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An expansion in orthogonal polynomials of binomial-random variables for inhomogeneous transport in disordered media

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Abstract. A general method is presented for expanding random functions in orthogonal polynomials of binomial-random variables for transport in randomly inhomogeneous media. The expansion projects the stochastic equation onto the statistically orthogonal polynomials of binomial variables. It generates an infinite set of coupled equations for the determination of kernels in the expansion where randomness is removed at the outset. The expansion in orthogonal polynomials is applied to inhomogeneous transport in bond-disordered resistor networks (bond model). The expression for the effective conductivity is obtained, to order c^2 (c being the fraction of broken bonds), by truncating the infinite set of coupled equations for kernels after the third term. It is found that the expression agrees with that derived from the two-bond approximation. The expansion in orthogonal polynomials is also applied to the clumped-bond model and the continuum model. Truncated equations are derived to govern the kernels in the expansions.

1. Introduction

The properties of randomly inhomogeneous physical systems have recently been investigated intensively by both experimental and theoretical methods. The system can be simulated by a continuum model or by a resistor network model. Numerical computations of the conductivity have been performed using Monte Carlo techniques (Kirkpatrick 1973, Seager and Pike 1974, Webman *et al* 1975, Winterfeld *et al* 1981). Various theoretical methods, including the perturbation expansion (Hori and Yonezawa 1974, 1975a, b, 1977, Blackman 1976, Ahmed and Blackman 1979), the variational approach (Hori 1973a, b, Willemse and Caspers 1979), the effective-medium approximation (EMA) (Bruggeman 1935, Landauer 1952, Kirkpatrick 1973, Watson and Leath 1974, Bernasconi and Wiesmann 1976) and the percolation theory (Shante and Kirkpatrick 1971, Last and Thouless 1971, Essam 1972), were used to analyse the overall properties of randomly inhomogeneous materials. The single-vertex EMA, two-vertex EMA and three-vertex EMA, derived from the diagrammatic expansions, were shown to be equivalent to those obtained by effective-medium methods for a single bond, two bonds and three bonds, respectively, in the lattice model (Nagatani 1981a, b). In the non-self-consistent treatment, the approximations result in the expression of the effective conductivity as an integral power series of the fraction of broken bonds, and correspond to the group expansion for the continuum model derived by Jeffrey (1973, 1974).

Statistical theories of turbulence have been developed involving the diagrammatic expansions (Wyld 1961, Edwards 1964, Edwards and McComb 1969, Leslie 1973) and

Wiener–Hermite expansions (Siegel *et al* 1964, Imamura *et al* 1965, Meecham and Jeng 1968, Crow and Canavan 1970). Wiener (1939, 1958) has proposed the novel method of expanding random fields as an orthogonal polynomial series in powers of the white noise. The terms in Wiener’s expansion have the form of Hermite polynomials in the white-noise function. The feature that distinguishes the Hermite polynomials is that they are orthonormal with respect to a weighting function which has the form of a Gaussian probability distribution of unit variance.

In this paper, we present orthogonal polynomials of binomial-random variables for transport in randomly inhomogeneous media. The polynomials are orthogonal under the weighting function which represents the multiple-binomial distribution function. We expand random functions in orthogonal polynomials of binomial variables and obtain truncated equations for the determination of kernels in the expansion. We represent the effective conductivity in terms of the kernels. The effective conductivity is calculated by deriving the approximate solutions of kernels. In § 2 we give orthogonal polynomials of binary-random variables and summarise the outline of the expansion. Application to the bond model is given in § 3. Truncated equations are derived for kernels, and the effective conductivity is evaluated by the approximate solution of kernels. In § 4 we apply the expansion in orthogonal polynomials to the clumped-bond model and to the continuum model.

2. Outline of expansion

As the basis for constructing our series, we use the ‘binomial-random function’ $a(x_i)$ of a discrete-valued index x_i expressing the position of the space. For any fixed x_i , $a(x_i)$ is a binary-random variable having zero mean and is independent of $a(x_j)$ whenever $x_i \neq x_j$. The $a(x_i)$ is then defined by

$$\langle a(x_i) \rangle = 0 \tag{2.1}$$

$$\langle a(x_i)a(x_j) \rangle = \langle a(x_i)^2 \rangle \delta_{x_i x_j} \tag{2.2}$$

where the angle brackets denote an ensemble average and $\delta_{x_i x_j}$ is the Kronecker delta, equal to one when $x_i = x_j$, to zero otherwise.

We define the polynomials $B^{(n)}$ of binomial variables by

$$B^{(1)}(x_1) = a(x_1) \quad B^{(2)}(x_1, x_2) = (1 - \delta_{x_1 x_2}) \cdot a(x_1)a(x_2) \tag{2.3}$$

$$B^{(n)}(x_1, x_2, \dots, x_n) = a(x_1)(1 - \delta_{x_1 x_n}) \prod_{k=1}^{n-1} (1 - \delta_{x_k x_{k+1}}) \cdot a(x_{k+1}) \quad \text{for } n \geq 3.$$

The $B^{(n)}$ are orthogonal under the weighting function which represents the multiple-binomial distribution function:

$$\langle B^{(n)}(x_1, x_2, \dots, x_n) \cdot B^{(m)}(x'_1, x'_2, \dots, x'_m) \rangle = \begin{cases} 0 & \text{for } n \neq m \\ \left((1 - \delta_{x_1 x_n}) \prod_{i=1}^{n-1} (1 - \delta_{x_i x_{i+1}}) \right) \left((1 - \delta_{x'_1 x'_n}) \prod_{j=1}^{n-1} (1 - \delta_{x'_j x'_{j+1}}) \right) \\ \times \left(\sum_{\substack{\text{distinct} \\ \text{pairings}}} \prod_{\substack{\text{exogamous} \\ \text{pairs}}} \langle a(x_i)^2 \rangle \delta_{x_i x'_j} \right) & \text{for } n = m. \end{cases} \tag{2.4}$$

Here the symbols are to be interpreted as follows:

$$\prod_{\substack{\text{exogamous} \\ \text{pairs}}} \delta_{x_i x'_j}$$

is a product in which the x_i (or x'_j) index from x_1 (or x'_1) to x_n (or x'_n) appears just once as a subscript of the Kronecker delta multiplicand, subject to the restriction that each pair coupled in a delta function is 'exogamous' in the sense that the two partners in it come from different sets, (x_1, x_2, \dots, x_n) and $(x'_1, x'_2, \dots, x'_n)$. In the summation, such a product appears just once for each distinct way of arranging all x variables.

The expansion of a random function f in orthogonal polynomials is given by

$$\begin{aligned} f(x) = \langle f(x) \rangle + \sum_{x_1} K^{(1)}(x; x_1) \cdot B^{(1)}(x_1) + \frac{1}{2!} \sum_{x_1, x_2} K^{(2)}(x; x_1, x_2) \\ \times B^{(2)}(x_1, x_2) + \dots + \frac{1}{n!} \sum_{x_1, x_2, \dots, x_n} K^{(n)}(x; x_1, x_2, \dots, x_n) \\ \times B^{(n)}(x_1, x_2, \dots, x_n) + \dots \end{aligned} \tag{2.5}$$

where the summations over x_n range over all positions of the space. Here it must be borne in mind that the kernels K are ordinary functions of their arguments, while the B 's are random functions. The statistical properties of f will be determined by its moments, i.e. by exception values of the form

$$\langle f(x') f(x'') \dots f(x^{(n)}) \rangle. \tag{2.6}$$

The computation of such an expansion can, by commuting the $\langle \rangle$ operation with the sums in (2.6), be reduced to the evaluation of sums of products of K 's, since the exception values of products of B 's are invariably combinations of Kronecker δ 's.

The application of the expansion (2.5) to stochastic equations involves three steps. Firstly, random functions are replaced by the expansion (2.5). Secondly, the resulting expression is multiplied by any one of the orthogonal polynomials of binomial variables. Thirdly, the product is averaged over the ensemble of binomial variables. The ensemble average projects the stochastic equation onto the statistically orthogonal polynomials of the binomial variable. These three steps extract an equation of the kernel that appears in (2.5) as the coefficient of the particular polynomial used in the first step. Applied to each polynomial in turn, the extraction process generates an infinite set of coupled equations for the determination of the infinite set of kernels in (2.5). Randomness is thereby removed from the problem at the outset, and one can concentrate on finding approximate solutions for the kernels. The expansion is computationally useful if it can be truncated after a few terms.

3. Application to inhomogeneous transport in the bond model

We consider the problem of electrical conduction in bond-disordered resistor networks in which bonds are broken at random (bond model). The models are an infinite square resistor network and an infinite simple cubic resistor network. We consider the imperfect lattice in terms of perturbations from the perfect reference lattice, which is defined as a network of conductances g_0 across each of which is a field $E^0 (= \langle E \rangle)$. Making use of the Green function formalism (Blackman 1976, Ahmed and Blackman

1979, Nagatani 1981a, b), the electric field E_i of any one bond i can be expressed as

$$E_i = E^0 + \sum_j \Gamma_{ij} \Delta_j E_j \tag{3.1}$$

where $\Delta_j = (g_j - g_0)/g_0$, g_j is the conductance of a bond j in which each bond has a probability $1 - p = c$ of taking the value $g_j = 0$ and a probability $p = 1 - c$ of taking a finite value g_0 , subscripts label bonds, and Γ_{ij} is a bond-bond Green function that depends on the type of lattice, the separation of bond i and j , and their relative orientation. We shall apply the expansion (2.5) to the stochastic equation (3.1). The random function E_i can be expanded in orthogonal polynomials of binomial-random variables as

$$\frac{E_i}{E^0} = 1 + \sum_j K_{ij}^{(1)} \cdot B_j^{(1)} + \frac{1}{2!} \sum_j \sum_k K_{ijk}^{(2)} \cdot B_{jk}^{(2)} + \frac{1}{3!} \sum_j \sum_k \sum_m K_{ijkm}^{(3)} \cdot B_{jkm}^{(3)} + \dots \tag{3.2}$$

where

$$\begin{aligned} B_j^{(1)} &= \Delta_j + c & B_{jk}^{(2)} &= (1 - \delta_{jk})(\Delta_j + c)(\Delta_k + c) \\ B_{jkm}^{(3)} &= (1 - \delta_{jk})(1 - \delta_{km})(1 - \delta_{mj})(\Delta_j + c)(\Delta_k + c)(\Delta_m + c) & \dots \end{aligned} \tag{3.3}$$

$\langle \Delta_i \rangle = -c$ and, in the summations, j, k and m range over all bonds of the lattice.

In equation (3.1) the electric field E_i is replaced by (3.2). Applying each polynomial to the resulting expression in turn, the products are averaged over the ensemble of binomial variables. We then obtain an infinite set of coupled equations for the determination of kernels in (3.2). For the sake of computational usefulness, if it is truncated after the third term in (3.2), we obtain

$$K_{im}^{(1)} = \Gamma_{im} - c \sum_j \Gamma_{ij} K_{jm}^{(1)} + (2c - 1) \cdot \Gamma_{im} K_{mm}^{(1)} + (c - c^2) \sum_j \Gamma_{ij} K_{jim}^{(2)} (1 - \delta_{jm}) \tag{3.4}$$

$$K_{imn}^{(2)} = \Gamma_{im} K_{mn}^{(1)} + \Gamma_{in} K_{nm}^{(1)} - c \sum_j \Gamma_{ij} K_{jmn}^{(2)} + (2c - 1) \Gamma_{im} K_{mnn}^{(2)} + (2c - 1) \Gamma_{in} K_{nmm}^{(2)}. \tag{3.5}$$

The expression for effective conductivity g^* is given by

$$\Delta^* \equiv \langle \Delta_i E_i \rangle / E^0 = -c + (c - c^2) K_{ii}^{(1)} \tag{3.6}$$

where $\Delta^* = (g^* - g_0)/g_0$.

We solve equations (3.4) and (3.5) for the kernel $K^{(1)}$. For simplicity, we derive the solution of the kernel $K^{(1)}$ to the first order of the concentration c of broken bonds. For the second kernel $K_{jim}^{(2)}$, we obtain from equation (3.5)

$$K_{jim}^{(2)} = \left(\frac{\Gamma_0(1 + \Gamma_0) - (\Gamma_{mj})^2}{(1 + \Gamma_0)^2 - (\Gamma_{mj})^2} \right) \cdot K_{jm}^{(1)} + \left(\frac{\Gamma_{jm}}{(1 + \Gamma_0)^2 - (\Gamma_{mj})^2} \right) \cdot K_{mj}^{(1)} + O(c). \tag{3.7}$$

By the substitution of equation (3.7) in equation (3.4), the first kernel $K_{im}^{(1)}$ is given by

$$\begin{aligned} K_{im}^{(1)} &= \frac{\Gamma_{im}}{1 + \Gamma_0} + \frac{2\Gamma_0 \Gamma_{im}}{(1 + \Gamma_0)^2} \cdot c + \sum_j \left(\Gamma_{ij} - \frac{\Gamma_{im} \Gamma_{mj}}{1 + \Gamma_0} \right) \frac{\Gamma_{jm}}{1 + \Gamma_0} \\ &\times \left[-1 + \left(\frac{\Gamma_0(1 + \Gamma_0) + \Gamma_{jm} - (\Gamma_{mj})^2}{(1 + \Gamma_0)^2 - (\Gamma_{mj})^2} \right) (1 - \delta_{jm}) \right] \cdot c + O(c^2). \end{aligned} \tag{3.8}$$

Substituting equation (3.8) in equation (3.6), we obtain

$$\frac{g^*}{g_0} = 1 - \frac{1}{1 + \Gamma_0} \cdot c - \frac{\Gamma_0}{(1 + \Gamma_0)^2} \cdot c^2 + \sum_{\substack{j \\ (j \neq i)}} \left(\frac{-(\Gamma_{ij})^2 / (1 + \Gamma_0)^3 + (\Gamma_{ij})^3 / (1 + \Gamma_0)^4}{1 - (\Gamma_{ij})^2 / (1 + \Gamma_0)^2} \right) \cdot c^2 + O(c^3). \tag{3.9}$$

Our expression (3.9) for the effective conductivity agrees with that derived by the two-bond approximation (Nagatani 1981a). We see immediately that the truncation after the third term in the expansion (3.2) gives the exact value to order c^2 .

4. Expansions for the clumped-bond and continuum models

We present expansions in orthogonal polynomials of binomial variables for the clumped-bond model (Nagatani 1982) and for the continuum model (Hori and Yonezawa 1977). We derive truncated coupled equations for the determination of kernels in expansions.

4.1. Clumped-bond model

We consider the electrical conduction in clumped-bond-disordered resistor networks where clumps of bonds are broken at random in square and simple cubic resistor networks. The electric field $E_{a(i)}$ of any one bond i within the clump a is determined by

$$E_{a(i)} = E^0 + \sum_b \sum_{j=1}^n \Gamma_{a(i)b(j)} \Delta_b E_{b(j)} \tag{4.1}$$

where $\Delta_b = (g_b - g_0) / g_0$, g_b is the conductance of the bond in the clump b in which each clump has a probability c of taking the value $g_b = 0$ and a probability $1 - c$ of taking a finite value g_0 , the subscripts $b(j)$ represent the bond j in the clump b , $\Gamma_{a(i)b(j)}$ is the bond-bond Green function between the bond i in the clump a and the bond j in the clump b , and, in the summations, b and j range over all clumps of the lattice and over all bonds within a single clump respectively.

We apply the expansion (2.5) to the stochastic equation (4.1). The random function $E_{a(i)}$ can be expanded in orthogonal polynomials of binary-random variables as

$$\frac{E_{a(i)}}{E^0} = K_{a(i)}^{(0)} + \sum_b K_{a(i)b}^{(1)} \cdot B_b^{(1)} + \frac{1}{2!} \sum_b \sum_c K_{a(i)bc}^{(2)} \cdot B_{bc}^{(2)} + \frac{1}{3!} \sum_b \sum_c \sum_d K_{a(i)bcd}^{(3)} \cdot B_{bcd}^{(3)} + \dots \tag{4.2}$$

where

$$\begin{aligned} B_b^{(1)} &= \Delta_b + c & B_{bc}^{(2)} &= (1 - \delta_{bc})(\Delta_b + c)(\Delta_c + c) \\ B_{bcd}^{(3)} &= (1 - \delta_{bc})(1 - \delta_{cd})(1 - \delta_{db})(\Delta_b + c)(\Delta_c + c)(\Delta_d + c) & \dots \end{aligned} \tag{4.3}$$

$\langle \Delta_a \rangle = -c$ and, in the summations, b , c and d range over all clumps of the lattice.

In equation (4.1) the electric field $E_{a(i)}$ is replaced by (4.2). Applying each polynomial to the resulting expression in turn, and averaging over the ensemble of binomial variables, we obtain an infinite set of coupled equations for kernels in (4.2). If

it is truncated after the third term in (4.2), we obtain

$$K_{a(i)}^{(0)} = 1 - c \sum_b \sum_{j=1}^n \Gamma_{a(i)b(j)} K_{b(j)}^{(0)} + (c - c^2) \sum_b \sum_{j=1}^n \Gamma_{a(i)b(j)} K_{b(j)b}^{(1)} \tag{4.4}$$

$$K_{a(i)m}^{(1)} = \sum_{j=1}^n \Gamma_{a(i)m(j)} K_{m(j)}^{(0)} - c \sum_b \sum_{j=1}^n \Gamma_{a(i)b(j)} K_{b(j)m}^{(1)} + (2c - 1) \sum_{j=1}^n \Gamma_{a(i)m(j)} K_{m(j)m}^{(1)} + (c - c^2) \sum_b \sum_{j=1}^n \Gamma_{a(i)b(j)} K_{b(j)bm}^{(2)} (1 - \delta_{bm}) \tag{4.5}$$

$$K_{a(i)md}^{(2)} = \sum_{j=1}^n \Gamma_{a(i)m(j)} K_{m(j)d}^{(1)} + \sum_{j=1}^n \Gamma_{a(i)d(j)} K_{d(j)m}^{(1)} - c \sum_b \sum_{j=1}^n \Gamma_{a(i)b(j)} K_{b(j)md}^{(2)} + (2c - 1) \sum_{j=1}^n \Gamma_{a(i)m(j)} K_{m(j)md}^{(2)} + (2c - 1) \sum_{j=1}^n \Gamma_{a(i)d(j)} K_{d(j)dm}^{(2)}. \tag{4.6}$$

The effective conductivity g^* is given by

$$g^*/g_0 = 1 - c + (c - c^2) K_{a(i)a}^{(1)}/K_{a(i)}^{(0)}. \tag{4.7}$$

If one finds approximate solutions for the kernels, one can derive the expression for the effective conductivity.

4.2. Continuum model

We consider electrical conduction in a 2D (or 3D) inhomogeneous medium with spatially fluctuating conductivity. A randomly continuous medium can be represented by the cell model which was first proposed by Miller (1969a, b) and discussed in detail by Brown (1974) and Hori (1975). In the cell model, the space is completely covered by non-overlapping cells within which the material property is constant. Cells are distributed in a manner such that the material is statistically homogeneous. The material property of a cell is statistically independent of that of any other cell. The equivalent expression for the electric fields in the continuum model is

$$E_i(\alpha(x_1)) = E^0 + \sum_{\beta} \int dx_2 \Gamma_{ij}(\alpha(x_1), \beta(x_2)) \Delta_{\beta} E_j(\beta(x_2)) \tag{4.8}$$

where $\Delta_{\beta} = (g_{\beta} - g_0)/g_0$, g_{β} is the conductance of the cell in which each cell has a probability c of taking the value $g_{\beta} = 0$ and a probability $1 - c$ of taking a finite value g_0 , $\alpha(x_1)$ represents the position x_1 within the cell α , subscripts i and j indicate the Cartesian components, the integral is extended over the space within a single cell, and, in the summation, β ranges over all cells of the whole space. The bond labels of equation (4.1) are replaced by a continuous variable x and a subscript i to indicate the Cartesian components. The Green functions $\Gamma_{ij}(\alpha(x_1), \beta(x_2))$ appropriate to equation (4.8) are given by Hori and Yonezawa (1977). We apply the expansion (2.5) to the stochastic equation (4.8). The random function $E_i(\alpha(x_1))$ can be expanded as

$$\frac{E_i(\alpha(x_1))}{E^0} = K_i^{(0)}(\alpha(x_1)) + \sum_{\beta} K_i^{(1)}(\alpha(x_1), \beta) \cdot B_{\beta}^{(1)} + \frac{1}{2!} \sum_{\beta} \sum_{\gamma} K_i^{(2)}(\alpha(x_1), \beta, \gamma) \cdot B_{\beta\gamma}^{(2)} + \dots \tag{4.9}$$

where

$$B_{\beta}^{(1)} = \Delta_{\beta} + c \quad B_{\beta\gamma}^{(2)} = (1 - \delta_{\beta\gamma})(\Delta_{\beta} + c)(\Delta_{\gamma} + c) \quad \dots \quad (4.3')$$

$\langle \Delta_{\beta} \rangle = -c$ and, in the summations, β and γ range over all cells of the whole space.

In equation (4.8) the electric field $E_i(\alpha(x_1))$ is replaced by (4.9). Applying each polynomial to the resulting expression in turn, and averaging over the ensemble of binomial variables, we obtain an infinite set of coupled equations for kernels. If it is truncated after the third term in (4.9), we obtain

$$K_i^{(0)}(\alpha(x_1)) = 1 - c \sum_{\beta} \int dx_2 \Gamma_{ij}(\alpha(x_1), \beta(x_2)) \cdot K_j^{(0)}(\beta(x_2)) + (c - c^2) \sum_{\beta} \int dx_2 \Gamma_{ij}(\alpha(x_1), \beta(x_2)) \cdot K_j^{(1)}(\beta(x_2), \beta) \quad (4.10)$$

$$K_i^{(1)}(\alpha(x_1), \gamma) = \int dx_2 \Gamma_{ij}(\alpha(x_1), \gamma(x_2)) \cdot K_j^{(0)}(\gamma(x_2)) - c \sum_{\beta} \int dx_2 \Gamma_{ij}(\alpha(x_1), \beta(x_2)) \cdot K_j^{(1)}(\beta(x_2), \gamma) + (2c - 1) \int dx_2 \Gamma_{ij}(\alpha(x_1), \gamma(x_2)) \cdot K_j^{(1)}(\gamma(x_2), \gamma) + (c - c^2) \sum_{\beta} \int dx_2 \Gamma_{ij}(\alpha(x_1), \beta(x_2)) \cdot K_j^{(2)}(\beta(x_2), \beta, \gamma) \cdot (1 - \delta_{\beta\gamma}) \quad (4.11)$$

$$K_i^{(2)}(\alpha(x_1), \gamma, \delta) = \int dx_2 \Gamma_{ij}(\alpha(x_1), \gamma(x_2)) \cdot K_j^{(1)}(\gamma(x_2), \delta) + \int dx_2 \Gamma_{ij}(\alpha(x_1), \delta(x_2)) \cdot K_j^{(1)}(\delta(x_2), \gamma) - c \sum_{\beta} \int dx_2 \Gamma_{ij}(\alpha(x_1), \beta(x_2)) \cdot K_j^{(2)}(\beta(x_2), \gamma, \delta) + (2c - 1) \int dx_2 \Gamma_{ij}(\alpha(x_1), \gamma(x_2)) \cdot K_j^{(2)}(\gamma(x_2), \gamma, \delta) + (2c - 1) \int dx_2 \Gamma_{ij}(\alpha(x_1), \delta(x_2)) \cdot K_j^{(2)}(\delta(x_2), \delta, \gamma). \quad (4.12)$$

The effective conductivity g^* is given by

$$g^*/g_0 = 1 - c + (c - c^2) \cdot K_i^{(1)}(\alpha(x_1), \alpha) / K_i^{(0)}(\alpha(x_1)). \quad (4.13)$$

If one finds approximate solutions for the kernels, one can derive the expression for the effective conductivity. Comparing the clumped-bond model with the continuum model, we see that the clumped-bond model presents the continuum model in the limiting case where the number of bonds in a clump is infinite. It is not easy to derive solutions of kernels for the continuum model, but one may derive solutions of kernels for the clumped-bond model.

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