may transform coefficients in the other direction (28), (29).

We consider a more restricted class of Ito processes in section 7, the *Ito diffusions*, which are solutions to an Ito stochastic differential equation (SDE) given in (31). Then a transformation of an Ito diffusion is again an Ito diffusion, and in this case, the general Ito's formula (25) takes a particularly simple form (32), henceforth called *Ito's formula*. The drift vector and diffusion matrix of the transformed Ito SDE are computed by a second-order scalar differential operator L (33) and a first-order vector differential operator D (34) associated with the original Ito SDE. Then we state a scaling relation for Ito diffusions, where the Ito SDE for a scaled Ito diffusion (35) is given in (36) and (38).

In section 8 we elaborate the definition of a hypersurface as a level set of a smooth function F, and then give the construction of Ito diffusions on a hypersurface by the imbedding method in theorem 1. The basic idea is to start with an Ito diffusion X_t on $\mathbb{R}^n$, satisfying an Ito SDE (31), and to choose the diffusion matrix and drift vector in such a way (conditions (40) and (41)) that an Ito diffusion starting on the hypersurface remains on the hypersurface for all times, which is equivalent to $\mathrm{d}F(X_t) = 0$ in the sense of Ito's calculus. To be noted is that the diffusions are defined in the ambient space $\mathbb{R}^n$, so no local parametrization of the hypersurface is needed. Moreover, the diffusions may be simulated using standard numerical methods for Ito SDEs.

In section 9 we define Brownian motion on a hypersurface by choosing the diffusion matrix $B(X)$ to be the projection onto the tangent space at X (43), hence, satisfying (41), and then choosing the drift vector $A(X)$ to be the normal vector at X, satisfying (40).

In section 10 we assume that the hypersurface has a local parametrization $f(x^1, \ldots, x^{n-1})$, and want to find an Ito SDE for the local coordinates x_t defined by (45). We extend the local parametrization to a local flattening diffeomorphism $f(x^1, \ldots, x^n)$ defined by the property (46), define local basis vectors f_i and dual basis vectors f^i, define metric tensors (51) and compute the coefficients of the Ito SDE by Ito's formula (54), transformed to the x-coordinates by the chain rule (49) and the decompositions (48) and (55). The resulting transformations of L and D to local coordinates are given in (56) and (59), and the resulting Ito SDE for x_t is given in (65). Finally, we define a standard Brownian motion in local coordinates in (66) and get an Ito SDE in local coordinates driven by a local standard Brownian motion in (67).

As noted previously, the main objective is to compute certain time correlation functions relevant to spin relaxation theory. They are introduced in section 11.

In section 12 we consider a specific surface studied in the literature, which we call the *Rippled surface* [10,11]. We find a local parametrization in which the standard Brownian motion coincides with the local Brownian motion. We may then reduce the computation of functionals of the standard Brownian motion of the Rippled surface to a standard Brownian motion on a finite interval with periodic boundary conditions. As a consequence we get our main result in theorem 3, a generalized Fourier series representation of correlation functions on the Rippled surface. In particular, we get the decay rates explicitly in (86) and also an explicit calculation of order parameters in (94).

In the appendix, order parameters for the Rippled surface are given (appendix B) and elliptic integrals are specified (appendix C).

2. Brownian motion

In this section, we review the theory of Brownian motion in $\mathbb{R}^n$. This is a stochastic process on $\mathbb{R}^n$, i.e., a mapping $W : \mathbb{R}_+ \times \Omega \to \mathbb{R}^n$, usually written as a parametrized family of random variables $W_t : \Omega \to \mathbb{R}^n$, $t \in \mathbb{R}_+$, over some sample space Ω. Physically, for $n = 3$ (three-dimensional space) this is a description of the irregular motion of small particles in suspensions, on a timescale much larger then the autocorrelation time of the velocity, cf. [12].

A stochastic process W_t is said to be a Brownian motion (with diffusion constant $K > 0$) starting at $X_0 \in \mathbb{R}^n$ if

1. $W_0 = X_0$.

2. It has stationary, independent increments, i.e., $W_t - W_s$ and $W_{t+h} - W_{s+h}$ have the same distributions for all $s, t, h > 0$, and $W_{t_1} - W_{t_0}, W_{t_2} - W_{t_1}, \ldots, W_{t_k} - W_{t_{k-1}}$ are independent random variables for all $0 \leqslant t_0 < t_1 < \cdots < t_k$, $k \in \mathbb{N}$.

3. For every $t > 0$, W_t has a Gaussian distribution with mean $m = 0$ and covariance matrix $C = 2KtI$, i.e., $W_t = (W_t^1, W_t^2, \ldots, W_t^n)$ have the probability density

$$f_{W_t}(X) = \left((2\pi)^n \det(C)\right)^{-1/2} \mathrm{e}^{-(1/2)(X-m)\cdot C^{-1}(X-m)}$$
$$= (4\pi Kt)^{-n/2} \mathrm{e}^{-\|X\|^2/(4Kt)}, \quad X \in \mathbb{R}^n. \tag{1}$$

4. It has continuous sample paths, i.e., $t \mapsto W_t(\omega)$ is almost surely continuous.

Let us first note that since W_t has stationary increments, $W_t - W_s$ and W_{t-s} have the same distributions,

$$f_{W_t - W_s} = f_{W_{t-s}}, \quad t > s,$$

hence, the increment $W_t - W_s$ is Gaussian with mean X_0 and covariance matrix $2K(t-s)I$.

Furthermore, since W_t has independent increments,

$$f_{W_{t_0},\ldots,W_{t_k}}(X_0, \ldots, X_k) = f_{W_{t_0}}(X_0) f_{W_{t_1} - W_{t_0}}(X_1 - X_0) \cdots f_{W_{t_k} - W_{t_{k-1}}}(X_k - X_{k-1}).$$

Consequently, conditional probability densities can be computed as

$$f_{W_{t_k}|W_{t_0},\ldots,W_{t_{k-1}}}(X_k \mid X_0, \ldots, X_{k-1}) \equiv \frac{f_{W_{t_0},\ldots,W_{t_k}}(X_0, \ldots, X_k)}{\int f_{W_{t_0},\ldots,W_{t_k}}(X_0, \ldots, X_{k-1}, Y)\, \mathrm{d}Y}$$
$$= f_{W_{t_k} - W_{t_{k-1}}}(X_k - X_{k-1})$$
$$= f_{W_{t_k}|W_{t_0}}(X_k|X_{k-1}). \tag{2}$$

Hence, W_t is a *Markov process*. Moreover, for conditional expectations we get

$$E(W_{t_k}|W_{t_0}, \ldots, W_{t_{k-1}}) \equiv \frac{f_{W_{t_0},\ldots,W_{t_k}}(X_0, \ldots, X_k)}{\int Y f_{W_{t_k}|W_{t_0},\ldots,W_{t_{k-1}}}(Y \mid X_0, \ldots, X_{k-1})\, \mathrm{d}Y}$$
$$= X_{k-1}, \tag{3}$$

i.e., with the usual identification of conditional expectations with functions of the conditioning variables ($W_{t_0}, \ldots, W_{t_{k-1}}$ in this case),

$$E(W_{t_k}|W_{t_0}, \ldots, W_{t_{k-1}}) = W_{t_{k-1}}. \tag{4}$$

Hence, W_t is a *martingale*. Finally, $(W_{t_0}, W_{t_1} - W_{t_0}, \ldots, W_{t_k} - W_{t_{k-1}})$ is Gaussian with mean 0 and covariance matrix

$$C(W_{t_0}, W_{t_1} - W_{t_0}, \ldots, W_{t_k} - W_{t_{k-1}}) = 2Kt_0 I \oplus (t_1 - t_0)I \oplus \cdots \oplus (t_k - t_{k-1})I, \tag{5}$$

so, by the transformation properties of multidimensional Gaussian variables, $(W_{t_0}, W_{t_1}, \ldots, W_{t_k})$ is also Gaussian with mean 0, and the covariance matrix may be computed according to

$$C(W_{t_0}, W_{t_1}, \ldots, W_{t_k}) = 2KM\left(t_0 I \oplus (t_1 - t_0)I \oplus \cdots \oplus (t_k - t_{k-1})I\right)M^{\mathrm{T}}, \tag{6}$$

where M is the matrix of the mapping $\mathbb{R}^{n(k+1)} \to \mathbb{R}^{n(k+1)}: (X_0, \ldots, X_k) \mapsto (X_0, X_0 + X_1, \ldots, X_0 + X_1 + \cdots + X_k)$. This covariance matrix consists of a $(k+1) \times (k+1)$ block matrix C_{ij} where each block C_{ij} is an $n \times n$ matrix given by $C_{ij} = 2Kt_{\min(i,j)}I$. Consequently,

$$E(W_s \cdot W_t) = 2Kn \min(s, t). \tag{7}$$

Moreover, Brownian motion W_t on $\mathbb{R}^n$ with diffusion constant K starting at X_0 has the scaling property that

$$\widetilde{W}_t = LW_{Tt} \tag{8}$$

is a Brownian motion on $\mathbb{R}^n$ with diffusion constant KL^2T, starting at LX_0. Thus, we may choose time scale T such that the diffusion constant is $K = 1/2$, and then we say that we have a *standard Brownian motion*. In this case we denote the conditional probability density

$$p(X, t \mid X_0, t_0) = \big(2\pi(t - t_0)\big)^{-n/2} \exp\left(-\frac{|X - X_0|^2}{2(t - t_0)}\right), \tag{9}$$

where $t, t_0 \in \mathbb{R}_+$ and $X, X_0 \in \mathbb{R}^n$. The rigorous mathematical definition of Brownian motion was given by Norbert Wiener in 1923 [13], where Brownian motion is defined in terms of a measure on the space of continuous paths on $\mathbb{R}^n$, and this is usually called the *canonical Brownian motion*. Let us consider the definition of the Wiener measure W in some detail. The Wiener-measurable sets are generated (as a σ-algebra) by sets of paths specified by the condition that they pass through a finite number of measurable sets $E_1, \ldots, E_k$ in $\mathbb{R}^n$ (Borel sets) at a finite number of specified time instants $0 < t_1 < \cdots < t_k$, and the Wiener measure of such a *cylinder set* is computed by the formula

$$\begin{aligned} &W\big(\{\omega\colon \omega(t_1) \in E_1, \ldots, \omega(t_k) \in E_k\}\big) = \\ &\quad \int_{E_1} \cdots \int_{E_k} p(X_1, t_1 \mid X_0, t_0) p(X_2, t_2 \mid X_1, t_1) \cdots p(X_k, t_k \mid X_{k-1}, t_{k-1}) \, \mathrm{d}X_1 \cdots \mathrm{d}X_k. \end{aligned} \tag{10}$$

The Wiener measure defines a Markov process on the path space with transition function $p(X, t \mid X_0, t_0)$, namely, the *coordinate process*

$$W_t(\omega) = \omega(t). \tag{11}$$

For more details on Browian motion and Wiener measure, see, for example, [12,14–16].

Note that the Wiener measure assigns values to *sets* of continuous paths, not individual paths themselves, and that singleton sets $\{\omega\}$ have Wiener measure zero. A property of a path is said to be a *sample path property* for Brownian motion, or to hold *almost surely*, if the property holds for all paths except for a set of paths with Wiener measure 0. For example, the famous Lévy–Hölder condition (cf. [17, p. 36] and [16, p. 30]) says that

$$\limsup_{t_2 - t_1 = \varepsilon \searrow 0, 0 \leqslant t_1 < t_2 < 1} \frac{|\omega(t_2) - \omega(t_1)|}{\sqrt{2\varepsilon \ln(1/\varepsilon)}} = 1 \tag{12}$$

is a sample path property. Also, it follows from the Lévy condition above that to be continuous, nowhere differentiable, and of infinite variation is a sample path property.

3. The Ito integral

We would like to define a path integral

$$I_t(\omega) = \int_0^t f(\tau, \omega)\, \mathrm{d}W_\tau(\omega) \tag{13}$$

of an $m \times n$-matrix-valued functional $f(\tau, \omega)$ over a continuous path ω, but since such a path is almost surely of infinite variation, the usual Lebesgue–Stieltjes definition does not apply. However, the sums do converge in a mean square sense, more precisely, in the space of square-integrable functions with respect to the Wiener measure, provided the functional $f(t, \omega)$ depends only on the values of $W_s(\omega)$ for $s \leqslant t$ in a precise, measure-theoretic sense (the functional is said to be *adapted* to W_t) and

$$\int_0^t \left\| f(\tau, \omega) \right\|^2 \mathrm{d}\tau < \infty \tag{14}$$

almost surely, cf. [18, p. 35] and [6, p. 24]. The Ito integral was first introduced by Ito in [4]. The convergence of the approximating sums is a consequence of the *Ito isometry* [18, p. 26–29]

$$E\left(\left\| \int_0^t f(\tau, \omega)\, \mathrm{d}W_\tau(\omega) \right\|^2 \right) = E\left(\int_0^t \left\| f(\tau, \omega) \right\|^2 \mathrm{d}\tau \right), \tag{15}$$

where $E(X)$ denotes the expectation $\int X(\omega)\, \mathrm{d}W(\omega)$ of the stochastic variable X, and $\| \cdot \|$ denotes the usual vector or matrix norm, i.e., $\| f \|^2$ is the sum of the square of each element. We consider a simple example.

Example 1. Let W_t be a standard one-dimensional Brownian motion. Consider the Ito integral $\int_0^t W_\tau\, \mathrm{d}W_\tau$ and the approximating sum $S_k = \sum_{j=0}^{k-1} W_{\tau_j}(W_{\tau_{j+1}} - W_{\tau_j})$, where $\tau_j = jt/k$, $j = 0, 1, \ldots, k$. The approximating sum may be written as $S_k = W_t^2/2 - a/2$, where $a = \sum_{j=0}^{k-1}(W_{t_{j+1}} - W_{t_j})^2$. Using the fact that $E((W_{\tau\, j+1} - W_{\tau_j})^2) = E(W^2_{\tau_{j+1} - \tau_j}) = \tau_{j+1} - \tau_j$ we get $E(a) = t$. To compute the variance of a, we first get $a - E(a) = \sum_{j=0}^{k-1}(W_{\tau_{j+1}} - W_{\tau_j})^2 - (\tau_{j+1} - \tau_j)$. Then, expanding the square of the sum in $E((a - E(a))^2)$ and using the fact that W_t has independent increments we get the variance of a, $\sum_{j=0}^{k} E(((W_{\tau_{j+1}} - W_{\tau_j})^2 - (\tau_{j+1} - \tau_j))^2)$. Finally, expanding the squares and using the fact that $E((W_{\tau_{j+1}} - W_{\tau_j})^4) = 3(\tau_{j+1} - \tau_j)^2$ we get $E((a - E(a))^2) = 2 \sum_{j=0}^{k-1}(\tau_{j+1} - \tau_j)^2$. Hence, the variance converges to 0 as $k \to \infty$, and the Ito integral is $\int_0^t W_\tau\, \mathrm{d}W_\tau = W_t^2/2 - E(a)/2 = W_t^2/2 - t/2$.

The definition of I_t in the mean square sense for each fixed $t > 0$ is analogous to the definition of the classical L^2-spaces. Thus, the Ito integral I_t is an equivalence class of $\mathbb{R}^m$-valued functionals on the continuous paths, and $I_t(\omega)$ is almost surely defined.

The Ito integral I_t defines a stochastic process on $\mathbb{R}^m$, if f is an $m \times n$ matrix. The process I_t is easily seen to be adapted, and from the important fact that I_t is a *martingale* (cf. [18]) it follows that continuity with respect to t is a sample path property for I_t (one says that I_t has *continuous sample paths*), cf. [6, p. 24].

4. Transformations of Brownian motion

Obviously, the method of computing Ito integrals from the definition, used in example 1, is rather awkward. We should have an analog of the fundamental theorem of calculus. This is provideed by the special case of the *Ito formula* (17) below. If g is a function $\mathbb{R} \times \mathbb{R}^n \to \mathbb{R}$ with continuous second derivatives, and $f(\tau, \omega) = g(\tau, W_\tau(\omega))$ in the Ito integral above, then it follows by the approximation procedure defining the Ito integral and properties of the Brownian motion, that

$$g(t, W_t(\omega)) = g(0,0) + \int_0^t \left(\frac{\partial g}{\partial t}\big(\tau, W_\tau(\omega)\big) + \frac{1}{2}(\nabla \cdot \nabla g)\big(\tau, W_\tau(\omega)\big)\right) \mathrm{d}\tau + \int_0^t (\nabla g)\big(\tau, W_\tau(\omega)\big) \cdot \mathrm{d}W_t(\omega). \tag{16}$$

This formula is a special case of *Ito's formula* (25) below, and is usually written in differential form,

$$\mathrm{d}g(t, W_t) = \left(\frac{\partial g}{\partial t}(t, W_t) + \frac{1}{2}(\nabla \cdot \nabla g)(t, W_t)\right) \mathrm{d}t + (\nabla g)(t, W_t) \cdot \mathrm{d}W_t. \tag{17}$$

It is convenient to summarize this formula in terms of a Taylor expansion

$$\begin{aligned} \mathrm{d}g = {} & \frac{\partial g}{\partial t}\,\mathrm{d}t + (\nabla g) \cdot \mathrm{d}W + \frac{1}{2}\frac{\partial^2 g}{\partial t^2}\,\mathrm{d}t^2 \\ & + \frac{1}{2}\left(\nabla \frac{\partial g}{\partial t}\right) \mathrm{d}W_t\,\mathrm{d}t + \frac{1}{2}(\nabla \otimes \nabla g) : \mathrm{d}W_t \otimes \mathrm{d}W_t \\ & + \frac{1}{6}(\nabla \otimes \nabla \otimes \nabla g) :: \mathrm{d}W_t \otimes \mathrm{d}W_t \otimes \mathrm{d}W_t + \cdots \end{aligned} \tag{18}$$

and the following *basic rules for the Ito calculus*:

$$\mathrm{d}W_t \otimes \mathrm{d}W_t = I\,\mathrm{d}t, \qquad \mathrm{d}W\,\mathrm{d}t = 0, \qquad \mathrm{d}t\,\mathrm{d}t = 0, \qquad \mathrm{d}W_t \otimes \mathrm{d}W_t \otimes \mathrm{d}W_t = 0. \tag{19}$$

Example 2. We have now a simpler method to compute the integral $\int_0^t W_\tau\,\mathrm{d}W_\tau$. Choose $g(t, X) = X^2/2$ (which would be a primitive function of our integrand X in classical calculus). Ito's formula (17) yields $W_t^2 = g(W_t) = \int_0^t g'(W_\tau)\,\mathrm{d}W_\tau + (1/2)g''(W_\tau)\,\mathrm{d}\tau = \int_0^t W_\tau\,\mathrm{d}W_\tau + (1/2)t$.

5. Ito processes

The formula (17) leads to the notion of an m-dimensional *Ito process* driven by n-dimensional Brownian motion W_t, which is an m-dimensional stochastic process X_t given by a sum of a usual integral and an Ito integral,

$$X_t = X_0 + \int_0^t A(\tau, \omega)\,\mathrm{d}\tau + B(\tau, \omega) \cdot \mathrm{d}W_\tau. \tag{20}$$

This is usually written is the differential form

$$\mathrm{d}X_t = A(t, \omega)\,\mathrm{d}t + B(t, \omega) \cdot \mathrm{d}W_t. \tag{21}$$

Here, A is a vector, the *drift vector*, and B is a matrix, the *diffusion matrix*, of the Ito process. For a review of the tensor notation used, see appendix. For the integral of the right-hand side of (20) to be defined, we require that

$$\int_0^t \left\| A(\tau, \omega) \right\| + \left\| B(\tau, \omega) \right\|^2 \mathrm{d}\tau < \infty \tag{22}$$

for all $t > 0$ almost surely, and that A, B are adapted, cf. [18, pp. 34 and 44].

6. Ito's calculus

Suppose that X_t is an m-dimensional Ito process (21), and that $x : \mathbb{R}^m \to \mathbb{R}^k$ is a twice continuously differentiable vector-valued function. Then it follows from the definition of the Ito integral and the basic rules (18) and (19) that $x_t = x(X_t)$ is a k-dimensional Ito process driven by the same n-dimensional Brownian motion W_t as X_t, and satisfying the equation

$$\mathrm{d}x_t = \mathrm{d}X_t \cdot (\nabla \otimes x)(X_t) + \frac{1}{2}(\mathrm{d}X_t \otimes \mathrm{d}X_t) : (\nabla \otimes \nabla \otimes x)(X_t), \tag{23}$$

and (19) amounts to

$$\mathrm{d}X_t \otimes \mathrm{d}X_t = (A\,\mathrm{d}t + B \cdot \mathrm{d}W_t) \otimes (A\,\mathrm{d}t + B \cdot \mathrm{d}W_t) = \left(B \cdot B^{\mathrm{T}}\right) \mathrm{d}t. \tag{24}$$

Hence, we obtain

$$\mathrm{d}x_t = a(t, \omega)\,\mathrm{d}t + b(t, \omega) \cdot \mathrm{d}W_t, \tag{25}$$

so x_t is an Ito process on $\mathbb{R}^k$ with drift vector

$$a(t, \omega) = A(t, \omega) \cdot (\nabla \otimes x)\big(X_t(\omega)\big) + \frac{1}{2}\big(B(t, \omega) \cdot B^{\mathrm{T}}(t, \omega)\big) : (\nabla \otimes \nabla \otimes x)\big(X_t(\omega)\big) \tag{26}$$

and diffusion matrix

$$b(t, \omega) = (\nabla \otimes x)^{\mathrm{T}}\big(X_t(\omega)\big) \cdot B(t, \omega). \tag{27}$$

In case $m = n$ and x is a diffeomorphism, (25) provides a change of variables formula for Ito processes, and we say that x_t is the Ito process obtained from X_t by the change of variables $x = x(X)$. In this case, $\nabla \otimes x$ is invertible, and we can compute A, B in terms of a, b, namely,

$$B(t,\omega) = J^{\mathrm{T}}\big(X_t(\omega)\big) \cdot b(t,\omega) \tag{28}$$

and

$$A(t,\omega) = a(t,\omega) \cdot J\big(X_t(\omega)\big) - \frac{1}{2}\big(B \cdot B^{\mathrm{T}}\big)(t,\omega) : J\big(X_t(\omega)\big) \cdot (\nabla \otimes x)^{-1}\big(X_t(\omega)\big), \tag{29}$$

where J is the Jacobian of $X \mapsto x$,

$$J(X) = (\nabla \otimes x)^{-1}(X).$$

In case x is a scalar function ($m = 1$), Ito's formula can be written

$$\mathrm{d}x_t = \mathrm{d}X_t \cdot (\nabla x)(X_t) + \frac{1}{2}\big(B \cdot B^{\mathrm{T}}\big)\,\mathrm{d}t : (\nabla \otimes \nabla x)(X_t). \tag{30}$$

7. Ito diffusions

If A and B in an Ito process X_t in (21) depends only on $X_t(\omega)$ itself, we say that (21) is an *Ito stochastic differential equation*:

$$\mathrm{d}X_t(\omega) = A\big(X_t(\omega)\big)\,\mathrm{d}t + B\big(X_t(\omega)\big) \cdot \mathrm{d}W_t, \tag{31}$$

and we say that X_t is an *Ito diffusion*. Under natural conditions on A and B, the existence and uniqueness of initial value problems for an Ito diffusion satisfying (31) can be established. We refer to [18] for details.

Suppose that X_t is an Ito diffusion satisfying (31), and $x_t = x(X_t)$ defined as above. Then x_t is also an Ito diffusion, satisfying the Ito stochastic differential equation

$$\mathrm{d}x_t = Lx(X_t)\,\mathrm{d}t + \mathrm{d}W_t \cdot Dx(X_t), \tag{32}$$

where L and D are *differential operators* defined by

$$Lx(X) = A(X) \cdot (\nabla \otimes x)(X) + \frac{1}{2}\big(B(X) \cdot B^{\mathrm{T}}(X)\big) : (\nabla \otimes \nabla \otimes x)(X) \tag{33}$$

and

$$Dx(X) = B^{\mathrm{T}} \cdot (\nabla \otimes x)(X). \tag{34}$$

Moreover, X_t fullfills a *scaling relation* similar to the well-known Brownian scaling, namely, that the process

$$LX_{Tt} \tag{35}$$

is equal in distribution with an Ito diffusion $\widetilde{X}_t$ satisfying the Ito equation

$$\mathrm{d}\widetilde{X}_t = \widetilde{A}\big(\widetilde{X}_t\big)\,\mathrm{d}t + \widetilde{B}\big(\widetilde{X}_t\big)\,\mathrm{d}\widetilde{W}_t. \tag{36}$$

Here $\widetilde{W}_t$ is a standard Brownian motion obtained by the Brownian scaling

$$\widetilde{W}_t = T^{-1/2} W_{Tt}, \tag{37}$$

and the scaled drift vector and diffusion matrix is

$$\widetilde{A}(\widetilde{X}) = LTA(\widetilde{X}/L), \qquad \widetilde{B}(\widetilde{X}) = LT^{1/2}B(\widetilde{X}/L). \tag{38}$$

8. Ito diffusions on hypersurfaces

By a smooth hypersurface in $\mathbb{R}^n$ we mean a level set $F^{-1}(c)$ of a smooth function $F:\mathbb{R}^n \to \mathbb{R}$ such that $\nabla F(X) \neq 0$ for all $X \in F^{-1}(c)$ (cf. [19]). Hence, with this definition all hypersurfaces are orientable (cf. [20, p. 146]). Moreover, a hypersurface in $\mathbb{R}^n$ is a smooth imbedding in $\mathbb{R}^n$ of codimension 1 as a consequence of the implicit function theorem (cf. [21, p. 31]). The values $c \in \mathbb{R}$ for which $F^{-1}(c)$ is a hypersurface are called *regular values* for F. By Sard's theorem (cf. [22, p. 11]), the set of values which are not regular has Lebesgue measure 0. Hence, $F^{-1}(c)$ is a hypersurface for a dense set of values $c \in \mathbb{R}$. We assume henceforth that $c = 0$ is a regular value, and denote $F^{-1}(0)$ by M. The following theorem gives a necessary and sufficient condition for the Ito diffusion X_t in (31) to be on M.

Theorem 1 (Imbedding method). Assume that X_t is an Ito diffusion on $\mathbb{R}^n$ given by (31), and that 0 is a regular value for a given smooth function $F:\mathbb{R}^n \to \mathbb{R}$. Let $M = F^{-1}(0)$, and let be defined by

$$N(X) = \frac{\nabla F(X)}{\|\nabla F(X)\|} \tag{39}$$

the corresponding normal vector field, defined in a neighbourhood of M. Also assume that $X_0 \in M$. Then $X_t \in M$ for all $t > 0$ almost surely, if and only if A and B in (31) fulfill the conditions

$$A(X) \cdot N(X) + \frac{1}{2}\big(B(X) \cdot B^{\mathrm{T}}(X)\big) : (\nabla \otimes N)(X) = 0 \tag{40}$$

for all $X \in M$, and

$$B^{\mathrm{T}}(X) \cdot N(X) = 0 \tag{41}$$

for all $X \in M$. Moreover, if (40) and (41) hold, the differential operators L, defined by (33), and D, defined by (34), are well-defined differential operators on M.

Proof. Let $x_t = F(X_t)$. Then by Ito's formula (32), $\mathrm{d}x_t = LF(X_t)\,\mathrm{d}t + \mathrm{d}W_t \cdot DF(X_t)$. By uniqueness of solutions to Ito SDE's (cf. [18]), $x_t = 0$ almost surely if and only if $\mathrm{d}x_t = 0$. This is equivalent to $LF(X_t) = 0$ and $DF(X_t) = 0$ by the independence of the Ito differentials $\mathrm{d}W_t$ and the ordinary differential $\mathrm{d}t$ (interpreted as Ito integrals, as usual). Obviously, $DF(X) = 0$ on M is equivalent to (41) in view of (39). Furthermore, provided (41) holds, $LF(X) = 0$ on M is equivalent to (40) since

$$(\nabla \otimes N) = \left(\frac{\nabla \otimes \nabla F}{\|\nabla F\|} + \nabla\left(\frac{1}{\|\nabla F\|}\right) \otimes \nabla F\right)$$

and

$$\left(B \cdot B^{\mathrm{T}}\right) : \left(\nabla\left(\frac{1}{\|\nabla F\|}\right) \otimes \nabla F\right) = \left(B^{\mathrm{T}} \cdot \nabla\left(\frac{1}{\|\nabla F\|}\right)\right) \cdot \left(B^{\mathrm{T}} \cdot \nabla F\right) = 0. \qquad (42)$$

If $\phi : \mathbb{R}^n \to \mathbb{R}$ is a function which is constant on M, then $\nabla\phi = \psi N$ on M for some smooth function $\psi : \mathbb{R}^n \to \mathbb{R}$, and

$$D\phi = \psi B^{\mathrm{T}} \cdot N = 0$$

on M by (41), which shows that D is a well-defined linear operator on M. Furthermore,

$$L\phi = \psi\left(A \cdot N + \frac{1}{2}\left(B \cdot B^{\mathrm{T}}\right) : (\nabla \otimes \nabla N)\right) + \frac{1}{2}\left(B^{\mathrm{T}} \cdot B\right) : (\nabla\psi \otimes N) = 0$$

on M by (40) and a similar computation as (42), which shows that L is a well-defined linear operator on M. This proves the theorem. □

Remark 1. The condition (41) means that the range of $B(X)$ should be in the tangent space of M at X for all $X \in M$, and the condition (40) means a specification of the normal component of the drift vector, in terms of the diffusion matrix B. Hence, the diffusion matrix is singular (has rank $n-1$), and the probability density of X_t is a singular measure, supported on the hypersurface (in fact, having a smooth probability density on the surface). Also, we see that the conditions on A and B depends on N, hence, independent of the particular choice of function F representing M as a level set. With this imbedding method, Ito diffusions on M may be numerically simulated by standard methods for Ito diffusions in $\mathbb{R}^n$, cf. [23,24]. Applications of this method to problems in relaxation theory are in progress and will be reported elsewhere. Related work of the authors may be found in [25].

9. Brownian motion on hypersurfaces

In this section we use the imbedding method of theorem 1 to define a natural generalization of standard Brownian motion to a smooth $(n-1)$-dimensional imbedded surface in $\mathbb{R}^n$. By the scaling relation in section 7, we may also define Brownian motion with a diffusion constant on the hypersurface.

To define Brownian motion on M, we choose $B(X)$ to be the projection onto the tangent plane of the level set M of F at X, i.e.,

$$B(X) = I - N(X) \otimes N(X). \qquad (43)$$

Clearly, this choice of B satisfies (41). Then we choose $A(X)$ be the a normal vector field, hence, completely specified by (40), i.e.,

$$A = -\frac{1}{2}\big(B(X) \cdot B^{\mathrm{T}}(X)\big) : (\nabla \otimes N)(X)N(X). \tag{44}$$

The restriction of the vector-valued first-order operator D and the scalar-valued second-order operator $2L$ to the level set M are called the *covariant derivative* or *gradient* on M, and the *Laplace–Beltrami operator* on M, respectively.

10. Local coordinates

So far we have considered the $(n-1)$-dimensional hypersurface imbedded in $\mathbb{R}^n$, as an implicitly defined surface, which often is convenient. However, sometimes we are given local coordinates for the imbedded hypersurface, which we consider in this section.

We henceforth assume that X_t is a standard Brownian motion on M, as defined in section 9. Let $f : U \to M$ be a local coordinate patch on M. We will calculate the Ito equation for X_t in local coordinates, i.e., the Ito equation for x_t where

$$f(x_t) = X_t. \tag{45}$$

Given the local parametrization $f(x^1, \ldots, x^{n-1}) \in \mathbb{R}^n$ and a function $F : \mathbb{R}^n \to \mathbb{R}$ such that $F(f(x^1, \ldots, x^{n-1})) \equiv 0$, we extend f to a mapping $\mathbb{R}^n \to \mathbb{R}^n$ such that in a neighbourhood of $f(U)$,

$$F\big(f\big(x^1, \ldots, x^{n-1}, x^n\big)\big) = x^n, \tag{46}$$

i.e., $f(\cdot, x^n)$ is a parametrization of the level set of F at level x^n (for all x^n in some open interval containing 0). The extension $f(x^1, \ldots, x^n)$ is defined as

$$f\big(x^1, \ldots, x^n\big) = \phi\big(x^n\big),$$

where ϕ is the unique solution to the initial value problem

$$\frac{\mathrm{d}\phi(t)}{\mathrm{d}t} = \frac{\nabla F(\phi)}{\|\nabla F(\phi)\|^2}, \qquad \phi(0) = f\big(x^1, \ldots, x^{n-1}\big).$$

Next, we do a change of coordinates by the diffeomorphism f constructed above. To compute derivatives in the x-coordinates we apply the chain rule,

$$\nabla_X = (\nabla_X \otimes x) \cdot \nabla_x = (\nabla_x \otimes X)^{-1} \cdot \nabla_x.$$

Let the vectors $f_1, \ldots, f_n$ be the row vectors of $\nabla_x \otimes X$, i.e., $f_j = \partial f/\partial x^j$. Clearly, $f_j(x^1, \ldots, x^n)$, $j = 1, \ldots, n-1$, are tangent vector fields to the level sets $F = x^n$, and $f_n(x^1, \ldots, x^n)$ is a normal vector field to the same level set. Moreover, $f_1, \ldots, f_n$

are linearly independent, and hence, constitute a frame in $\mathbb{R}^n$, since f is a local diffeomorphism. We define the dual basis $f^1, \ldots, f^n$ as the column vectors of $(\nabla_x \otimes X)^{-1}$, hence,

$$f^i \cdot f_j = \delta^i_j, \tag{47}$$

and we have the natural decomposition of the identity matrix,

$$I = \sum_{i=1}^{n} f^i \otimes f_i = \sum_{i=1}^{n} f_i \otimes f^i. \tag{48}$$

Moreover, the chain rule can be written

$$\frac{\partial}{\partial x^j} = f_j \cdot \nabla, \quad j = 1, \ldots, n, \quad \text{or equivalently,} \quad \nabla = \sum_{i=1}^{n} f^i \frac{\partial}{\partial x^i}. \tag{49}$$

Also, differentiation of (47) yields

$$\frac{\partial f^i}{\partial x^k} \cdot f_j = -f^i \cdot \frac{\partial f_j}{\partial x^k}. \tag{50}$$

The matrices

$$G = (\nabla \otimes X) \cdot (\nabla \otimes X)^{\mathrm{T}} \quad \text{and} \quad G^{-1} \tag{51}$$

are called the contravariant and covariant metric tensors, and we denote their elements

$$g_{ij} = f_i \cdot f_j, \qquad g^{ij} = f^i \cdot f^j. \tag{52}$$

The metric tensor G is thus decomposed into a "tangential" and a "normal" part

$$G = G_{\parallel} \oplus G_{\perp} = \begin{pmatrix} G_{\parallel} & 0 \\ 0 & G_{\perp} \end{pmatrix}, \tag{53}$$

where $G_{\parallel}$ is the usual covariant metric tensor of the level set.

We have seen by Ito's formula (32), applied to the Ito diffusion X_t and the mapping $x(X)$, that x_t is an Ito diffusion with drift vector a and diffusion matrix b given by

$$a(x) = Lx\big(X(x)\big), \qquad b(x) = Dx\big(X(x)\big). \tag{54}$$

Hence, to compute a and b we must transform L and D to the x-coordinates. From the decomposition (48) and the fact that $\{f_1, \ldots, f_{n-1}\}$ as well as $\{f^1, \ldots, f^{n-1}\}$ span the tangent space we have that the projection onto the tangent space is

$$B = \sum_{i=1}^{n-1} f^i \otimes f_i = \sum_{i=1}^{n-1} f_i \otimes f^i. \tag{55}$$

The operator D in local coordinates is then

$$D = B^{\mathrm{T}} \cdot \nabla = \sum_{j=1}^{n} \big(f^j \otimes f_j\big) \cdot \nabla = \sum_{j=1}^{n} f^j (f_j \cdot \nabla) = \sum_{j=1}^{n} f^j \frac{\partial}{\partial x^j}. \tag{56}$$

To transform L to local coordinates, first note that since B is a projection we have $B^{\mathrm{T}} = B$ and $B^2 = B$, hence,

$$B \cdot B^{\mathrm{T}} = B. \tag{57}$$

By a similar computation as (42), we may write A in the form

$$A = -\frac{1}{2}\big(B \cdot B^{\mathrm{T}}\big) : \big(\nabla \otimes f^n\big) f_n \tag{58}$$

and then use (57), (48), (49) and (50) to compute the first-order term of L,

$$A \cdot \nabla = \frac{1}{2} \sum_{i=1}^{n-1} \sum_{j=1}^{n} g^{ij} \frac{\partial f_j}{\partial x^i} \cdot f^n \frac{\partial}{\partial x^n}.$$

A similar computation shows that the second-order term of L is

$$\frac{1}{2}\big(B \cdot B^{\mathrm{T}}\big) : (\nabla \otimes \nabla) = \frac{1}{2} \sum_{i=1}^{n-1} \sum_{j=1}^{n} g^{ij} \left(\frac{\partial^2}{\partial x^j \partial x^k} - \sum_{k=1}^{n} \frac{\partial f_i}{\partial x^j} \cdot f^k \frac{\partial}{\partial x^k} \right).$$

Hence, when adding the first- and second-order terms to compute L the $\partial/\partial x^n$-terms cancel and we get

$$L = \frac{1}{2} \sum_{i,j=1}^{n-1} g^{ij} \left(\frac{\partial^2}{\partial x^i \partial x^j} - \sum_{k=1}^{n-1} \frac{\partial f_i}{\partial x^j} \cdot f^k \frac{\partial}{\partial x^k} \right). \tag{59}$$

The absence of $\partial/\partial x^n$ is a reflection of the fact that L is a differential operator on M. We introduce the common notation

$$\Gamma_{ij}^k \equiv \frac{\partial f_i}{\partial x^j} \cdot f^k \tag{60}$$

which are commonly called the *Christoffel symbols*. Hence, in view of the decomposition (48),

$$\frac{\partial f_i}{\partial x^j} = \sum_{k=1}^{n} \Gamma_{ij}^k f_k. \tag{61}$$

Now we may compute the drift vector and diffusion matrix in local coordinates,

$$a = Lx = -\frac{1}{2} \sum_{i,j,k=1}^{n-1} g^{ij} \Gamma_{ij}^k e_k \tag{62}$$

and

$$b = Dx = \sum_{i=1}^{n-1} f^i \otimes e_i, \tag{63}$$

where $(e_1, \ldots, e_n) = I$, i.e., e_j, $j = 1, \ldots, n$ is the standard basis in $\mathbb{R}^n$. Miraculously, the Christoffel symbols may be computed from the metric tensor components,

$$\Gamma^k_{ij} = \frac{1}{2} g^{kl} \left(\frac{\partial g_{lj}}{\partial x_i} + \frac{\partial g_{il}}{\partial x^j} - \frac{\partial g_{ij}}{\partial x^l} \right). \tag{64}$$

Substituting (62) and (63) in (54) and using (48) and (52) we get the following Ito equations for the local coordinates of a standard Brownian motion on M:

$$\mathrm{d}x^i_t = -\frac{1}{2} \Gamma^i_{jk} g^{jk}\, \mathrm{d}t + g^{ij} (f_j \cdot \mathrm{d}W_t), \quad i = 1, \ldots, n-1. \tag{65}$$

This is an $(n-1)$-dimensional Ito equation driven by an n-dimensional standard Brownian motion. For computational purposes it is advantageous to reformulate it to an Ito equation driven by an $(n-1)$-dimensional standard Brownian motion. To this end, let the Ito diffusion w_t in the patch U be defined by

$$\mathrm{d}w^i_t = \left(g^{1/2}\right)_{ij} f^j \cdot \mathrm{d}W_t, \tag{66}$$

where $((g^{1/2})_{ij}) = G^{1/2}$ is the symmetric positive square root of G. Then

$$\mathrm{d}w^i_t\, \mathrm{d}w^k_t = \left(g^{1/2}\right)_{ij} \left(g^{1/2}\right)_{kl} g^{jl}\, \mathrm{d}t = \delta^{ik}\, \mathrm{d}t.$$

Consequently, w_t is a Brownian motion in the local coordinate patch, cf. [18, p. 145]. Hence, x_t is given by the Ito equation

$$\mathrm{d}x^i_t = -\frac{1}{2} \Gamma^i_{jk} g^{jk}\, \mathrm{d}t + \left(g^{1/2}\right)^{ij} \mathrm{d}w^j_t, \tag{67}$$

where $((g^{1/2})^{ij}) = (G^{-1})^{1/2} = G^{-1/2}$ is the symmetric positive square root of G^{-1}.

11. Correlation functions

Interaction of the anistropic molecular environment with an ensemble of nuclear spins whose is described by a semiclassical Hamiltonian, which consists of spin operators $\widehat{A}$, acting on spin degrees of freedom (wave functions), and classical lattice functions F, introducing stochastic time dependence in the Hamiltonian. Both are expressed in spherical tensor components $\widehat{A}^I_k$, F^I_k, $k = -I, \ldots, I$, and $I = 0, 1, 2, \ldots$, such that

$$H(t) = \sum_I \sum_{k=-I}^{I} (-1)^k \widehat{A}^I_{-k} F^I_k(t). \tag{68}$$

The spherical tensor components could be evaluated either in a fixed laboratory frame, in which the spherical tensor components of the tensor operator A are constant, or in a fixed molecular frame, in which the spherical tensor components of the lattice function are constant. Assume that the components in (68) are evaluated in the laboratory frame. The lattice function components are then stochastic functions because of molecular reorientation and translations [26–30]. It is convenient to introduce a local director frame d on the surface where the surface normal defines the z-axis of the d-frame. Local molecular reorientations are then taken into account by the Euler angles Ω_{dM}, describing the rotation from the director frame d to the molecular fixed principal frame M, whereas the reorientation due to lateral diffusion is taken into account by the Euler angles Ω_{Ld} for the rotation from the lab frame L to the local director frame d. The lab frame spherical tensor components of F in the lab frame are, thus,

$$F_m^{L,I}(t) = \sum_{k,\ell=-I}^{I} D_{mk}^{I*}\big(\Omega_{Ld}(t)\big) D_{k\ell}^{I*}\big(\Omega_{dP}(t)\big) F_\ell^{M,I}.$$

Here the superscripts refer to components in the lab frame L, the local director frame d and the molecular fixed frame M, respectively.

Generally a Hamiltonian which is only modulated by translational diffusion along a surface is obtained by introducing a partially averaged F, denoted by an overbar,

$$\overline{F_m^{L,I}(t)} = \sum_{k,\ell=-I}^{I} D_{mk}^{I*}\big(\Omega_{Ld}(t)\big) \overline{D_{k\ell}^{I*}(\Omega_{dP})} F_\ell^{M,I}.$$

This formulation presupposes a time scale separation between local reorientation and lateral diffusion [28]. Furthermore, symmetry arguments often apply, resulting in

$$\sum_{\ell=-I}^{I} \overline{D_{k\ell}^{I*}(\Omega_{dM})} F_\ell^{M,I} = \delta_{k0} \overline{D_{00}^{I*}(\Omega_{dM})} F_0^{M,I}$$

when a cylindrically symmetric tensor $F^{M,I}$ is assumed. Thus, only one spherical component of the partially averaged tensor is nonzero and modulated as the spin bearing molecule is moving along the curved interface. This stochastic time-dependent process is, thus, described by the orientation of the local normal present in the Wigner rotation matrix element $D_{m0}^{I*}(\Omega_{Ld}(t))$.

With these observations, the Hamiltonian H can be interpreted as a noncommutative Fourier series on the rotation group [31, p. 256], where the molecule dynamics enter through the orientational Euler angles Ω_{Ld}:

$$\begin{aligned} H(t) &= \sum_I \sum_{k=-I}^{I} (-1)^k \widehat{A}_{-k}^{L,I} \overline{D_{00}^{I*}(\Omega_{dM})} F_0^{M,I} D_{k0}^{I}\big(\Omega_{Ld}(t)\big) \\ &= \sum_I (2I+1) \operatorname{tr}\Big(\widehat{H}(I) D^I\big(\Omega_{Ld}(t)\big)\Big), \end{aligned} \tag{69}$$

where the Fourier coefficients are

$$\widehat{H}(I)_{k\ell} = (-1)^k \frac{\widehat{A}_{-k}^{L,I} \overline{D_{00}^{I*}(\Omega_{dM})} F_0^{M,I} \delta_{0\ell}}{(2I+1)}. \tag{70}$$

Remark 2. The Wigner rotation matrices are irreducible representations of the rotation group, so by the "great orthogonality theorem" of Weyl [32], elements of the matrices are orthogonal with respect to the invariant measure of the rotation group,

$$\frac{2I+1}{8\pi^2}\int_0^{2\pi}\int_0^{2\pi}\int_0^{\pi} D^I_{ii'}(\Omega)D^{J*}_{jj'}(\Omega)\sin(\beta)\,\mathrm{d}\beta\,\mathrm{d}\alpha\,\mathrm{d}\gamma = \delta_{IJ}\delta_{ii'}\delta_{jj'}, \tag{71}$$

and the Fourier coefficients of $H(t) = \widetilde{H}(\Omega(t))$ may be computed by

$$\widehat{H}(I) = \frac{1}{8\pi^2}\int_0^{2\pi}\int_0^{2\pi}\int_0^{\pi} \widetilde{H}(\alpha,\beta,\gamma)D^{I\dagger}(\alpha,\beta,\gamma)\sin(\beta)\,\mathrm{d}\beta\,\mathrm{d}\alpha\,\mathrm{d}\gamma, \tag{72}$$

where $A^\dagger$ denotes the conjugate transpose of A, i.e., $(A^\dagger)_{ij} = A^*_{ji}$, cf. [31].

Experimental data are often connected to autocorrelation functions of the lattice functions (for example, in the regime of the BWR theory of spin relaxation, all spin relaxation rates are determined in this way). This motivates the study of correlation functions of the following general form:

$$C^I_{mn}(\rho,t) = \left\langle D^I_{m0}(\Omega_0)D^{I*}_{n0}(\Omega_t)\right\rangle, \tag{73}$$

where $\Omega_t = (\alpha_t, \beta_t, 0)$ is the stochastic process obtained by computing spherical angles (β,α) for the surface normal at X_t, the canonical Brownian motion on M, with probability distribution $\rho(X)$ for X_0 on M.

12. The Rippled surface

In this section we will compute relevant correlation functions for the Rippled surface [10,11] defined by the parametrization

$$\left(X^1, X^2\right) \mapsto \left(X^1, X^2, \frac{a}{k}\sin\left(kX^1\right)\right). \tag{74}$$

It is periodic with period $2\pi/k$ in the X^1-direction.

Theorem 2.

1. Define the function $\phi : \mathbb{R} \to \mathbb{R}$ by

$$\phi(X) = \frac{E(\mathrm{i}a) - E(\cos(kX), \mathrm{i}a)}{k} \tag{75}$$

for $0 \leqslant X \leqslant \pi/k$, and

$$\phi(X) = \left\lfloor \frac{kX}{\pi} \right\rfloor \frac{2E(\mathrm{i}a)}{k} + \phi\left(X - \left\lfloor \frac{kX}{\pi} \right\rfloor \frac{\pi}{k}\right) \tag{76}$$

otherwise. Then ϕ is smooth, strictly increasing and

$$\phi'(X) = \sqrt{1 + a^2\cos^2(kX)} \tag{77}$$

and

$$\phi\left(X + \frac{m\pi}{k}\right) = \phi(X) + \frac{2mE(\,\mathrm{i}a)}{k} \tag{78}$$

for all $m \in \mathbb{Z}$.

2. Let X_t be a standard Brownian motion on M. Define the mapping $f : \mathbb{R}^2 \to \mathbb{R}^3$ by

$$f\big(x^1, x^2\big) = \left(\phi^{-1}\big(x^1\big), x^2, \frac{a}{k}\sin\big(k\phi^{-1}\big(x^1\big)\big)\right). \tag{79}$$

Then f is a parametrization of the Rippled surface (74), and the process x_t defined by $X_t = f(x_t)$ as in section 10 is a two-dimensional standard Brownian motion.

Proof. 1. Equation (77), valid for $x \neq m\pi/k, m \in \mathbb{Z}$, is obtained by differentiation of the elliptic integral and simplification. Furthermore, ϕ is continuous at $X = m\pi/k$, $m \in \mathbb{Z}$, since

$$\lim_{X\to\pi/k-}\phi(X) - \lim_{X\to 0+}\phi(X) = \int_0^{\pi/k}\sqrt{1 + a^2\cos(kx)^2}\,\mathrm{d}x = \frac{2E(\,\mathrm{i}a)}{k}, \tag{80}$$

which also proves (78). Since $\phi'(X)$ is extended to $X = m\pi/k, m \in \mathbb{Z}$, by (77) as a continuous function, it follows that the formula (77) for the derivative of ϕ is valid for $X = m\phi/k$, $m \in \mathbb{Z}$, also. Hence, ϕ' is smooth. Moreover, ϕ is strictly increasing and bijective, since the derivative is bounded between two positive constants.

2. Clearly, (79) is a reparametrization of (74). We get, in the notation of section 10,

$$f_1(x^1, x^2) = \begin{pmatrix} 1 \\ 0 \\ -a\cos(k\phi^{-1}(x^1)) \end{pmatrix}\frac{\mathrm{d}\phi^{-1}}{\mathrm{d}x^1}, \qquad f_2(x^1, x^2) = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}. \tag{81}$$

The tangential part of the metric tensor is

$$\begin{aligned} G_\| &= \begin{pmatrix} f_1\cdot f_1 & f_1\cdot f_2 \\ f_2\cdot f_1 & f_2\cdot f_2 \end{pmatrix} \\ &= \begin{pmatrix} (1 + a^2\cos^2(2\pi X^1(x^1))(\mathrm{d}\phi^{-1}/\mathrm{d}x^1)^2 & 0 \\ 0 & 1 \end{pmatrix} \\ &= \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \end{aligned} \tag{82}$$

where the last equality follows from (77), since

$$\frac{\mathrm{d}\phi^{-1}}{\mathrm{d}x^1} = \frac{1}{(\mathrm{d}\phi/\mathrm{d}X^1)} = \frac{1}{\sqrt{1 + a^2\cos^2(kX^1)}}.$$

Hence, $\Gamma^k_{ij} = 0$ by (64), and subsitution in (67) gives the Ito equation

$$\mathrm{d}x_t = \mathrm{d}w_t$$

for x_t. Hence, $\mathrm{d}x_t$ is a standard Brownian motion. □

Remark 3. Here $E(\mathrm{i}a)$ and $E(z, \mathrm{i}a)$ denotes ellipic integrals, see table 1 in appendix C, and cf. [33] for more information. Depending on the choice of branch cuts for $E(z, \mathrm{i}a)$ at $z = \pm 1$, the formula for $\phi(X)$ may have singularities at $x = m\pi/k$, $m \in \mathbb{Z}$, but a continuous branch can always be computed by the formulas (75) and (76), where $\lfloor X \rfloor$ denotes the largest integer $\leqslant X$.

We are now ready to formulate the main theorem of this paper, a representation formula for correlation functions on the Rippled surface.

Theorem 3. Let $q(X) = q(X^1)$ and $r(X) = r(X^1)$ be complex-valued functions defined on the Rippled surface (74), independent of X^2 and periodic in X^1 with period $2\pi/k$. Then the correlation function

$$C(q, r)(t) \equiv \langle q(X_0) r^*(X_t) \rangle \tag{83}$$

has the generalized Fourier series representation

$$C(q, r)(t) = \sum_{m=-\infty}^{\infty} c_m(\rho q) c_m^*(r) \mathrm{e}^{-\lambda_m t}, \tag{84}$$

where the Fourier coefficients are given by

$$c_m(q) = \frac{1}{\sqrt{\ell}} \int_0^{2\pi/k} \mathrm{e}^{-(2\pi \mathrm{i}/\ell) m \phi(X^1)} q\big(X^1\big) \, \mathrm{d}\phi\big(X^1\big) \tag{85}$$

and

$$\lambda_m = \frac{2\pi^2 m^2}{\ell^2} \tag{86}$$

and

$$\ell = \frac{4E(\mathrm{i}a)}{k} \tag{87}$$

and

$$\rho\big(X^1\big) = \sum_{j \in \mathbb{Z}} \int_{-\infty}^{\infty} f_{X_0}\left(X^1 + \frac{2\pi j}{k}, X^2\right) \mathrm{d}X^2. \tag{88}$$

Usually we choose f_{X_0} such that the "reduced" probability distribution ρ on the interval $[0, 2\pi/k]$ is constant, $\rho(X^1) \equiv k/2\pi$.

Proof. First note that Rippled surface is periodic in x^1 with period ℓ. Since $x_t^1 = w_t^1$ and $x_t^2 = w_t^2$ are independent, and we are computing correlation function of quantities which are independent of x^2, we can average over one-dimensional trajectories x_t^1 only. Moreover, by the periodicity in x^1 it suffices to compute trajectories on the interval $[0, \ell]$ with periodic boundary conditions, and initial distribution ρ obtained by summing over all periods (88). For one-dimensional Brownian motion with periodic boundary conditions on the finite interval $[0, \ell]$ there is a well-known representation of the conditional probability density $p(x, t|y, 0)$ as Fourier series, namely,

$$p(x, t \mid y, 0) = \frac{1}{\ell} \sum_{m=-\infty}^{\infty} \mathrm{e}^{2\pi \mathrm{i}\, m(x-y)/\ell - 2\pi^2 m^2 t/\ell^2}. \tag{89}$$

Consequently,

$$\begin{aligned}
\langle q(x_0^1) r^*(x_t^1)\rangle &= \int\int p(x^1, t \mid y^1, 0)\rho(\phi^{-1}(y^1)) q(\phi^{-1}(y^1)) r^*(\phi^{-1}(x^1))\, \mathrm{d}x^1\, \mathrm{d}y^1 \\
&= \frac{1}{\ell} \sum_{m=-\infty}^{\infty} \mathrm{e}^{-2\pi^2 m^2 t/\ell^2} \Bigg[\bigg(\int_0^\ell \mathrm{e}^{(2\pi i/\ell)mx^1} q(\phi^{-1}(x^1))\, \mathrm{d}x^1\bigg) \\
&\qquad \times \bigg(\int_0^\ell \mathrm{e}^{-(2\pi \mathrm{i}/\ell)my^1} \rho(\phi^{-1}(y^1)) q(\phi^{-1}(y^1))\, \mathrm{d}y^1\bigg)\Bigg].
\end{aligned}$$

Making the change of variables $x^1 = \phi(X^1)$, $y^1 = \phi(Y^1)$ yields the representation formula (84). □

Remark 4. If we choose p, q to be Wigner rotation matrix elements like in the correlation functions (73), they can in general can be written in terms of reduced rotation matrices (cf. [34, p. 22–24])

$$D_{j0}^2(\alpha, \beta) = \mathrm{e}^{-\mathrm{i} j\alpha} d_{j0}^2(\beta),$$

and for the Rippled surface we get

$$D_{00}^2 = \frac{1}{2}\left(\frac{2 - a^2\cos(kX^1)^2}{1 + a^2\cos(kX^1)^2}\right), \tag{90}$$

$$D_{10}^2 = \frac{\sqrt{6}}{2}\left(\frac{\cos(kX^1)}{1 + a^2\cos(kX^1)^2}\right), \tag{91}$$

$$D_{20}^2 = \frac{\sqrt{6}}{4}\left(\frac{a^2\cos(kX^1)^2}{1 + a^2\cos(kX^1)^2}\right). \tag{92}$$

Using the periodicity (78) we may write the Fourier coefficients (85) as

$$c_m(q) = \frac{1}{\sqrt{\ell}} \int_0^{\pi/k} \mathrm{e}^{(-2\pi i/\ell)m\phi,(X^1)} \left(q(X^1) + (-1)^m q\left(X^1 + \frac{\pi}{k}\right)\right) \mathrm{d}\phi(X^1), \tag{93}$$

where ϕ is given by (75). In particular, for the Wigner rotation matrix elements (90) we see that

$$c_m(D^2_{j0}) = 0$$

if m and j have the opposite parity (odd/even or even/odd). In particular, for $m = 0$ we can obtain the averages

$$\langle D^2_{j0}\rangle = \frac{1}{\ell}\int_0^{2\pi/k} D^2_{j0}\sqrt{1 + a^2\cos\bigl(kX^1\bigr)^2}\,\mathrm{d}X^1,$$

in closed form,

$$\langle D^2_{00}\rangle = \frac{1}{2}\left(\frac{3K(\mathrm{i}a) - E(\mathrm{i}a)}{E(\mathrm{i}a)}\right), \tag{94}$$

$$\langle D^2_{10}\rangle = 0, \tag{95}$$

$$\langle D^2_{20}\rangle = \frac{\sqrt{6}}{4}\left(\frac{E(\mathrm{i}a) - K(\mathrm{i}a)}{E(\mathrm{i}a)}\right). \tag{96}$$

For definitions of the elliptic integrals E and K, see appendix C. Plots of these averages as functions of a can be found in the appendix. The integrals were obtained by first computing primitive functions symbolically (with Maple V Release 4) and then taking differences, taking into account the discontinuities of the primitive functions at $x = 1/2$.

Appendix A. Notation

- $\mathbb{R}$ denotes the set of real numbers.
- $\mathbb{R}^n = \{(x_1, \ldots, x_n)\colon\ x_1, \ldots, x_n \in \mathbb{R}\}$ denotes the n-dimensional space, where n is a positive integer. The dimension of a hypersurface is $n - 1$.
- $\mathbb{R}_+ = \{x \in \mathbb{R} : x > 0\}$ is the set of positive real numbers.
- $\mathbb{Z}$ denotes the set of integers.
- $\lfloor x \rfloor$ denotes the largest integer which is less than or equal to the real number x.
- z^* denotes the complex conjugate of the complex number z. In case z is a vector or a matrix, z^* denotes elementwise complex conjugation.
- W_t denotes a Brownian motion in $\mathbb{R}^n$, with components $(W_t^1, \ldots, W_t^n)$.
- I is the identity matrix, with dimension evident from context.
- ω is a sample in a probability space where random variables are defined. For canonical Brownian motion on $\mathbb{R}^n$, ω is a continuous path on $\mathbb{R}^n$ (i.e., a continuous mapping $\omega : \mathbb{R} \to \mathbb{R}^n$).
- $E(X)$ or $\langle X\rangle$ is the expectation of the random variable X.
- $p(X, t \mid X_0, t_0)$ is the conditional probability density for a standard Brownian motion, defined in (9).

- $\cdot$ denotes a general tensor contraction product, applicable to two vectors (ordinary scalar product), a matrix and a vector (ordinary matrix product), defined in general by

$$(A \cdot B)_{i_1 \ldots i_{k-1} j_2 \ldots j_l} = \sum_{m=1^n} A_{i_1 \ldots i_{k-1} m} B_{m j_2 \ldots j_l}.$$

- $:$ denotes a double contraction,

$$(A : B)_{i_1 \ldots i_{k-2} j_3 \ldots j_l} = \sum_{m_1, m_2 = 1}^{n} A_{i_1 \ldots i_{k-2} m_1 m_2} B_{m_1 m_2 j_3 \ldots j_l}.$$

- $::$ denotes a triple contraction (analogous to $:$).
- $\|A\|$ denotes the norm of the vector or matrix A, i.e., $\|A\| = (A \cdot A)^{1/2}$ for vectors, $\|A\| = (A : A)^{1/2}$ for matrices.
- $\otimes$ denotes the tensor product, defined by

$$(A \otimes B)_{i_1 \ldots i_k j_1 \ldots j_l} = A_{i_1 \ldots i_k} B_{j_1 \ldots j_l}.$$

- $\nabla = (\partial/\partial X^1, \ldots, \partial/\partial X^n)$ denotes the gradient operator in $\mathbb{R}^n$, acting to the right. For example,

$$f(\nabla \otimes \nabla) g = f \begin{pmatrix} \dfrac{\partial^2 g}{\partial X^1 \partial X^1} & \cdots & \dfrac{\partial^2 g}{\partial X^1 \partial X^n} \\ \vdots & \ddots & \vdots \\ \dfrac{\partial^2 g}{\partial X^n \partial X^1} & \cdots & \dfrac{\partial^2 g}{\partial X^n \partial X^n} \end{pmatrix}.$$

- $\oplus$ denotes the direct sum of matrices, so

$$A \oplus B = \begin{pmatrix} A & 0 \\ 0 & B \end{pmatrix}.$$

Appendix B. Order parameters for Rippled surface

Averages of some Wigner rotation matrix elements are given in figures 1–4 for the Rippled surface, with parametrization

$$X^3 = \frac{a}{k} \sin\bigl(k X^1\bigr).$$

The averages are functions of the nondimensional parameter a.

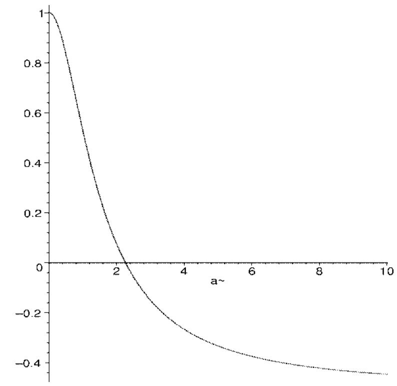

Figure 1. $\langle D^2_{00} \rangle$ versus a.

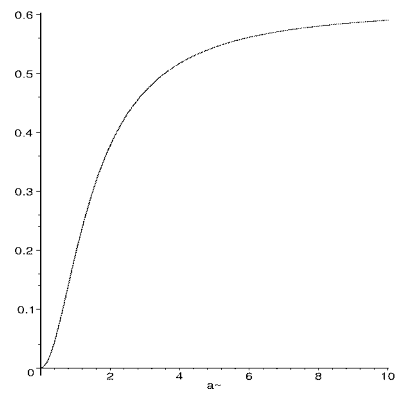

Figure 2. $\langle D^2_{22} \rangle$ versus a.

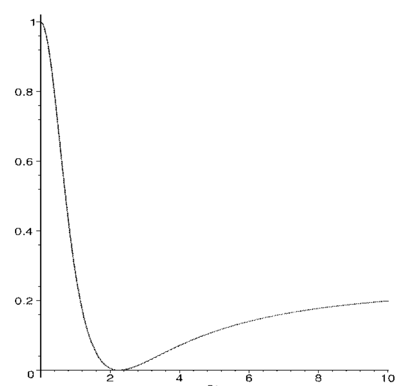

Figure 3. $S_0 = \langle D^2_{00} \rangle$ versus a.

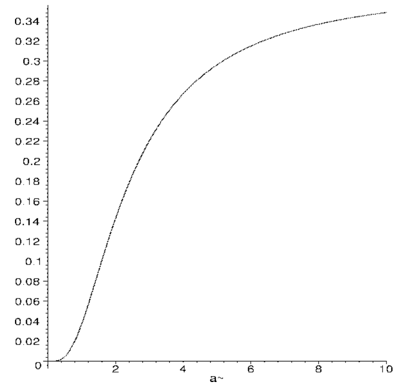

Figure 4. $S_2 = \langle D_{22}^2 \rangle$ versus a.

Table 1
Elliptic integrals.

Type	Definition	Maple
Incomplete, first kind	$F(z,k) = \int_0^z \frac{1}{\sqrt{(1-t^2)(1-k^2t^2)}}\,\mathrm{d}t$	`EllipticF(z,k)`
Complete, first kind	$K(k) = F(1,k)$	`EllipticK(k)`
Incomplete, second kind	$E(z,k) = \int_0^z \frac{\sqrt{1-k^2t^2}}{\sqrt{1-t^2}}\,\mathrm{d}t$	`EllipticE(z,k)`
Complete, second kind	$E(k) = E(1,k)$	`EllipticE(k)`

Appendix C. Elliptic integrals

For the elliptic integrals used in the paper, see table 1. Formulas involving elliptic integrals were obtained with the computer algebra program Maple from Waterloo Maple Software, and the corresponding Maple functions are given in the third column.

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