

# Stochastic Analysis: Classical and Quantum

Perspectives of White Noise Theory

Takeyuki Hida  
editor

0211.6-53

S264

2004

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Meijo University, Nagoya, Japan  
1–5 November 2004

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*Meijo University, Nagoya, Japan*  
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E200602046

 **World Scientific**

NEW JERSEY • LONDON • SINGAPORE • BEIJING • SHANGHAI • HONG KONG • TAIPEI • CHENNAI

*Published by*

World Scientific Publishing Co. Pte. Ltd.

5 Toh Tuck Link, Singapore 596224

USA office: 27 Warren Street, Suite 401-402, Hackensack, NJ 07601

UK office: 57 Shelton Street, Covent Garden, London WC2H 9HE

**British Library Cataloguing-in-Publication Data**

A catalogue record for this book is available from the British Library.

**STOCHASTIC ANALYSIS: CLASSICAL AND QUANTUM  
Perspectives of White Noise Theory**

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ISBN 981-256-526-4

Printed in Singapore by B & JO Enterprise

# Stochastic Analysis: Classical and Quantum

Perspectives of White Noise Theory

## Preface

We felt that time has come for a new epoch in stochastic analysis. Indeed various fields in mathematics as well as related fields in science continue to cross-fertilize each other, while keeping good relationships with probability theory. There, dominant roles have been played by stochastic analysis (classical and quantum).

It therefore seems to be a good opportunity to organize a conference on important topics in stochastic analysis. Almost three decades has passed since white noise analysis was launched, we thus plan to have perspectives of the theory on this occasion.

Consequently, the conference “Stochastic Analysis: Classical and Quantum – Perspectives of White Noise Theory” took place at Meijo University, Nagoya, Japan for the period of November 1–5, 2004.

The organizers of the conference were extremely happy to see many eminent mathematicians having contributed to the success of the conference and cultivated new ideas. To our great pleasure, important papers presented at the conference are published in the Proceedings of the conference. As such, we are grateful to the respective authors and to the referees of those papers.

We acknowledge gratefully the general support of Meijo University and Ministry of Education, Culture, Sports, Science and Technology for the conference.

Special thanks are also due to Professors M. Röckner, L. Streit and T. Shimizu who gave financial support together with me for the publication of this Proceedings. Finally, I wish to note the great help given by members of the local organizing committee: Professors M. Hitsuda, S. Ihara, K. Saito and Si Si. In particular, it is to be mentioned that this Proceedings would not appear without the help of Professor Si Si who handled the aspect of editing.

July 2005

Takeyuki Hida

## Organizing Committee of the Conference

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# White Noise Functional Approach to Polymer Entanglements

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## A b s t r a c t

The Hida-Streit white noise path integral is used to investigate the entanglement probabilities of two chainlike macromolecules where one polymer lies on a plane and the other perpendicular to it. To simulate the data contained in the lineal structure of a polymer of length  $L$  which lies on the plane, a potential,  $V = f(s) \vartheta$ , is introduced where,  $f = df/ds$ ,  $0 \leq s \leq L$ , and  $f(s)$  a modulating function. Using the  $T$ -transform in white noise calculus, entanglement probabilities are calculated which show a significant influence of chirality or the “handedness” of the polymer. The freedom to choose the modulating function  $f(s)$ , which gives rise to different entanglement probabilities, allows one to control and predict the coiling behavior of polymers. As examples, we consider two cases: (a)  $f(s) = k \cos(\nu s)$ , and (b)  $f(s) = ks^p$ .

## 1 Introduction

Investigations in biochemistry reveal that protein molecules are able to carry out their biological functions only when they are folded into specific three-dimensional structures [1]. For instance, enzymes, which are essentially protein molecules, have highly specific shapes which allow them to receive their targets as a lock receives a key. Understanding this molecular recognition process, which depends on the structure of proteins, acquires importance since almost all chemical processes within a living organism rely on enzyme catalysis. What are the rules involved in forming protein structures? What are the factors which determine the manner in which proteins fold? One essential factor which has been identified is the one-dimensional sequence of data embodied in the repeating units of macromolecules. It has been noted that the genetic code is translated from DNA sequences to amino acid sequences, and this

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one-dimensional sequence of data influences the highly specific shapes of proteins. Moreover, chirality, or “handedness,” of macromolecules also plays an important role in the globular structure of proteins. It is known, for instance, that amino acids in proteins are “left-handed,” and that the chirality of amino acids manifests in the helical structures of the proteins they form. These observations give rise to more specific questions. How can the sequence of data in the lineal structure of macromolecules allow us to predict or determine a protein’s three-dimensional structure? To what extent does chirality influence the folding or unfolding of proteins?

In this paper, we present a simple model which may shed light into these questions. In particular, we look at a model which incorporates the following features observed in a macromolecule:

- (1) the ability of a macromolecule to use the one-dimensional sequence of data in its repeating units to influence its globular structure, and,
- (2) the chirality of the polymer which influences the three-dimensional structure of a macromolecule.

We start with a polymer entanglement scenario originally studied by Edwards [2] and Prager and Frisch [3]. We then extend this system [4] by simulating the data contained in the repeating units of the entangled polymer using a potential of the form,  $V = f(s) \vartheta$ , where  $f = df/ds$ , and  $\vartheta$  is an angular variable about the  $z$ -axis. Here,  $f(s)$  is a modulating function where,  $0 \leq s \leq L$ , and  $L$  is the length of the polymer. We shall see that for any modulating function  $f(s)$ , the “handedness” of the winding polymer has a significant effect on the entanglement probabilities. In particular, we look at two cases (a)  $f(s) = k \cos(\nu s)$ , and (b)  $f(s) = ks^p$ , where  $k$  is a positive constant and  $p = \pm 1, \pm 2, \pm 3, \dots$ . Our calculations are greatly facilitated by first parametrizing the probability function in terms of the white noise variable, as was done by Hida and Streit [5] for the case of quantum propagators. The white noise functional can then be evaluated in a straightforward manner using the  $T$ -transform of white noise calculus [7]-[9].

## 2 Two Chainlike Macromolecules

In 1967, S. F. Edwards [2] and, independently, S. Prager and H. L. Frisch [3], solved the entanglement problem of two chainlike macromolecules in the absence of intermolecular forces. The problem consists of a polymer on a plane whose motion is constrained by a straight polymer orthogonal to the plane, since the macromolecules cannot cross each other. The polymer on the plane which starts at  $\mathbf{r}_0$  and ends at  $\mathbf{r}_1$  has fixed

endpoints, and can be viewed as a random walk with paths that can entangle, clockwise or counterclockwise, around the straight polymer which intersects the origin of the plane. Employing polar coordinates  $\mathbf{r} = (r, \vartheta)$  for this problem, S. F. Edwards [2] used the Wiener representation of the random walk in which the probability is represented by,

$$P(\mathbf{r}_1, \mathbf{r}_0) = \int \exp \left[ -\frac{1}{l} \int_0^L (d\mathbf{r}/ds)^2 ds \right] \mathcal{D}^2[\mathbf{r}], \quad (2.1)$$

where the integral is taken over all paths  $\mathbf{r}(s)$  such that  $\mathbf{r}(0) = \mathbf{r}_0$  and  $\mathbf{r}(L) = \mathbf{r}_1$ . Here, we represent the polymer of length  $L$  as consisting of  $N$  freely hinged individual molecules, each of length  $l$  such that  $L = Nl$ . In view of the point singularity, a set of topologically equivalent configurations can be characterized by a winding number  $n$ , where  $n = 0, \pm 1, \pm 2, \dots$ , indicating the number of times the polymer turns around the straight polymer intersecting the plane at the origin ( $n \geq 0$ , signifies  $n$  turns counterclockwise, and  $n \leq -1$  means  $|n + 1|$  turns clockwise).

### 3 Entanglement with an Intermolecular Potential $V(r)$

In 1977, F. W. Wiegel [6] extended this entanglement problem to include an intermolecular force where the repeating units of the entangled polymer interact with the straight polymer. For any potential  $V(r)$  which has a minimum at some radius  $R$ , Wiegel obtained a low-temperature limit for the entanglement probabilities given by,

$$W(n) = (R/l) \sqrt{4\pi/N} \exp(-4\pi^2 n^2 R^2 / Nl^2) \quad ; \quad (N \gg 1). \quad (3.1)$$

For example, the potential of the form,  $V = Cr^2 + D/r^2$  ( $C > 0, D > 0$ ), was considered where  $R = (D/C)^{1/4}$  is a radius where the potential has a minimum. With this potential, the force is repulsive at short distances and attractive at large distances. Wiegel then obtained the entanglement probabilities for this harmonically bound polymer to be that of Eq. (3.1). For low temperatures, he also noted that the configurations of the polymer are confined to a narrow strip in the immediate vicinity of a circle around the origin with radius  $R$ . Below, we shall use these observations of Wiegel which we refer to as the generic case.

### 4 White Noise Path Integral Approach

Let us now familiarize ourselves with the white noise path integral approach by using it to arrive at Eq. (3.1). Since we are interested in

the number of possible windings around the origin that the polymer on the plane undergoes, we can simplify the calculation by fixing the radial variable to  $r = R$ , i.e.,  $\mathbf{r} = (R, \vartheta)$ , and use  $\vartheta$  to track the number of turns, clockwise or counterclockwise, around the origin. As mentioned in the previous section, a fixed radial part describes the entanglement scenario in the low temperature limit [6] for any polymer interaction potential  $V(r)$  which has a minimum at some value  $r = R$ . For the generic case, Eq. (2.1) reduces to,

$$P(\vartheta_1, \vartheta_0) = \int \exp \left[ -\frac{1}{l} \int_0^L R^2 \left( \frac{d\vartheta}{ds} \right)^2 ds \right] \mathcal{D}[R d\vartheta], \quad (4.1)$$

with,  $\vartheta_1 = \vartheta(L)$  and  $\vartheta_0 = \vartheta(0)$ . The paths  $\vartheta$  can be parametrized as,

$$\begin{aligned} \vartheta(L) &= \vartheta_0 + \left( \sqrt{l/R} \right) B(L) \\ &= \vartheta_0 + \left( \sqrt{l/R} \right) \int_0^L \omega(s) ds, \end{aligned} \quad (4.2)$$

where  $B(s)$  is a Brownian motion parametrized by  $s$ , and  $\omega(s)$  a random white noise variable. With Eq. (4.2), the integrand in  $P(\vartheta_1, \vartheta_0)$  becomes,

$$\exp \left[ -\frac{1}{l} \int R^2 \left( \frac{d\vartheta}{ds} \right)^2 ds \right] = \exp \left[ - \int \omega(s)^2 ds \right]. \quad (4.3)$$

Noting that the polymer can wind  $n$  times, clockwise or counterclockwise, we use the Donsker delta function

$$\delta(\vartheta(L) - \vartheta_1 + 2\pi n), \quad (4.4)$$

to fix the endpoint  $\vartheta_1$ , where  $n = 0, \pm 1, \pm 2, \dots$ . Since  $P(\vartheta_1, \vartheta_0)$  is now expressed as a white noise functional, the integration over  $\mathcal{D}[R d\vartheta]$  becomes an integration over,  $N_\omega d^\infty \omega = \exp \left[ (1/2) \int \omega(s)^2 ds \right] d\mu(\omega)$ , where  $d\mu(\omega)$  is the Gaussian white noise measure. Eq. (4.1) can now be written as,

$$P(\vartheta_1, \vartheta_0) = \int \sum_{n=-\infty}^{+\infty} I_0 \delta(\vartheta(L) - \vartheta_1 + 2\pi n) d\mu(\omega), \quad (4.5)$$

where

$$I_0 = N \exp \left( -\frac{1}{2} \int_0^L \omega(s)^2 ds \right). \quad (4.6)$$

The evaluation of  $P(\vartheta_1, \vartheta_0)$  is facilitated by using the Fourier representation of the  $\delta$  - function, i.e.,

$$P(\vartheta_1, \vartheta_0) = \frac{1}{2\pi} \sum_{n=-\infty}^{+\infty} \int \exp [i\lambda (\vartheta_0 - \vartheta_1 + 2\pi n)] \\ \times \int \exp \left( i\lambda \left( \sqrt{l}/R \right) \int_0^L \omega(s) ds \right) I_0 d\mu(\omega) d\lambda. \quad (4.7)$$

Observing that the integration over  $d\mu(\omega)$  is just the  $T$ -transform of  $I_0$  [7]-[9], we obtain,

$$P(\vartheta_1, \vartheta_0) = \frac{1}{2\pi} \sum_{n=-\infty}^{+\infty} \int \exp [i\lambda (\vartheta_0 - \vartheta_1 + 2\pi n)] \\ \times \exp (-\lambda^2 lL/4R^2) d\lambda \\ = \sum_{n=-\infty}^{+\infty} P_n. \quad (4.8)$$

Here, the  $P_n$  is the probability function for polymer configurations which entangle  $n$  - times around the origin. The remaining integral in  $P_n$  is a Gaussian integral over  $\lambda$ . We have,

$$P_n = \frac{1}{2\pi} \int \exp [i\lambda (\vartheta_0 - \vartheta_1 + 2\pi n) - \lambda^2 (lL/4R^2)] d\lambda \\ = \sqrt{R^2/lL\pi} \exp [-(R^2/lL) (\vartheta_0 - \vartheta_1 + 2\pi n)^2]. \quad (4.9)$$

Also, applying Poisson's sum formula,

$$\frac{1}{2\pi} \sum_{n=-\infty}^{+\infty} \exp (in\phi) = \sum_{m=-\infty}^{+\infty} \delta (\phi + 2\pi m), \quad (4.10)$$

to Eq. (4.8), we get,

$$\begin{aligned}
P(\vartheta_1, \vartheta_0) &= \frac{1}{2\pi} \sum_{m=-\infty}^{+\infty} \int \delta(\lambda + m) \\
&\quad \times \exp [i\lambda (\vartheta_0 - \vartheta_1) - \lambda^2(lL/4R^2)] d\lambda \\
&= \frac{1}{2\pi} \sum_{m=-\infty}^{+\infty} \exp [-im(\vartheta_0 - \vartheta_1) - m^2(lL/4R^2)]. \quad (4.11)
\end{aligned}$$

For an arbitrary initial starting point we may set,  $\vartheta_0 = \vartheta_1$ , and the probability that the polymer winds  $n$  - times is,

$$\begin{aligned}
W(n) &= P_n/P(L) \\
&= \frac{\sqrt{R^2/lL\pi} \exp [-(2\pi nR)^2/lL]}{\frac{1}{2\pi} \sum_{m=-\infty}^{+\infty} \exp [-m^2(lL/4R^2)]}. \quad (4.12)
\end{aligned}$$

For a very long polymer,  $L = Nl \gg 1$ , the dominant term in the denominator is for  $m = 0$ . Hence,

$$W(n) = (R/l)\sqrt{4\pi/N} \exp (-4\pi^2 n^2 R^2/Nl^2); \quad (N \gg 1), \quad (4.13)$$

which agrees with the result, Eq. (3.1), obtained by Wiegel [6].

## 5 Length-dependent Potentials

We shall now generalize the system discussed in the previous section by adding a length-dependent potential,  $V = f(s) \vartheta$ , acting on the polymer on the plane as it entangles around the second straight polymer at the origin [4]. Here,  $f = df/ds$ , where  $f(s)$  is the modulating function. The potential  $V$  is added to the “kinetic part” of Eq. (4.1) such that the probability function becomes,

$$P_V(\vartheta_1, \vartheta_0) = \int \exp \left\{ -\frac{1}{l} \int_0^L \left[ R^2 \left( \frac{d\vartheta}{ds} \right)^2 + lf(s) \vartheta \right] ds \right\} \mathcal{D}[R d\vartheta]. \quad (5.1)$$

The nature of the potential may be understood in the following way. Firstly, one may associate with it a length-dependent force given by,  $F = -\nabla V = -f(s)/R$ . Secondly, the effect of the potential term may also be understood by rewriting it as,

$$\begin{aligned}
\int_0^L f(s) \vartheta ds &= \int_0^L \frac{d}{ds} (f\vartheta) ds - \int_0^L f \left( \frac{d\vartheta}{ds} \right) ds \\
&= f(L) \vartheta(L) - f(0) \vartheta(0) - \int_0^L f \vartheta ds \quad . \quad (5.2)
\end{aligned}$$

The first two terms are constants given by the values of  $f$  and  $\vartheta$  at the endpoints. The last term, on the other hand, shows that one essentially has a “velocity-dependent potential” in view of  $\dot{\vartheta}$ . Moreover, from Eq. (5.2), one may have the case,  $f(s) = 0$  with  $f \neq 0$ , such that the nonzero  $f$  may still manifest in the probability function. For the case,  $f = 0$ , one obtains the results of the generic case discussed in the previous section. An example of a constant nonzero  $f$  may be illustrated if one takes,  $f = (q\Phi_0/2\pi)$ , where  $q$  is the net charge of each repeating unit of the polymer which winds around the straight polymer that contains a constant magnetic flux  $\Phi_0$  oriented along the  $z$ -axis. This choice leads to an effective potential,  $f \dot{\vartheta} = q\mathbf{A} \cdot \dot{\mathbf{r}}$ , which resembles that of an Aharonov-Bohm setup where  $\mathbf{A}$  is the vector potential for the constant magnetic flux  $\Phi_0$  [4, 10].

Using again the parametrization Eq. (4.2), we obtain an expression similar to Eq. (4.7) but modified by the potential Eq. (5.2) of the form,

$$\begin{aligned}
P_V(\vartheta_1, \vartheta_0) &= \exp [f(0) \vartheta(0) - f(L) \vartheta(L)] \\
&\times \frac{1}{2\pi} \sum_{n=-\infty}^{+\infty} \int_{-\infty}^{+\infty} \exp [i\lambda (\vartheta_0 - \vartheta_1 + 2\pi n)] \\
&\times \int \exp \left\{ i \int_0^L \left( \sqrt{l}/R \right) (\lambda - if) \omega(s) ds \right\} \\
&\times I_0 d\mu(\omega) d\lambda \quad . \quad (5.3)
\end{aligned}$$

The integration over  $d\mu(\omega)$  is again just the  $T$  - transform of  $I_0$  which yields,

$$\begin{aligned}
P_V(\vartheta_1, \vartheta_0) &= \exp [f(0) \vartheta(0) - f(L) \vartheta(L)] \\
&\times \frac{1}{2\pi} \sum_{n=-\infty}^{+\infty} \int_{-\infty}^{+\infty} \exp [i\lambda (\vartheta_0 - \vartheta_1 + 2\pi n)] \\
&\times \exp \left\{ - (l/4R^2) \int_0^L (\lambda - if)^2 ds \right\} d\lambda \\
&= \sum_{n=-\infty}^{+\infty} P_n .
\end{aligned} \tag{5.4}$$

The Gaussian integral over  $\lambda$  in  $P_n$  can be evaluated to give,

$$\begin{aligned}
P_n &= \sqrt{\frac{R^2}{\pi lL}} \exp [f(0) \vartheta(0) - f(L) \vartheta(L)] \exp \left[ \left( \frac{l}{4R^2} \int_0^L f^2 ds \right) \right] \\
&\times \exp \left[ -\frac{R^2}{lL} \left( \vartheta_0 - \vartheta_1 + 2\pi n + \frac{l}{2R^2} \int_0^L f ds \right)^2 \right] .
\end{aligned} \tag{5.5}$$

Employing the Poisson sum formula to Eq. (5.4), and integrating  $\lambda$  yields,

$$\begin{aligned}
P_V(\vartheta_1, \vartheta_0) &= \frac{1}{2\pi} \exp [f(0) \vartheta(0) - f(L) \vartheta(L)] \sum_{m=-\infty}^{+\infty} \exp [-im (\vartheta_0 - \vartheta_1)] \\
&\times \exp \left\{ -\frac{m^2 lL}{4R^2} - \frac{iml}{2R^2} \int_0^L f ds + \frac{l}{4R^2} \int_0^L f^2 ds \right\} .
\end{aligned} \tag{5.6}$$

From these, we obtain the probability that the polymer entangles  $n$  times as, (setting,  $\vartheta_0 = \vartheta_1$ ),

$$\begin{aligned}
W(n) &= P_n / P_V \\
&= \frac{R}{l} \sqrt{\frac{4\pi}{N}} \frac{\exp \left[ -\frac{R^2}{Nl^2} \left( 2\pi n + \frac{l}{2R^2} \int_0^L f ds \right)^2 \right]}{\theta_3 \left( \frac{l}{4R^2} \int_0^L f ds \right)} ,
\end{aligned} \tag{5.7}$$



where  $\theta_3(u)$  is the theta function [11],

$$\theta_3(u) = 1 + 2 \sum_{m=1}^{+\infty} q^{m^2} \cos(2mu), \quad (5.8)$$

with  $u = (l/4R^2) \int f ds$ , and  $q = \exp(-Nl^2/4R^2)$ .

## 6 Chirality of Entangled Polymers

Let us now consider the effect of the “handedness” of a polymer on the coiling probabilities of a macromolecule. As is normally the case, we define “handedness” in a way that a “right-handed” polymer would have a mirror-image which is “left-handed.” We may write Eq. (5.7) as,

$$W(n) = W_s \exp \left[ - \left( \frac{2\pi n}{L} \right) \int_0^L f ds \right], \quad (6.1)$$

where  $W_s$ , symmetric in  $n$ , is of the form,

$$W_s = \frac{R}{l} \sqrt{\frac{4\pi}{N}} \frac{\exp \left[ -\frac{4\pi^2 n^2 R^2}{Nl^2} - \frac{1}{4NR^2} \left( \int_0^L f ds \right)^2 \right]}{\theta_3 \left( \frac{l}{4R^2} \int_0^L f ds \right)}. \quad (6.2)$$

From these equations the following observations may be made:

(1) It is clear from Eq. (6.1) that the entanglement probability  $W(n)$  significantly changes depending on whether  $n$  is a positive or a negative number. If we designate clockwise winding ( $n \leq -1$ ) as “right-handed,” and anti-clockwise winding ( $n \geq 0$ ) as “left-handed,” then for  $f > 0$ , a “right-handed” polymer is more likely to have configurations with large values of winding number  $n$  than “left-handed” ones. In particular, for winding numbers  $\pm n$ , the corresponding “right” and “left-handed” entanglements differ by an exponential factor, i.e.,  $W(-n)/W(n) = \exp \left[ (4\pi n/L) \int f ds \right]$ .

(2) We also see from Eq. (6.1), that a change in sign of the modulating function, from  $f$  to  $-f$ , gives a similar effect as that of  $n$  to  $-n$ , i.e., from “left-handed” to “right-handed”. Since the role of the modulating function  $f$  is that of simulating the data contained in the lineal structure of the polymer, it appears that the choice of the sign of  $f$  is one way of incorporating the observation that the “handedness” of