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Approximation of a Conditional Wiener Integral

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ABSTRACT

An approximation for conditional Wiener integrals, similar to Cameron's "Simpson's Rule" for unconditional Wiener integrals, is developed. An alternate derivation of Konheim and Miranker's prescription for the development of higher-order formulas is presented.

I. INTRODUCTION

With the growing power of computing machinery, the connection between the diffusion equation and the Schrödinger equation is being exploited for numerical computations. Our particular interest has been in quantum statistical mechanical computations which use this connection [1]–[3], others have used it for the computation of atomic wavefunctions [4]. In one instance this is the only method which has provided useful numerical solutions; namely, the three-particle computations on helium. In the case of the quantum statistical mechanical computations the Wiener integral is the mathematical foundation supporting the numerical work which is, primarily, an evaluation of a certain Wiener integral. Thus an interest has developed in techniques for making this evaluation and here certain of these techniques are discussed.

There are two rather distinct aspects to these computations: one involves a direct approximation of a Wiener integral; the other involves a Monte Carlo sampling procedure. Here attention is directed at the first of these. One method for direct approximation of a Wiener integral is based on a functional Taylor series expansion [5], a form of which is known as the Wigner–Kirkwood expansion.

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This is the method which has been used in the three-particle computations. Another method is a "Simpson rule" for Wiener integrals developed by Cameron [6] and a generalization of this developed by Konheim and Miranker [7]. The Simpson rule approach does not seem to have been employed in any interesting physics computations.

Cameron's Simpson rule cannot be used directly for the type of Wiener integral which arises in the quantum statistical mechanical computations. Here a simple extension of Cameron's idea is used to obtain a corresponding rule for these computations. The application of the Konheim–Miranker generalization is also described here along with an alternate derivation of their result.

II. Notation and Background

Let $r(\tau)$ denote a continuous function of τ, with $r(0) = 0$; $r(\tau)$ is called the path variable, or simply the path, and τ is called the time variable, or simply the time. The function $r(\tau; n)$ is regarded as an approximation of $r(\tau)$ and is, in particular, a piecewise-straight function of time with breaks in slope at

$$\tau_0 < \tau_1 < \cdots < \tau_{n-1} < \tau_n . \tag{1}$$

Also,

$$\begin{gathered} \tau_0 = 0, \qquad \tau_n = \beta, \\ r(0) = r(0; n) = 0, \qquad r(\beta) = r(\beta; n) = R, \end{gathered} \tag{2}$$

are regarded as constants in the limiting process below, and the notation

$$r_i \equiv r(\tau_i\,; n) \tag{3}$$

is used. The conditional Wiener integral of a functional of the path, say, $F[r(\tau)]$, is defined as the limit

$$E\{F[r(\tau)] | r(\beta) = R\} = \lim_{n\to\infty} \int_{-\infty}^{+\infty} \cdots \int_{-\infty}^{+\infty} F[r(\tau; n)]\, d\mu_n , \tag{4}$$

where

$$d\mu_n = (2\pi\beta)^{1/2} \exp\left(\frac{R^2}{2\beta}\right) \prod_{i=0}^{n-1} \left\{(2\pi(\tau_{i+1} - \tau_i)^{-1/2} \exp\left(\frac{-(r_{i+1} - r_i)^2}{2(\tau_{i+1} - \tau_i)}\right)\right\} \prod_{i=1}^{n-1} dr_i . \tag{5}$$

The measure $d\mu_n$ is a joint Gaussian probability and the normalization is such that

$$E\{1 \mid r(\beta) = R\} = 1. \tag{6}$$

Loosely speaking, this integral is an average of the functional $F[r(\tau)]$, where the average is taken over all continuous functions $r(\tau)$ with $r(0) = 0$, $r(\beta) = R$ and the infinitesimals $r(\tau + \delta) - r(\tau)$ are governed by the joint Gaussian distribution shown in Eq. (5). Sometimes the functional depends on other functions of the time as well as the path, as in

$$F[ar(\tau) + g(\tau)], \tag{7}$$

where $r(\tau)$ is the path, $g(\tau)$ is some function of time and a is some constant. In such a case the measure is still defined as in Eq. (5); confusion as to which variable is the path in an expression, such as

$$E\{F[ar(\tau) + g(\tau)] \,|\, r(\beta) = R\}, \tag{8}$$

can be avoided by noting that the end-point condition, here $r(\beta) = R$, always exhibits the path variable on the left of the equality. The limit in Eq. (4) is independent of the manner of subdivision of the time interval, so long as the points of subdivision become dense as $n \to \infty$, but for convenience

$$\tau_{i+1} - \tau_i = \beta/n \tag{9}$$

is assumed in the discussion below.

Several properties of the conditional Wiener integral which play an important role in these computations are reviewed below. The first of these concerns a change in the time scale. Suppose that a new time variable, τ', is defined by the relation

$$\tau' = p\tau, \tag{10}$$

then

$$E\{F[r(\tau)] \mid r(\beta) = R\} = E\left\{F\left[\frac{1}{p^{1/2}}\, r(\tau')\right] \mid r(\beta') = p^{1/2}R\right\}. \tag{11}$$

The second of these properties concerns a change in the path variable. Suppose that a new path variable, $r'(\tau)$, is defined by the relation

$$r'(\tau) = r(\tau) + A + \tau B, \tag{12}$$

then

$$E\{F[r(\tau)] \mid r(\beta) = R\} = E\{F[r'(\tau) - A - \tau B] \mid r'(\beta) = A + \beta B + R\}. \tag{13}$$

These two properties can be combined to reduce all conditional Wiener integrals to a standard form in which the time interval is (0,1) and the end-point condition is $r(1) = 0$; thus,

$$E\{F[r(\tau)] \,|\, r(\beta) = R\} = E\{F[\beta^{1/2}r(\tau) + \tau R] \,|\, r(1) = 0\}. \tag{14}$$

A third property concerns the conditional Wiener integral of functionals of the form $\prod_{i=1}^{p} r(\tau_i)$. The basic relations are

$$E\left\{\prod_{i=1}^{2p-1} r(\tau_i) \mid r(1) = 0\right\} = 0, \tag{15}$$

$$E\left\{\prod_{i=1}^{2p} r(\tau_i) \mid r(1) = 0\right\} = \sum \prod b(\tau_i\,, \tau_k), \tag{16}$$

$$b(\tau_i\,,\tau_k) = \tau_i(1 - \tau_k), \qquad (\tau_i \leqslant \tau_k), \tag{17}$$

where the sum and product on the right of Eq. (16) are to be understood as follows: let $\tau_1\,, \tau_2\,,..., \tau_{2p}$ be arranged into p pairs; then the product contains p factors of the form $b(\tau_i\,, \tau_k)$, one for each pair; the sum is understood to extend over all such pairings; no τ_i appears in more than one pair and the pair $(\tau_i\,, \tau_k)$ is not distinguished from $(\tau_k\,, \tau_i)$. To clarify the interpretation of Eq. (16) the result for $p = 2$ is

$$\begin{aligned} &E\{r(\tau_1)r(\tau_2)r(\tau_3)r(\tau_4) \mid r(1) = 0\} \\ &\quad = b(\tau_1\,, \tau_2)b(\tau_3\,, \tau_4) + b(\tau_1\,, \tau_3)b(\tau_2\,, \tau_4) + b(\tau_1\,, \tau_4)b(\tau_2\,, \tau_3) \\ &\quad = \tau_1(1 - \tau_2)\tau_3(1 - \tau_4) + \tau_1(1 - \tau_3)\tau_2(1 - \tau_4) + \tau_1(1 - \tau_4)\tau_2(1 - \tau_3), \end{aligned} \tag{18}$$

where $\tau_1 \leqslant \tau_2 \leqslant \tau_3 \leqslant \tau_4$ is understood.

Our interest is centered on functionals of the form

$$F[r(\tau)] = \exp\left(-\int_0^\beta V(r(\tau))\, d\tau\right). \tag{19}$$

The reason for this is that the conditional Wiener integral of this functional is known [8] to be the Green's function for the Bloch equation

$$H\phi = -\partial\phi/\partial\beta. \tag{20}$$

More specifically, let H be the Hamiltonian operator

$$H = -\frac{1}{2}\frac{d^2}{dr^2} + V(r); \tag{21}$$

then

$$\begin{aligned} &(2\pi\beta)^{-1/2} \exp\left(-\frac{(R' - R)^2}{2\beta}\right) E\{F[r(\tau) + R] \mid r(\beta) = R' - R\} \\ &\quad = \sum_i \Psi_i^*(R)\Psi_i(R')e^{-\beta E_i}\,, \end{aligned} \tag{22}$$

where the functional is given by Eq. (19) and $\{\Psi_i\}$ and $\{E_i\}$ are the eigenvectors and eigenvalues of the Hamiltonian operator, Eq. (21). In the context of quantum statistics, Eq. (22) is the basic formula linking a conditional Wiener integral with the density matrix elements. Although the formulas displayed here apply to a one-dimensional, one-particle problem, they apply equally well, *mutatis mutandis*, to a three-dimensional, N-particle system; the appropriate equations for this extension have been displayed elsewhere [3]. For simplicity most of the discussion below applies to the one-dimensional (and one-particle) case.

The functional in Eq. (19) can be written

$$F[r(\tau)] = \prod_{i=0}^{n-1} f_i[r(\tau)], \tag{23}$$

$$f_i[r(\tau)] = \exp\left(-\int_{\tau_i}^{\tau_{i+1}} V(r(\tau))\, d\tau\right). \tag{24}$$

This property has an extremely useful consequence; it allows the conditional Wiener integral to be similarly factored, in particular

$$E\{F[r(\tau)] \mid r(1) = 0\} = \int\cdots\int \prod_{i=0}^{n-1} E\left\{f_i\left[\frac{1}{n^{1/2}} r(\tau) + r_i(1-\tau) + r_{i+1}\tau\right] \middle| r(1) = 0\right\} d\mu_n, \tag{25}$$

where: $d\mu_n$ is defined in Eq. (5); $\tau_i = 0$, $\tau_{i+1} = 1$ and $d(\tau/n)$ replaces $d\tau$ in f_i. The important feature in this result is the factor $1/n^{1/2}$ making it possible to treat $r(\tau)/n^{1/2}$ as small for large n and to use an expansion in powers of this quantity. This statement must be read in a probabilistic context; $r(\tau)$ can become arbitrarily large, but the measure of the set of paths for which $|r(\tau)| > M$ for some τ can be made as small as we please by making M sufficiently large. In computations the result expressed in Eq. (25) is used in the following way: an approximation, based on the fact that $r(\tau)/n^{1/2}$ is small, is constructed for each factor

$$E\left\{f_i\left[\frac{1}{n^{1/2}} r(\tau) + r_i(1-\tau) + r_{i+1}\tau\right] \middle| r(1) = 0\right\}, \tag{26}$$

and Monte Carlo sampling is then used to evaluate the n-fold Riemann integral. Here we are concerned with the first part of this process, namely the determination of a suitable approximation for the factor Eq. (26).

III. Simpson Rule for Conditional Wiener Integrals

Following the approach of Cameron [6], we seek an approximation for the conditional Wiener integral which depends on the choice of a function $\rho(u, \tau)$ having the property that

$$E\{f[x(\tau)] \mid x(1) = 0\} = \frac{1}{2}\int_{-1}^{1} f[\rho(u, \tau)]\, du, \tag{27}$$

when the functional is a polynomial of some degree, that is, when

$$\begin{aligned} f[x(\tau)] = h_0 &+ \int_0^1 x(\tau)h_1(\tau)\, d\tau + \int_0^1\int_0^1 x(\tau_1)x(\tau_2)h_2(\tau_1, \tau_2)\, d\tau_1\, d\tau_2 \\ &+ \cdots + \int_0^1\int_0^1 \cdots \int_0^1 x(\tau_1)x(\tau_2)\cdots x(\tau_n)h_n(\tau_1, \tau_2, \ldots, \tau_n)\, d\tau_1\, d\tau_2 \cdots d\tau_n . \end{aligned} \tag{28}$$

In Eq. (27) it is seen that the essential computation features are that the path is replaced by a function of two variables, u and τ, and the Wiener integration is replaced by integration (Lebesgue) with respect to the variable u.

When the functional is a polynomial it follows, by an exchange of order of integration, that

$$\begin{aligned} E\{f[x(\tau)] \mid x(1) = 0\} = h_0 &+ \int_0^1 E\{x(\tau) \mid x(1) = 0\}\, h_1(\tau)\, d\tau \\ &+ \int_0^1\int_0^1 E\{x(\tau_1)x(\tau_2) \mid x(1) = 0\}\, h_2(\tau_1, \tau_2)\, d\tau_1 d\tau_2 \\ &+ \cdots + \int_0^1\int_0^1 \cdots \int_0^1 E\{x(\tau_1)x(\tau_2)\cdots x(\tau_n) \mid x(1) = 0\} \\ & h_n(\tau_1, \tau_2, \ldots, \tau_n)\, d\tau_1\, d\tau_2 \cdots d\tau_n . \end{aligned} \tag{29}$$

The exchange of the order of the Wiener integration and the τ-integrations is justified as follows: for any k, $h_k(\tau_1, \tau_2, \ldots, \tau_k)$ is a constant with respect to the Wiener integration, and $x(\tau_1)\, x(\tau_2) \cdots x(\tau_k)$ is integrable in the product space composed of the domain of the paths and the domains of $\tau_1, \tau_2, \ldots, \tau_k$; consequently, $x(\tau_1)\, x(\tau_2) \cdots x(\tau_k)\, h_k(\tau_1, \tau_2, \ldots, \tau_k)$ is integrable in the product space and Fubini's theorem allows exchange of the order of integration. As a consequence of Eq. (29) we can formulate the property described in Eq. (27) by

$$E\{x(\tau_1)x(\tau_2) \cdots x(\tau_k) \mid x(1) = 0\} = \frac{1}{2}\int_{-1}^{1} \rho(u, \tau_1)\rho(u, \tau_2) \cdots \rho(u, \tau_k)\, du, \tag{30}$$

for $k = 1, 2, \ldots, n$. The values of these Wiener integrals are well known and were displayed earlier in Eqs. (15) and (16).

Now consider the function

$$\rho(u, \tau) = \begin{cases} -\tau \text{ when } \tau < u \text{ and } u \geqslant 0, \\ 1 - \tau \text{ when } \tau > u \text{ and } u \geqslant 0, \\ -\rho(-u, \tau) \text{ when } u < 0. \end{cases} \tag{31}$$

It is easy to verify the following results:

$$\frac{1}{2}\int_{-1}^{1} \rho(u, \tau)\, du = 0, \tag{32}$$

$$\frac{1}{2}\int_{-1}^{1} \rho(u, \tau_1)\rho(u, \tau_2)\, du = \tau_1(1 - \tau_2) \qquad (\tau_1 \leqslant \tau_2), \tag{33}$$

$$\frac{1}{2}\int_{-1}^{1} \rho(u, \tau_1)\rho(u, \tau_2)\rho(u, \tau_3)\, du = 0 \qquad (\tau_1 \leqslant \tau_2 \leqslant \tau_3) \tag{34}$$

$$\begin{aligned} &\frac{1}{2}\int_{-1}^{1} \rho(u, \tau_1)\rho(u, \tau_2)\rho(u, \tau_3)\rho(u, \tau_4)\, du \\ &\quad = \tau_1(1 - \tau_4)(1 - 2\tau_2 - \tau_3 + 3\tau_2\tau_3) \qquad (\tau_1 \leqslant \tau_2 \leqslant \tau_3 \leqslant \tau_4). \end{aligned} \tag{35}$$

Thus Eq. (30) is satisfied for $k \leqslant 3$, and we conclude that $\rho(u, t)$, defined by Eq. (31), will satisfy Eq. (27) when the functional is a polynomial of degree three; also, it will not be satisfied when the functional is a polynomial of degree four. The analogy with the Simpson rule for Riemann integrals is clear, and it is for this reason that we follow Cameron and call the approximation

$$E\{f[x(\tau)] \mid x(1) = 0\} \cong \frac{1}{2}\int_{-1}^{1} f[\rho(u, \tau)]\, du \tag{36}$$

the Simpson rule for conditional Wiener integrals, where now the functional is arbitrary.

Since there is nothing to suggest uniqueness for $\rho(u, \tau)$, it is natural to ask if there is any other $\rho(u, \tau)$ satisfying the same conditions. Let us, for example, consider

$$\rho(u, \tau) = \begin{cases} \alpha_1 - \beta_1\tau \text{ when } \tau < u \text{ and } u \geqslant 0, \\ \alpha_2 - \beta_2\tau \text{ when } \tau > u \text{ and } u \geqslant 0, \\ -\rho(-u, \tau) \text{ when } u < 0. \end{cases} \tag{37}$$

This is an obvious generalization of Eq. (31). With this choice of $\rho(u, \tau)$, straightforward integration shows that

$$\begin{aligned}\frac{1}{2}\int_{-1}^{+1} &\rho(u, \tau_1)\rho(u, \tau_2)\,du \\ &= \tau_1(\alpha_2 - \beta_2\tau_1)(\alpha_2 - \beta_2\tau_2) + (\alpha_1 - \beta_1\tau_1)(\alpha_2 - \beta_2\tau_2)(\tau_2 - \tau_1) \\ &\quad + (\alpha_1 - \beta_1\tau_1)(\alpha_1 - \beta_1\tau_1)(1 - \tau_2), \qquad (38)\end{aligned}$$

and a comparison with the desired value, $\tau_1(1 - \tau_2)$, shows that the conditions

$$\alpha_1 = 0, \qquad \beta_1 = 1, \qquad \alpha_2 = 1, \qquad \beta_2 = 1 \qquad (39)$$

are necessary; a trivial alternative is obtained by reversing the signs of α_1, β_1, α_2, β_2. Thus among functions linear in τ, with a single discontinuity, and antisymmetric in u, the function defined in Eq. (31) is the only one which yields a Simpson rule. Further generalization by adding discontinuities, and replacement of the linear function in τ by a polynomial of degree greater than one, also does not seem to lead to a new Simpson rule.

Another way to carry out this search is by consideration of the Fourier series representation of the path. This representation is [9]

$$x(\tau) = \sqrt{2}\sum_{j=1}^{\infty} \frac{\xi_j}{j\pi} \sin(j\pi\tau), \qquad (40)$$

where the ξ_j's are independent Gaussian random variables with mean zero and variance one. The sense in which this representation is to be understood is that

$$E\{f[x(\tau)] \mid x(1) = 0\} = \lim_{n\to\infty} \int\int \cdots \int f\left(\sum_{j=1}^{n} \frac{\xi_j}{j\pi} \sin(j\pi\tau)\right) d\mu_n(\xi), \qquad (41)$$

where

$$d\mu_n(\xi) = \prod_{i=1}^{n} (2\pi)^{-1/2} \exp(-\xi_i^2/2)\, d\xi_i\,. \qquad (42)$$

The Fourier series representation of the function $\rho(u, \tau)$ defined in Eq. (31) is

$$\rho(u, \tau) = \begin{cases} 2\sum_{j=1}^{\infty} \dfrac{\cos(j\pi u)}{j\pi} \sin(j\pi\tau) & (u \geqslant 0), \\ -\rho(-u, \tau) & (u < 0). \end{cases} \qquad (43)$$

The comparison of Eq. (43) with Eq. (40) is interesting. It is seen that the cosine functions replace the Gaussian random variables; therefore, it is natural to consider

$$\eta(u, \tau) = 2 \sum_{j=1}^{\infty} \frac{\sin(j\pi u)}{j\pi} \sin(j\pi\tau) \tag{44}$$

as an alternative to be used in the Simpson rule. It can be shown that [10]

$$\lim_{n\to\infty} \sum_{j=1}^{n} \frac{\cos(j\pi z)}{j\pi} = -\log |\, 2 \sin(z\pi/2) \,|, \tag{45}$$

where the convergence is uniform on the open interval (0,2). Consequently, $\eta(u, \tau)$ may be expressed

$$\eta(u, \tau) = \log \left| \frac{\sin((\tau + u)\pi/2)}{\sin((\tau - u)\pi/2)} \right|. \tag{46}$$

Now the question is: Are Eqs. (32), (33), and (34) satisfied when $\rho(u, \tau)$ is replaced by $\eta(u, \tau)$ of Eq. (46)? The answer is: Yes. To see this let us note first that the integrals

$$I_1 = \frac{1}{2} \int_{-1}^{1} \eta(u, \tau)\, du, \tag{47}$$

$$I_2 = \frac{1}{2} \int_{-1}^{1} \eta(u, \tau_1)\eta(u, \tau_2)\, du, \tag{48}$$

$$I_3 = \frac{1}{2} \int_{-1}^{1} \eta(u, \tau_1)\eta(u, \tau_2)\eta(u, \tau_3)\, du \tag{49}$$

exist since the singularities at $u = \tau$ and $-u = \tau$ are logarithmic. The function $\eta(u, \tau)$ is antisymmetric in u; hence

$$I_1 = I_3 = 0. \tag{50}$$

The evaluation of I_2 is simplified by making use of the relation

$$\begin{aligned} &(1/2) \int_{-1}^{1} \eta(u, \tau_1)\eta(u, \tau_2)\, du \\ &\quad = \lim_{n\to\infty} 2 \int_{-1}^{1} \left\{ \sum_{j=1}^{n} \frac{\sin(j\pi u)\sin(j\pi\tau_1)}{j\pi} \right\} \left\{ \sum_{k=1}^{n} \frac{\sin(k\pi u)\sin(k\pi\tau_2)}{k\pi} \right\} du, \end{aligned} \tag{51}$$

where the exchange of limits is allowed by the Lebesgue convergence theorem; notice, for instance, that the partial sums on the left of Eq. (45) can be bounded by a function $C \log z$ when z is near zero. Using the expression on the right side of Eq. (51) we have

$$2\int_{-1}^{1}\left\{\sum_{j=1}^{n}\frac{\sin(j\pi u)\sin(j\pi\tau_1)}{j\pi}\right\}\left\{\sum_{k=1}^{n}\frac{\sin(k\pi u)\sin(k\pi\tau_2)}{k\pi}\right\}du$$

$$=\sum_{j=1}^{n}(\cos(j\pi(\tau_2-\tau_1))-\cos(j\pi(\tau_1+\tau_2)))\Big/(j\pi)^2. \tag{52}$$

The right side of Eq. (52) can be expressed in terms of an integral using

$$\sum_{j=1}^{n}(\cos(j\pi z))\Big/(j\pi)^2 = -\int_0^z\left\{\sum_{j=1}^{n}(\sin(j\pi t))\Big/(j\pi)\right\}dt+\sum_{j=1}^{n}(j\pi)^{-2}, \tag{53}$$

where $z \geqslant 0$; consequently,

$$2\int_{-1}^{1}\left\{\sum_{j=1}^{n}\frac{\sin(j\pi u)\sin(j\pi\tau_1)}{j\pi}\right\}\left\{\sum_{k=1}^{n}\frac{\sin(k\pi u)\sin(k\pi\tau_2)}{k\pi}\right\}du$$

$$=\int_{\tau_2-\tau_1}^{\tau_2+\tau_1}\left\{\sum_{j=1}^{n}(\sin(j\pi t))\Big/(j\pi)\right\}dt. \tag{54}$$

The integrand can be summed [10], yielding

$$\lim_{n\to\infty}\sum_{j=1}^{n}(\sin(j\pi t))\Big/(j\pi)=(1-t)/2, \tag{55}$$

the convergence being uniform on the open interval (0,2); note that the sum vanishes at the end points.

We again use the Lebesgue convergence theorem and take the limit $n \to \infty$ first and then integrate over t in Eq. (54); this gives, with the help of Eq. (55),

$$I_2 = \tau_1(1-\tau_2). \tag{56}$$

Hence $\eta(u,\tau)$ could be used in place of $\rho(u,\tau)$ in Eq. (36); however, it appears that $\rho(u,\tau)$ would be easier to use in computations. Although we have not explored the point further, it seems that other such functions could be discovered by this line of reasoning; i.e., using orthogonal functions in place of the random variables in the series on the right side of Eq. (30) and then summing the series.

IV. Higher Rules for Conditional Wiener Integrals

Now we turn to the problem of finding an approximation for the Wiener integral which is exact for polynomial functionals of degree greater than three. Konheim and Miranker [7] have shown a way to obtain such an approximation; here an alternate derivation of their result is presented. Since the discussion is awkward to follow because of the combinatorics, it will simplify matters to consider first some special cases.

Let us define

$$\theta(u, \tau) = c_1 \rho(u_1, \tau) + c_2 \rho(u_2, \tau), \tag{57}$$

where, on the left, u is short for u_1, u_2 and on the right, the functions $\rho(u_1, \tau)$ and $\rho(u_2, \tau)$ are as defined by Eq. (31) and c_1, c_2 are certain constants to be determined. Now let us try to satisfy

$$E\{f(x(\tau)) \mid x(1) = 0\} = \frac{1}{4} \int_{-1}^{+1} \int_{-1}^{+1} f(\theta(u, \tau))\, du_1\, du_2 \tag{58}$$

when $f(x(\tau))$ is a polynomial functional of degree five. It is immediately evident that Eq. (58) is satisfied when $f(x(\tau))$ is constant or a product of an odd number of $x(\tau)$'s; notice that $\theta(u, \tau)$ is antisymmetric in u_1 and u_2. Consequently, only two cases, when $f(x(\tau))$ is a product of two $x(\tau)$'s and when $f(x(\tau))$ is a product of four $x(\tau)$'s, remain to be considered; this yields the conditions

$$\frac{1}{4} \int_{-1}^{+1} \int_{-1}^{+1} \theta(u, \tau_1)\theta(u, \tau_2)\, du_1\, du_2 = b(\tau_1, \tau_2), \tag{59}$$

$$\begin{aligned} \frac{1}{4} \int_{-1}^{1} \int_{-1}^{1} & \theta(u, \tau_1)\theta(u, \tau_2)\theta(u, \tau_3)\theta(u, \tau_4)\, du_1\, du_2 \\ &= b(\tau_1, \tau_2)b(\tau_3, \tau_4) + b(\tau_1, \tau_3)b(\tau_2, \tau_4) \\ &\qquad + b(\tau_1, \tau_4)b(\tau_2, \tau_3). \end{aligned} \tag{60}$$

The integration on the left of Eq. (59) is easily performed and this condition becomes

$$c_1^2 + c_2^2 = 1. \tag{61}$$

With the help of Eq. (57) the integral on the left side of Eq. (60) can be expressed as

$$\begin{aligned} &(c_1^4 + c_2^4) \int_0^1 \rho(u, \tau_1)\rho(u, \tau_2)\rho(u, \tau_3)\rho(u, \tau_4)\, du \\ &+ 2(c_1^2 c_2^2) \int_0^1 \int_0^1 (\rho(u_1, \tau_1)\rho(u_1, \tau_2)\rho(u_2, \tau_3)\rho(u_2, \tau_4) \\ &+ \rho(u_1, \tau_1)\rho(u_1, \tau_3)\rho(u_2, \tau_2)\rho(u_2, \tau_4) \\ &+ \rho(u_1, \tau_1)\rho(u_1, \tau_4)\rho(u_2, \tau_2)\rho(u_2, \tau_3))\, du_1\, du_2\, . \end{aligned} \tag{62}$$

It should be evident from this that the condition expressed by Eq. (60) is satisfied when

$$c_1^4 + c_2^4 = 0, \tag{63}$$

and

$$c_1^2 c_2^2 = \tfrac{1}{2}. \tag{64}$$

Equations (61), (63), and (64) are not independent; from Eq. (61),

$$(c_1^2 + c_2^2)^2 = 1, \tag{65}$$

which with Eq. (64) implies that Eq. (63) is satisfied. Now it is easy to see that Eqs. (61) and (64) are satisfied if c_1^2 and c_2^2 are the two roots of

$$z^2 - z + \tfrac{1}{2} = 0. \tag{66}$$

Consequently,

$$c_1^2 = \frac{1+i}{2}, \qquad c_2^2 = \frac{1-i}{2} \tag{67}$$

will satisfy the requirements. There is some freedom of choice in c_1 and c_2. The values assigned to c_1^2 and c_2^2 can be interchanged without affecting the result, and there are two choices for the square root. One assignment is

$$c_1 = 2^{-1/4} e^{i\pi/8}, \qquad c_2 = 2^{-1/4} e^{-i\pi/8}. \tag{68}$$

Thus it has been shown that

$$\begin{aligned} &E\{f(x(\tau)) \mid x(1) = 0\} \\ &= \frac{1}{4} \int_{-1}^{1} \int_{-1}^{1} f(2^{-1/4} e^{i\pi/8} \rho(u_1, \tau) + 2^{-1/4} e^{-i\pi/8} \rho(u_2, \tau))\, du_1\, du_2 \end{aligned} \tag{69}$$

is satisfied when $f(x(\tau))$ is a polynomial of degree five.

As the second example we consider an approximation which is exact for polynomials of degree seven. To this end we construct

$$\theta(u, \tau) = c_1 \rho(u_1, \tau) + c_2 \rho(u_2, \tau) + c_3 \rho(u_3, \tau), \tag{70}$$

analogous to Eq. (57), and attempt to satisfy

$$E\{f(x(\tau)) \mid x(1) = 0\} = \frac{1}{8} \int_{-1}^{1} \int_{-1}^{1} \int_{-1}^{1} f(\theta(u, \tau))\, du_1\, du_2\, du_3 \tag{71}$$

for polynomials of degree seven. This leads to conditions represented by Eqs. (59) and (60), *mutatis mutandis*, and the condition

$$\frac{1}{8}\int_{-1}^{1}\int_{-1}^{1}\int_{-1}^{1} \theta(u, \tau_1)\theta(u, \tau_2) \cdots \theta(u, \tau_6)\, du_1\, du_2\, du_3 = \sum b(\tau_1, \tau_2)b(\tau_3, \tau_4)b(\tau_5, \tau_6), \tag{72}$$

where the sum is to be interpreted as in Eq. (16). The new Eq. (59) now yields the condition

$$c_1^2 + c_2^2 + c_3^2 = 1, \tag{73}$$

the new Eq. (60) now yields the pair of conditions

$$c_1^4 + c_2^4 + c_3^4 = 0, \tag{74}$$

$$c_1^2c_2^2 + c_1^2c_3^2 + c_2^2c_3^2 = \tfrac{1}{2}, \tag{75}$$

and, finally, the Eq. (72) yields the three conditions

$$c_1^6 + c_2^6 + c_3^6 = 0, \tag{76}$$

$$c_1^4c_2^2 + c_1^2c_2^4 + c_1^4c_3^2 + c_1^2c_3^4 + c_2^4c_3^2 + c_2^2c_3^4 = 0, \tag{77}$$

$$c_1^2c_2^2c_3^2 = \frac{1}{3!}. \tag{78}$$

The expressions on the left of Eqs. (73), (75), and (78) are known as the elementary symmetric functions of c_1^2, c_2^2, and c_3^2. Denoting these elemenatry symmetric functions by σ_1, σ_2, and σ_3, we have

$$\sigma_1 = c_1^2 + c_2^2 + c_3^2, \tag{79}$$

$$\sigma_2 = c_1^2c_2^2 + c_1^2c_3^2 + c_2^2c_3^2, \tag{80}$$

$$\sigma_3 = c_1^2c_2^2c_3^2. \tag{81}$$

By the fundamental theorem on symmetric functions [11], any symmetric polynomial in c_1^2, c_2^2, c_3^2 can be expressed in terms of σ_1, σ_2, and σ_3. Therefore, among the conditions represented by Eqs. (73)–(78) which must be satisfied, Eqs. (73), (75), and (78) form an independent set. In terms of the σ's, the conditions which must be satisfied are

$$\begin{gathered} \sigma_1 = 1, \qquad \sigma_1^2 - 2\sigma_2 = 0, \qquad \sigma_2 = 1/2, \\ \sigma_1^3 - 6\sigma_1\sigma_2 + 12\sigma_3 = 0, \qquad \sigma_1\sigma_2 - 3\sigma_3 = 0, \qquad \sigma_3 = 1/3!\,. \end{gathered} \tag{82}$$

It is easy to verify that when σ_1, σ_2, σ_3 are given by the first, third, and last of these equations, then the remaining ones are satisfied. Finally, observe that the polynomial

$$z^3 - \sigma_1 z^2 + \sigma_2 z - \sigma_3 = 0 \tag{83}$$

has roots c_1^2, c_2^2, c_3^2; hence the particular values for c_1^2, c_2^2, and c_3^2 which we seek are given as the roots of the polynomial

$$z^3 - z^2 + \left(\frac{1}{2}\right) z - \left(\frac{1}{3!}\right) = 0. \tag{84}$$

These values will guarantee that Eq. (71) will be satisfied for polynomial functionals of degree seven.

Now let us turn to the general problem, namely we seek numbers $c_1, c_2, \ldots, c_n$ in

$$\theta(u, \tau) = c_1\rho(u_1, \tau) + c_2\rho(u_2, \tau) + \cdots + c_n\rho(u_n, \tau), \tag{85}$$

such that

$$E\{f(x(\tau)) \mid x(1) = 0\} = \frac{1}{2^n} \int_{-1}^{1} \int_{-1}^{1} \cdots \int_{-1}^{1} f(\theta(u, \tau))\, du_1\, du_2 \cdots du_n, \tag{86}$$

for $f(x(\tau))$ a polynomial functional of degree $2n + 1$.

It is evident from the special cases already considered that we will be led to a system of equations based on the even symmetric polynomials of $c_1^2, c_2^2, \ldots, c_n^2$. If we denote the kth elementary symmetric function by σ_k, then this system of equations is succinctly expressed by

$$\sigma_k = 1/k!, \qquad k = 1, 2, \ldots, n \tag{87}$$

and the requirement that the other symmetric polynomials which arise must vanish. The latter requirement is actually unnecessary since Eq. (87) implies that this requirement is satisfied. The proof is as follows. The symmetric polynomials which are required to vanish are homogeneous of degree n, and have the form

$$p(\alpha_1, \alpha_2, \ldots, \alpha_n) = \sum (c_1^2)^{\alpha_1}(c_2^2)^{\alpha_2} \cdots (c_n^2)^{\alpha_n} \tag{88}$$

where at least one α_i, say α_j, must satisfy the inequality

$$\alpha_j \geqslant 2. \tag{89}$$

Consider the powers of σ_1 and define $\Phi_2, \Phi_3, ..., \Phi_n$ by

$$\begin{aligned} \sigma_1 &= c_1^2 + c_2^2 + \cdots + c_n^2, \\ \sigma_1^2 &= 2!\sigma_2 + \Phi_2, \\ \sigma_1^3 &= 3!\sigma_3 + \Phi_3, \\ &\vdots \\ \sigma_1^n &= n!\sigma_n + \Phi_n. \end{aligned} \tag{90}$$

Since any symmetric polynomial can be expressed in terms of the elementary symmetric polynomials,

$$p(\alpha_1, \alpha_2, ..., \alpha_n) = f(\sigma_1, \sigma_2, ..., \sigma_n), \tag{91}$$

and by Eq. (90)

$$p(\alpha_1, \alpha_2, ..., \alpha_n) = g(\sigma_1, \Phi_2, ..., \Phi_n). \tag{92}$$

Now because of the inequality, Eq. (89), every term in $g(\sigma_1, \Phi_2, ..., \Phi_n)$ must contain a factor of Φ_i for some i, otherwise, it would contain a term σ_1^n which implies a term on the right of Eq. (88) with all $\alpha_i = 1$. But Eqs. (87) and (90) imply

$$\Phi_i = 0, \qquad (i = 2, 3, ..., n), \tag{93}$$

hence $p(\alpha_1, \alpha_2, ..., \alpha_n) = 0$. This completes the proof.

Finally, we observe that the polynomial

$$p_n(z) = z^n - \sigma_1 z^{n-1} + \sigma_2 z^{n-2} - \cdots + (-1)^n \sigma_n \tag{94}$$

has roots $c_1^2, c_2^2, ..., c_n^2$; hence, by the conditions expressed by Eq. (87), the values of $c_1^2, c_2^2, ..., c_n^2$ we seek are given by the roots of the polynomial

$$p_n(z) = z^n - z^{n-1} + \frac{1}{2!} z^{n-2} - \cdots + (-1)^n \frac{1}{n!}. \tag{95}$$

It is interesting to observe that $p_n(z)$ may be obtained by truncating the power series for $z^n e^{-1/z}$.

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