# Series expansion for the macroscopic conductivity of a random resistor network $\dagger$ 

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#### Abstract

The macroscopic conductivity $\sigma_{e}$ of a simple cubic, two-component, random resistor network is systematically expanded as a power series in the relative difference between the two basic conductances. Graphs are developed to aid in implementing the calculation. A single-bond $T$-matrix-type rearrangement of the series leads to various types of single-bond approximations, and to an improved graph expansion for $\sigma_{\mathrm{e}}$. The improved expansion is worked out up to seventh order, and used to discuss the singular properties of $\sigma_{c}$.


## 1. Introduction

Random resistor networks have received attention in recent years because they provide the simplest type of model for an inhomogeneous conductor. As such, the random resistor network has been used to discuss percolation conductivity in a macroscopically inhomogeneous medium (see, e.g., the review article by Kirkpatrick 1973), as well as the more difficult problem of hopping conduction between localised impurity states of electrons in microscopically dirty semiconductors (see Miller and Abrahams 1960, Ambegaokar et al 1971, Shklovskii and Efros 1971, Pollak 1972). It has even been invoked in an attempt to describe the metal-semiconductor transition in metal-ammonia solutions and in expanded liquid mercury and liquid caesium (see Cohen and Jortner 1974), though such uses have been severely criticised by Mott (1973).

Theoretical discussions of random resistor networks have been given by means of numerical solutions of finite networks (Kirkpatrick 1973), by a scaling theory (Straley 1976), by position-space renormalisation-group transformations (Stinchcombe and Watson 1976, Kirkpatrick 1977), by relating the resistor network to the zero-state Potts model (Dasgupta et al 1978), by a series expansion (Fisch and Harris 1978), and by various one-shot approximations such as effective-medium theory (EMT) (Kirkpatrick 1973), and mean-field theory (after properly defining an order parameter-see Stephen 1978). Of these methods, the only one which is a systematic expansion is the series method developed by Harris and Fisch for cubic and hypercubic networks made of two types of conductors $g$ and 0 . This is an expansion in powers of $p$, the probability for any conductor to be $g$.

[^0]It has recently been pointed out that the conductivity of a macroscopically inhomogeneous system has some characteristic analytical properties as a function of the conductivity ratios of its pure constituents (Bergman 1978a, b). In this article we attempt to exploit these properties in order to develop a systematic expansion for the macroscopic conductivity $\sigma_{\mathrm{e}}$ of a random, simple cubic network of conductors $g_{1}, g_{2}$ as a function of $g_{1} / g_{2}$ and for arbitrary values of $p$, the probability for any conductor to be $g_{1}$. It is hoped that such an expansion will eventually enable us to obtain quantitative results concerning the singularities of $\sigma_{\mathrm{e}}$. It is also hoped that similar expansions may be developed in the future for calculating the conductivity and other properties of real disordered composite materials.

In § 2, we formulate the problem and develop the basic expansion for the solution of the network, as well as for $\sigma_{\mathrm{e}}$, as a power series in $\left(g_{2}-g_{1}\right) / g_{2}$. In $\S 3$, we introduce graphs to aid in calculating all the contributions of a given order for $\sigma_{\mathrm{e}}$. By a standard $T$-matrix resummation procedure, the expansion is rearranged so it becomes an expansion around the EMT approximation for $\sigma_{\mathrm{e}}$. Using the rearranged expansion, explicit expressions are found for all the terms up to seventh order in the power series for $\sigma_{e}$. In § 4, those terms are used to analyse the singular properties of $\sigma_{\mathrm{e}}$. The results, though at present less accurate than those obtained by other methods, can in principle be improved by calculating more terms in the series. Furthermore, they bear upon the properties of $\sigma_{\mathrm{e}}$ as a function of $g_{1} / g_{2}$, and not merely for $g_{1} / g_{2}=0$, as is usually the case with all the other methods with the exception of the numerical simulations. In Appendix 1 we discuss the mathematical properties of as well as methods for evaluating certain matrix elements $\Gamma_{a b}$ that are used in the expansion. In Appendix 2 we give the decomposition of certain correlation functions used in the expansion. In Appendix 3 we give explicit expressions for the first seven terms in the power series for $\sigma_{\mathrm{e}}$.

## 2. Formulation of the problem and basic equations

We consider a random resistor network in the form of a three-dimensional, simple cubic lattice, where every bond between nearest-neighbour sites independently assumes one of the two conductances $g_{1}, g_{2}$ with probability $p, 1-p$ respectively. The method used to analyse this system is the discrete analogue of the method developed by Bergman (1979a, b) to treat a continuous two-phase medium.

We assume that the network fills the space between the infinitely large plates of a parallel plate condenser, which are at a distance $L$ from each other, and is subjected to


Figure 1. Schematic representation of the resistor network between the parallel plates of an infinite condenser. In this drawing, the distance between the plates is $L=3$. The sites $m$ and $k$ are surface sites.
a potential difference also equal to $L$ (see figure 1). Kirchoff's equations for the potentials $V_{j}$ at all the lattice sites are

$$
\begin{equation*}
\sum_{j} g_{i j}\left(V_{i}-V_{j}\right)=0 \tag{2.1}
\end{equation*}
$$

where the sum is over all the nearest neighbours to the site $i$, and where $i$ is an internal site (i.e., surface sites are excluded-there the potential is either 0 or $L$ ). The conductance $g_{i j}$ is either $g_{1}$ or $g_{2}$, and will be represented in the form

$$
\begin{equation*}
g_{i j}=g_{2} \varepsilon_{i j}\left(1-u \theta_{i j}\right) \tag{2.2}
\end{equation*}
$$

where

$$
\begin{align*}
& u \equiv 1-g_{1} / g_{2} \\
& \theta_{i j}= \begin{cases}1 & \text { if } g_{i j}=g_{1} \\
0 & \text { if } g_{i j}=g_{2}\end{cases}  \tag{2.3}\\
& \varepsilon_{i j}= \begin{cases}1 & \text { if } i, j \text { are nearest-neighbour sites } \\
0 & \text { otherwise. }\end{cases}
\end{align*}
$$

Obviously, $\theta_{i j}$ is a random bond-variable. Using this representation, Kirchoff's equations become

$$
\begin{equation*}
\sum_{i} \varepsilon_{i j}\left(V_{i}-V_{j}\right)=u \sum_{j} \theta_{i j}\left(V_{i}-V_{j}\right) \tag{2.4}
\end{equation*}
$$

We introduce the discrete lattice Green function $\gamma_{i}^{\prime}$ for the uniform network, defined by the equations

$$
\begin{equation*}
\sum_{j} \varepsilon_{i j}\left(\gamma_{i}^{\prime}-\gamma_{i}^{l}\right)=\delta_{i l} \tag{2.5}
\end{equation*}
$$

together with the requirement that $\gamma_{i}^{l}$ vanishes when $i$ is a surface site. The quantity $\gamma_{i}^{l}$ is the discrete analogue of the potential created at $i$ by a point charge at $l$. With the help of $\gamma_{i}^{l}$, (2.4) and the accompanying boundary condition can be transformed into a set of equations for the voltages across the individual conductors

$$
\begin{equation*}
V_{a}=Z_{a}+u \sum_{b} \Gamma_{a b} \theta_{b} V_{b} \tag{2.6}
\end{equation*}
$$

Here we have introduced the bond indices $a, b$, i.e.,

$$
\begin{equation*}
V_{a} \equiv V_{i j} \equiv V_{i}-V_{j} \quad Z_{a} \equiv Z_{i}-Z_{j} \quad \theta_{a} \equiv \theta_{i j} \tag{2.7}
\end{equation*}
$$

where $Z_{i}$ is the $z$-coordinate of the site $i$, and the discrete dipole-dipole interaction between two bonds

$$
\begin{equation*}
\Gamma_{a b} \equiv \Gamma_{i j, l m} \equiv \gamma_{i}^{l}-\gamma_{i}^{m}-\gamma_{j}^{l}+\gamma_{j}^{m} . \tag{2.8}
\end{equation*}
$$

The mathematical properties of $\Gamma_{a b}$, as well as convenient series for its numerical evaluation, are described in Appendix 1.

The effective or average uniform conductance per bond $g_{e}$ of the random network is defined by requiring the total current or the total dissipation (Joule heat) to be reproduced correctly. For convenience, we will take all the bonds of the network to have unit length, so that $Z_{a}=1$ if $a$ is a bond in the $z$ direction while $Z_{a}=0$ for bonds in the $x$ or $y$ direction. The average current density is then given by

$$
\begin{equation*}
g_{\mathrm{e}}=\frac{1}{N} \sum_{a} g_{a} V_{a} Z_{a} \tag{2.9}
\end{equation*}
$$

where $N$ is the total number of unit cells. Instead of $g_{e}$, it is more convenient to discuss the following quantity

$$
\begin{equation*}
f(u) \equiv 1-\frac{g_{e}}{g_{2}}=\frac{u}{N} \sum_{a} Z_{a} \theta_{a} V_{a} \equiv \frac{u}{N} Z \theta V, \tag{2.10}
\end{equation*}
$$

where we used equation (2.2) for $g_{a}$, and where we also introduced a symbolic notation for the summation over bond indices. Introducing a formal or a series solution of (2.6) for $V_{a}$, we can finally write $f(u)$ as
$f(u)=\frac{u}{N}\left(Z \theta \frac{1}{1-u \Gamma \theta} Z\right)=\frac{1}{N} Z\left(u \theta+u^{2} \theta \Gamma \theta+u^{3} \theta \Gamma \theta \Gamma \theta+\ldots\right) Z$.
The function $f(u)$ is completely analogous to the characteristic geometric function which was introduced by Bergman (1978a, b) to describe the macroscopic dielectric constant of a composite material. In the case of a random network, we must average every term of (2.11) over the distribution of $\theta_{a}$ in order to get an expansion for the average of $f(u)$. We will always discuss an infinitely large network, in which case $\gamma_{i}^{l}$ depends only upon the vector $i-l$. Consequently, $\Gamma_{a b}$ also depends only on the vector separation of the bonds $a$ and $b$ and on their orientations, and not on their absolute positions. Consequently, the ensemble average of

$$
\begin{equation*}
\left(\theta \frac{1}{1-u \Gamma \theta}\right)_{a b} \tag{2.15}
\end{equation*}
$$

also depends only on the orientations and vector separation of $a$ and $b$, and in (2.11) we can omit the sum on one of the outermost bond indices, at the same time omitting also the $1 / N$ factor.

## 3. Graph expansions for $\langle f(u)\rangle$

When the series of (2.11) is averaged over the distribution of the random variables $\theta_{a}$, each term will include a correlation function of the type

$$
\begin{equation*}
\left\langle\theta_{a} \theta_{b} \theta_{c} \theta_{d} \ldots\right\rangle \tag{3.1}
\end{equation*}
$$

For independently distributed bonds, each of these correlation functions may be decomposed into a sum of $\delta$-functions multiplied by polynomials in $p$, e.g.,

$$
\begin{align*}
& \left\langle\theta_{0}\right\rangle=p \\
& \left\langle\theta_{0} \theta_{1}\right\rangle=p^{2}+p(1-p) \delta_{01} \\
& \left\langle\theta_{0} \theta_{1} \theta_{2}\right\rangle=p^{3}+p^{2}(1-p)\left(\delta_{01}+\delta_{02}+\delta_{12}\right)+p(1-p)(1-2 p) \delta_{012}  \tag{3.2}\\
& \left\langle\theta_{0} \theta_{1} \theta_{2} \theta_{3}\right\rangle=p^{4}+p^{3}(1-p)\left(\delta_{01}+\ldots\right)+p^{2}(1-p)(1-2 p)\left(\delta_{012}+\ldots\right) \\
& +p(1-p)\left(1-6 p+6 p^{2}\right) \delta_{0123} \\
& +p^{2}(1-p)^{2}\left(\delta_{01} \delta_{23}+\delta_{02} \delta_{13}+\delta_{12} \delta_{03}\right),
\end{align*}
$$

where a symbol such as $\delta_{012}$ is equal to 1 if the bonds $0,1,2$ are all equal, and to 0 otherwise. The decomposition of higher-order correlation functions, up to $n=6$, is given in Appendix 2. Every order- $n$ correlation function is multiplied by a sum of a
product of $n-1$ matrix elements $\Gamma_{a b}$. Many of these sums either vanish due to (A1.13), or simplify due to (A1.8). The low-order terms of $\langle f(u)\rangle$ are thus readily found to be

$$
\begin{equation*}
\langle f(u)\rangle=u p+\frac{1}{3} u^{2} p(1-p)+\frac{1}{9} u^{3} p(1-p)(1+p)+\mathrm{O}\left(u^{4}\right) . \tag{3.3}
\end{equation*}
$$

In order to calculate higher-order terms in this expansion, we need to calculate non-trivial sums such as

$$
\begin{equation*}
\sum_{b}\left(\Gamma_{a b}\right)^{3} \tag{3.4}
\end{equation*}
$$

which have to be evaluated numerically. In order to facilitate the evaluation of the non-vanishing terms in the expansion, we characterise each one by an appropriate graph: We assign a vertex to every independent bond index $a$, and a line segment joining two vertices to represent every matrix element $\Gamma_{a b}$. The factor $Z_{a}$ is represented by a oneended (dangling) segment which emanates from the vertex $a$. The non-vanishing contributions to the first four orders in (2.11) are represented by the graphs of table 1. The rules for drawing these graphs are that every vertex must have an even number of lines attached to it, and all graphs are doubly connected, i.e., they cannot be separated into disconnected parts by removing a single line. The last rule follows from the fact that such an isolated line would have associated with it a single sum of the form of (A1.13), which vanishes. A further rule is that any vertex that has only two lines attached to it can

Table 1. All non-zero graphs and their contributions to the coefficient of $u^{n}, 1 \leqslant n \leqslant 4$, in the series for $\langle f(u)\rangle$. In column 3 there appear the $\delta$-function products which determine all the non-repeating covering paths $0,1, \ldots n-1$ of a given graph. The total number of such paths is the multiplicity of the graph.

| Order in <br> $u$ | Contributing <br> graphs | Non-repeating <br> covering paths |
| :--- | :--- | :--- | | Total contribution of the graph |
| :--- |
| $n=1$ |
| $n=2$ |

be ignored, and a line that includes any number of such vertices can be represented by a single factor $\Gamma_{a b}$. This follows from the idempotency property (A1.8).

Using these rules, every graph can be uniquely translated into a product of $\Gamma$ matrices. In general, however, the same topological $n$ th-order graph may represent more than one term in the decomposition of the order- $n$ correlation function. The total number of such terms represented by one graph can be obtained simply by counting the number of different continuous paths which cover the entire graph without traversing any line more than once. Every non-repeating covering path of this kind can be represented by a product of $\delta$-functions of vertices from 0 to $n-1$ which also determines the topology of the graph. All the $\delta$-function products which correspond to the same graph are similar in form, and thus carry the same p-polynomial in the decomposition of the correlation function. Their total number is equal to the multiplicity of the given $n$ th-order graph, and this number multiplied by the appropriate $p$-polynomial and by the characteristic $\Gamma$-product is the total contribution of that graph to the coefficient of $u^{n}$ in the series for $\langle f(u)\rangle$. In table 1, we show all the non-zero contributions up to order $n=4$. Together with each graph appear the $\delta$-function products which determine all the non-repeating covering paths, as well as the total contribution of that graph.

From table 1, and recalling that $\Gamma_{a a}=\frac{1}{3}$ (see equation (A1.9)), we can easily reproduce the first three terms in the power series for $\langle f(u)\rangle$, as in (3.3). For the fourth term we get, by summing all the four graphs,

$$
\begin{equation*}
u^{4}\left[\frac{1}{9} p(1-p)\left(\frac{1}{3}+p\right)+p^{2}(1-p)^{2} \sum_{1} Z_{0} \Gamma_{01}^{3} Z_{1}\right] \tag{3.5}
\end{equation*}
$$

If one tries to implement this expansion beyond fifth order, the number of graphs proliferates to such an extent that it becomes impossible to keep track of them all. Furthermore, it is clear even from the orders up to $n=4$, shown in table 1 , that most of the contributing graphs are trivial in the sense that they depend only on the diagonal matrix element $\Gamma_{00}=\frac{1}{3}$. In order to get a more manageable expansion, we rearrange the series of (2.11) by a $T$-matrix resummation procedure (see e.g., the review articles by Elliott et al 1974 and by Ehrenreich and Schwartz 1976). Defining
$\hat{\Gamma}_{a b} \equiv \Gamma_{a b}-\frac{1}{3} \delta_{a b} \quad \delta \theta_{a} \equiv \theta_{a}-\theta_{0} \quad \delta \kappa_{a} \equiv u \delta \theta_{a} /\left(1-u \theta_{0}-\frac{1}{3} u \delta \theta_{a}\right)$
where $\theta_{0}$ is some constant to be determined later, and where the matrix $\hat{\Gamma}_{a b}$ has vanishing diagonal elements, we can easily show that
$\frac{f(u)-u \theta_{0}}{1-u \theta_{0}}=\frac{1}{N}\left(Z \delta \kappa \frac{1}{1-\hat{\Gamma} \delta K} Z\right)=\frac{1}{N} Z(\delta \kappa+\delta \kappa \hat{\Gamma} \delta \kappa+\delta \kappa \hat{\Gamma} \delta \kappa \hat{\Gamma} \delta \kappa+\ldots) Z$.
As usual, one of the advantages of this form is that two adjacent factors must have different bond indices, and consequently they are statistically independent. In the single-bond approximation (SBA) we take all the factors in each product to be independent, and we thus get for the average of $f(u)$

$$
\begin{equation*}
\frac{\langle f(u)\rangle_{\mathrm{SBA}}-u \theta_{0}}{1-u \theta_{0}}=\frac{1}{N}\left(Z\langle\delta \kappa\rangle \frac{1}{1-\hat{\Gamma}\langle\delta \kappa\rangle} Z\right)=\frac{\langle\delta \kappa\rangle}{1+\frac{1}{3}\langle\delta \kappa\rangle}, \tag{3.8}
\end{equation*}
$$

where we used the fact that

$$
\begin{equation*}
\sum_{b} \hat{\Gamma}_{a b} Z_{b}=-\Gamma_{a a} Z_{a}=-\frac{1}{3} Z_{a} \tag{3.9}
\end{equation*}
$$

The simplest of the single-bond approximations is obtained if we choose $\theta_{0}=0$. In
that case, we find

$$
\begin{align*}
& \langle\delta \kappa\rangle=u p /\left(1-\frac{1}{3} u\right)  \tag{3.10}\\
& \langle f(u)\rangle \simeq u p /\left[1-\frac{1}{3} u(1-p)\right] .
\end{align*}
$$

This is just the Clausius-Mossotti approximation for $f(u)$ of a composite medium where the $g_{2}$ conductors are taken to be the host medium and the $g_{1}$ conductors are taken to be the inclusions.

Another possibility is to choose $\theta_{0}=p$, which leads to

$$
\begin{equation*}
\frac{\langle f(u)\rangle-u p}{1-u p} \cong \frac{\frac{1}{3} u^{2} p(1-p)}{1-\frac{1}{3} u(1+4 p)+\frac{1}{3} u^{2} p(1+p)} \tag{3.11}
\end{equation*}
$$

This approximation seems to be better than (3.10): whereas (3.10) only reproduces correctly the first two terms in the exact series of (3.3), (3.11) reproduces the third term as well.

Finally, we can choose $\theta_{0}$ so as to make the average of $\delta \kappa$ vanish. This leads to

$$
\begin{equation*}
\langle f(u)\rangle \simeq u \theta_{0}=\frac{3}{4}\left(1-\frac{1}{3} u+p u \pm\left[\left(1-\frac{1}{3} u\right)^{2}+p^{2} u^{2}-\frac{2}{3} p u(1+u)\right]^{1 / 2}\right) \tag{3.12}
\end{equation*}
$$

which is nothing else than the effective-medium approximation (EMT) for the random network. Since now $\langle\delta \kappa\rangle=0$, it is clear that the exact series for $\langle f(u)\rangle-u \theta_{0}$ will start with a fourth-order term in $\delta \kappa$ (and hence in $u$ ). All the lower-order terms on the RHS of (3.7) will vanish when averaged. Like (3.11), equation (3.12) is thus correct up to, and including, terms of order $u^{3}$, and we may hope that the resulting exact expansion for $\langle f(u)\rangle$ will perhaps be more manageable than the direct expansion described earlier.

Comparing equations (2.11) and (3.7), it is obvious that the two series have the same structure. Therefore the same graphs are used in both expansions. However, many of the graphs that appeared in expanding the average of (2.11) will give a vanishing contribution when expanding the average of (3.7): such will be the case with all graphs that have a vertex with only two lines attached to it, since such a vertex corresponds to an isolated single bond factor $\left\langle\delta \kappa_{a}\right\rangle=0$. Furthermore, no $\Gamma_{00}$ loops appear in the rearranged expansion, since $\hat{\Gamma}_{00}=0$.

In order to determine the contribution of an order- $n$ graph, we assign the factor $\hat{\Gamma}_{a b}$ to a line that connects the vertices $a$ and $b$, and sum over the positions and orientations of all the vertices except for the entry bond and the exit bond (the one or two vertices with a dangling line). The entry bond is held fixed, and though the position of the exit bond is summed over (unless it happens to coincide with the entry bond), its orientation is kept identical with that of the entry bond-we have taken it to lie along the $z$ axis.

Besides the $\hat{\Gamma}$-product discussed above, the contribution of every order- $n$ graph includes a product of single-bond averages $\left\langle\delta \kappa_{a}^{m}\right\rangle$, which arises from the decomposition of the order- $n$ correlation function $\left\langle\delta \kappa_{0} \delta \kappa_{1} \ldots \delta \kappa_{n-1}\right\rangle$ into a sum of non-repeating covering paths. When the graph is traversed, starting from one dangling line that is labelled by 0 and ending at the other one that is labelled by $n-1$, each vertex (bond) is followed by a different vertex, but each vertex is visited at least twice. The different covering paths belonging to the same graph all give the same kind of decomposition for the order- $n$ correlation function, and the same sum of $\hat{\Gamma}$-products. The total contribution of a given order- $n$ graph is thus the product of these two terms times the combinatorical factor, which is the total number of covering paths. Because of restrictions on the allowed covering paths, we find far fewer terms in this decomposition than we did in (3.2) or in Appendix 2.

The graphs are characterised by the number of vertices (or different bonds) $v$, and by one plus the number of internal (i.e., non-dangling) lines (or $\hat{\Gamma}$-factors) $n$. The number $n$ is also equal to the total number of factors appearing in the correlation function, and is therefore equal to the order of the graph. In order to ensure that all graphs and covering paths with given $n$ and $v$ were counted, we made an independent calculation of the total number $L_{v}(n)$ of covering paths of all $n, v$ graphs for $v=2,3,4$. These numbers were found to be

$$
\begin{array}{ll}
L_{2}(n)=1 & \text { for } n \geqslant 4, \text { zero otherwise } \\
L_{3}(n)=2^{n-1}-2 n+1 & \text { for } n \geqslant 6, \text { zero otherwise } \\
L_{4}(n)=\frac{1}{2}\left(3^{n-2}+15\right)-2^{n-1}-3(n-2) 2^{n-4}+2 n(n-3) & \text { for } n \geqslant 8, \text { zero otherwise } \tag{3.13}
\end{array}
$$

In this way, all the graphs and their combinatorical factors were found up to order $n=9$ (Kantor 1979). However, the sums of $\hat{\Gamma}$-products were only calculated completely up to order $n=7$. The reason for this is that the limiting factor in the calculations turns out to be the amount of computer time needed to calculate these long-range multiple sums. We were thus able to calculate double sums, which sufficed for graphs up to order $n=7$, but we were unable to complete the calculation of all the graphs of order $n=8$ and $n=9$, where triple sums also appear. The results for graphs of order $n=8$ and $n=9$ appear in Kantor's thesis (1979) and are available upon request.

The single-bond averages $\left\langle\delta \kappa^{m}\right\rangle$ which appear in table 2 are readily evaluated from (3.6), e.g.,
$\left\langle\delta \kappa_{0}^{2}\right\rangle=u^{2} p\left(\frac{1-\theta_{0}}{1-u \theta_{0}-\frac{1}{3} u\left(1-\theta_{0}\right)}\right)^{2}+u^{2}(1-p)\left(\frac{-\theta_{0}}{1-u \theta_{0}+\frac{1}{3} u \theta_{0}}\right)^{2}$.
Into this result we naturally have to substitute $\theta_{0}=\theta_{0}(u)$ from (3.12). Clearly, the resulting expansion for $\langle f(u)\rangle$ is not a power series in $u$. However, if the order- $n$ term in the expansion is itself expanded in powers of $u$, the leading term is $u^{n}$. In this way, a power series in $u$ can systematically be constructed for $\langle f(u)\rangle$. The results represented in table 2 allowed us to expand (3.7) up to order $\delta \kappa^{7}$, and thus to get the expansion of $\langle f(u)\rangle$ as a power series up to $u^{7}$. The technical aspects of the rearrangement of (3.7) in order to get the power series in $u$ are summarised in Appendix 3. The coefficients of the expansion are given there in the form of polynomials in $p$, so that the numerical values can be calculated for any $p$. For comparison, the corresponding expansion of $u \theta_{0}(u)$ (which is the EMT approximation for $\langle f(u)\rangle$ ) is also given. In $\S 4$, the power series which we obtained for $\langle f(u)\rangle$ in this way will be used to discuss the singularities of this function.

## 4. Analytic properties and asymptotic analysis of $\langle f(u)\rangle$

The three lowest orders in the exact expansion (see (A3.6)) coincide with those of the EMT approximation for $\langle f(u)\rangle$, namely, $u \theta_{0}(u)$. But even at higher orders, the differences between the coefficients of the two series are very small as can be seen from the example in table 3. This explains the good agreement between EMT and the results of numerical simulations even for values of $u$ as high as 0.9 (Kirkpatrick 1971), which could be expected to be outside the region of validity of EMT (i.e., $|u| \ll 1$ ).

Table 2. List of all contributing graphs and non-repeating covering paths and their contributions to the term of order $\delta \kappa^{n}$ in the expansion of (4.14).

| Order in <br> $\delta K n$ Contributing <br> graphs Correlation <br> functionCombinatorical <br> factor | Non-repeating <br> covering paths | Sum of $\hat{\Gamma}$ products |
| :--- | :--- | :--- | :--- | :--- | :--- |

[^1]In this way one obtains the second form for this sum.

Table 3. An example of the expansion coefficients of $\langle f(u)\rangle$ and $u \theta_{0}(u)$ for $p=0.60$.

| Order of $u$ | 0 | 1 | 2 | 3 | 4 | 5 | 6 | 7 |
| :--- | :--- | :--- | :--- | :--- | :--- | :--- | :--- | :--- |
| $u \theta_{0}(u)$ | 0 | 0.6 | 0.08 | 0.04267 | 0.02702 | 0.01896 | 0.01421 | 0.01114 |
| $\langle f(u)\rangle$ | 0 | 0.6 | 0.08 | 0.04267 | 0.02686 | 0.01868 | 0.01386 | 0.01076 |

The function $\theta_{0}(u)$ has a branch cut on a segment of the real axis $\left[u_{\mathrm{c} 1}, u_{\mathrm{c} 2}\right]$ given by:

$$
\begin{equation*}
u_{\mathrm{c} 1,2}=\frac{3(1+p) \mp 6[2 p(1-p)]^{1 / 2}}{(1-3 p)^{2}} \tag{4.1}
\end{equation*}
$$

The lower edge of this cut $u_{\mathrm{c} 1}$ is usually greater than 1 , being equal to 1 only at the EMT percolation threshold for the $g_{2}$ conductors $p_{\mathrm{c}}=\frac{2}{3}$ (note that the concentration of the $g_{2}$ conductors is $1-p$ ). We expect that the exact solution will have a qualitatively similar behaviour. That is, we expect $\langle f(u)\rangle$ to have a branch cut on the real axis with the lower edge $u_{\mathrm{cl}} \geqslant 1$, equality being achieved only at the true percolation threshold of the simple cubic, independent random bond lattice (Bergman and Imry 1977). The function $\langle f(u)\rangle$ should have no singularities outside the real $u$ axis, and the branch point $u_{\mathrm{c} 1}$ will be the closest singularity to the origin. We can therefore try to determine the location of $u_{\mathrm{c} 1}$ as well as the singular behaviour of $\langle f(u)\rangle$ there by an asymptotic analysis of the power series. We analysed our power series for $\langle f(u)\rangle$ using the method of Neville tables (see, for instance, Gaunt and Guttman 1974; in what follows, we will use their notation). We are looking for the convergence radius $u_{\mathrm{c} 1}$ of our series expansion

$$
\langle f(u)\rangle=\sum_{n} a_{n}(p) u^{n}
$$

which is given by $1 / u_{\mathrm{c} 1}=\lim _{n \rightarrow \infty} e_{n}^{0}$, where $e_{n}^{0} \equiv a_{n} / a_{n-1}$. The Neville tables relate to each sequence $\left\{e_{n}^{0}\right\}$ a set of sequences $\left\{e_{n}^{r}\right\}$ that are expected to converge more quickly to the same limit with increasing order $r=1,2,3$. The highest- $n$ term in each sequence, namely $e_{7}^{r}(r=1,2,3)$, was taken as an approximation to $1 / u_{c 1}$, with the expectation that, as $r$ increases, the approximation becomes more exact. These approximations are depicted as a function of $p$ in figure 2 . The curves for $r=1,2,3$ reach their maximum value at the concentrations $0.617,0.687$ and 0.755 , respectively. The last result is in good agreement with the best known value of the percolation threshold of the independent, random bond, simple cubic lattice, namely 0.7535 (Fisch and Harris 1977).

The successive approximations are not well converged, but comparing them with the lower branch point of $\theta_{0}(u)$ for different values of $p$, we can conclude that the true


Figure 2. Three successive approximations $e_{7}^{\frac{1}{7}}$ (dotted curve), $e_{7}^{2}$ (chain curve), $e_{7}^{3}$ (full curve) and the EMT approximation (broken curve) for $1 / u_{\mathrm{c} 1}$.
$u_{c 1}(p)$ stays closer to the value 1 . This result could have been expected because in the EMT approximation, $u_{\mathrm{c} 1}(p)$ has the following form near the percolation threshold:

$$
\begin{equation*}
u_{\mathrm{cl}}(p)-1 \simeq \frac{9}{8}\left(p-\frac{2}{3}\right)^{2} \tag{4.2}
\end{equation*}
$$

On the other hand, scaling arguments (Straley 1979) predict that the exponent of $u_{\mathrm{cl}}(p)$ near threshold should be $2.4 \pm 0.2$.

The method of Neville tables can also be used to estimate the exponent which characterises the singularity of $\langle f(u)\rangle$ at $u=u_{\mathrm{c} 1}$, but our expansion up to order $u^{7}$ turns out to be too short to determine this exponent with any reasonable accuracy. We have also applied the method of Pade approximants to the logarithmic derivative of $\langle f(u)\rangle$. This gave worse results than the previous method, probably due to the fact that the expected singularity in $\langle f(u)\rangle$ is a weak one (i.e., the function does not diverge at $\left.u_{\mathrm{c} 1}\right)$.

To summarise this section, we have been able to investigate the position of the branch cut singularity in $\langle f(u)\rangle$, although we have not been able to obtain quantitative information about the critical exponents. To do that we would need to calculate more terms in the series for $\langle f(u)\rangle$.

## Appendix 1

In this Appendix we discuss the mathematical properties of the matrices $\gamma_{i}^{l}$ and $\Gamma_{a b}$, and develop convenient series for the numerical evaluation of $\Gamma_{a b}$.

The discrete analogue of Green's theorem for the homogeneous network is

$$
\begin{equation*}
\sum_{i, j}\left[U_{i} \varepsilon_{i j}\left(V_{i}-V_{j}\right)-V_{i} \varepsilon_{i j}\left(U_{i}-U_{j}\right)\right]=\sum_{i, j}\left(V_{i} \varepsilon_{i j} U_{j}-U_{i} \varepsilon_{i j} V_{j}\right) \tag{A1.1}
\end{equation*}
$$

where on the Lhs, $j$ ranges over all sites while $i$ ranges only over all the internal sites (i.e., excluding surface sites). On the RHs, $j$ ranges only over the surface sites, while $i$ ranges over those internal sites which are nearest neighbours to surface sites. Obviously, the RHS is obtained by noting that the terms on the LHS for which both $i$ and $j$ are internal sites will cancel out when the sums are performed. If we substitute $U_{i}=\gamma_{i}^{l}$ and $V_{i}=\gamma_{i}^{m}$ in (A1.1), and remember that these quantities vanish at the surface, we find

$$
\begin{equation*}
\gamma_{m}^{l}-\gamma_{l}^{m}=0 \tag{A1.2}
\end{equation*}
$$

which is the discrete version of the reciprocity theorem.
In the case of an infinite network, it is easy to derive an expression for the Fourier transform of $\gamma_{l}^{m}$,

$$
\begin{equation*}
\gamma(k) \equiv \sum_{l} \gamma_{l}^{m} \exp [\mathrm{i} k .(\boldsymbol{m}-l)] \tag{A1.3}
\end{equation*}
$$

with the help of the Fourier transform of $\varepsilon_{i j}$,

$$
\begin{equation*}
\varepsilon(k)=\sum_{m} \varepsilon_{l m} \exp [\mathrm{i} k .(m-l)]=2 \sum_{\alpha=1}^{3} \cos k_{\alpha} \tag{A1.4}
\end{equation*}
$$

Taking the Fourier transform of equation (2.5) we get

$$
\begin{equation*}
\gamma(k)=\frac{1}{\varepsilon(0)-\varepsilon(k)}=\left(4 \sum_{\alpha=1}^{3} \sin ^{2} \frac{1}{2} k_{\alpha}\right)^{-1} \tag{A1.5}
\end{equation*}
$$

so that

$$
\begin{equation*}
\gamma_{i}^{m}=\int \frac{\mathrm{d}^{3} k}{(2 \pi)^{3}} \frac{\exp [-\mathrm{i} k \cdot(m-l)]}{4 \Sigma_{\alpha=1}^{3} \sin ^{2} \frac{1}{2} k_{\alpha}} \quad-\pi<k_{\alpha}<\pi \tag{A1.6}
\end{equation*}
$$

These quantities are special cases of the so-called lattice Green function for a simple cubic lattice. A summary of the properties of this function, as well as a list of references where selected values are tabulated, can be found in an article by Katsura et al (1971). Detailed double series for calculating these functions with arbitrary accuracy have been developed by Abe and Katsura (1973).

From (A1.6) and (2.8) we can derive a Fourier integral expression for our $\Gamma_{a b}$
$\Gamma_{a b} \equiv \Gamma_{\boldsymbol{R} \alpha, \boldsymbol{R}^{\prime} \beta}=\int \frac{\mathrm{d}^{3} k}{(2 \pi)^{3}} \frac{\sin \frac{1}{2} k_{\alpha} \sin \frac{1}{2} k_{\beta} \cos \left(k \cdot\left(\boldsymbol{R}-\boldsymbol{R}^{\prime}\right)\right)}{\Sigma_{\gamma=1}^{3} \sin ^{2} \frac{1}{2} k_{\gamma}} \quad-\pi<k_{\gamma}<\pi$,
where the symbol $\boldsymbol{R} \alpha$ denotes a bond pointing in the positive direction $\boldsymbol{e}_{\alpha}$, whose centre is at $\boldsymbol{R}$. From this expression, it is immediately clear that $\Gamma_{a b}$ is an idempotent matrix, i.e.,

$$
\begin{equation*}
\sum_{b} \Gamma_{a b} \Gamma_{b c}=\Gamma_{a c}, \tag{A1.8}
\end{equation*}
$$

and also that its diagonal elements are

$$
\begin{equation*}
\Gamma_{a a}=\frac{1}{3} . \tag{A1.9}
\end{equation*}
$$

In the limit of large separation, the lattice Green function $\gamma_{l}^{m}$ reduces to the ordinary Coulomb potential

$$
\begin{equation*}
\gamma_{l}^{m} \rightarrow \frac{1}{4 \pi|l-\boldsymbol{m}|}, \quad \text { for large }|\boldsymbol{l}-\boldsymbol{m}| \tag{A1.10}
\end{equation*}
$$

Similarly, the $\Gamma$-matrix reduces in that limit to the interaction between two dipoles

$$
\begin{equation*}
\Gamma_{\boldsymbol{R} \alpha, \boldsymbol{R}^{\prime} \beta} \rightarrow \frac{\partial}{\partial R_{\alpha}} \frac{\partial}{\partial R_{\beta}^{\prime}} \frac{1}{4 \pi\left|\boldsymbol{R}-\boldsymbol{R}^{\prime}\right|}, \quad \text { for large }\left|\boldsymbol{R}-\boldsymbol{R}^{\prime}\right| \tag{A1.11}
\end{equation*}
$$

By considering the behaviour of (A1.7) under the various transformations of the cubic point symmetry group at $\boldsymbol{R}^{\prime}$, we can easily show that when $\Gamma_{\boldsymbol{R} \alpha, \boldsymbol{R}^{\prime} \beta}$ is summed over the star of $\boldsymbol{R}-\boldsymbol{R}^{\prime}$ the result is zero unless $\boldsymbol{R} \alpha=\boldsymbol{R}^{\prime} \beta$. From this it follows that if we sum $\Gamma_{a b} Z_{b}$ over all the bonds $b \neq a$ in a cube surrounding $a$, the result will be zero. A different result is obtained if we sum $\Gamma_{R \alpha, R^{\prime} \beta}$ over all the sites $\boldsymbol{R}^{\prime}$ of the network (including $R^{\prime}=R$ ). This is due to the fact that the matrix elements $\Gamma_{R \alpha, R^{\prime} \beta}$ decrease with separation only as $\left|\boldsymbol{R}-\boldsymbol{R}^{\prime}\right|^{-3}$, so that the infinite sum is only semiconvergent. Thus, the value of such a sum depends on the shape of the network. Since the network as a whole does not have the shape of a cube, the previous method of summation is inappropriate. In order to obtain the sum in this case, we consider a uniform network where $\theta_{a}=1$ for all bonds $a$. The voltage distribution is then simply $V_{a}=Z_{a}$, and (2.6) becomes

$$
\begin{equation*}
Z_{a}=Z_{a}+u \sum_{b} \Gamma_{a b} Z_{b} \tag{A1.12}
\end{equation*}
$$

We conclude that

$$
\begin{equation*}
\sum_{b} \Gamma_{a b} Z_{b}=0 \tag{A1.13}
\end{equation*}
$$

for any orientation of the bond $a$.

We will now develop series for the numerical evaluation of the matrix elements $\Gamma_{a b}$. Several years ago, Abe and Katsura (1973) developed and published a number of series expansions for the lattice Green function of simple cubic and tetragonal lattices, in their notation

$$
\begin{equation*}
I(a ; l, m, n ; \gamma) \equiv \int_{0}^{\pi} \frac{\mathrm{d}^{3} r}{\pi^{3}} \frac{\cos l x \cos m y \cos n z}{a-\mathrm{i} \varepsilon-\gamma \cos x-\cos y-\cos z} \tag{A1.14}
\end{equation*}
$$

Obviously, our quantities $\gamma_{i}^{j}$ of (A1.6) are related to these integrals by

$$
\begin{align*}
& \gamma_{i}^{j}=\frac{1}{2} I(3 ; l, m, n ; 1)  \tag{A1.15}\\
& \boldsymbol{j}-\boldsymbol{i}=l \boldsymbol{e}_{x}+m \boldsymbol{e}_{y}+n \boldsymbol{e}_{z} .
\end{align*}
$$

Unfortunately, the point $a=3, \gamma=1$ is a singular point of $I$, and consequently the series expansion, which is a double series, converges rather slowly. Since we are really interested in $\Gamma_{a b}$ rather than in $\gamma_{i}^{j}$, we used the series for $I(3 ; l, m, n ; 1)$ (equation (3.3) from Abe and Katsura (1973)) to derive a series for $\Gamma$ with the help of (2.8) and (A1.15). In order to exhibit this series and discuss its properties, we need a more convenient notation. Representing the site vectors of $\Gamma_{i j, h k}$ by

$$
\begin{align*}
& \boldsymbol{i}=\boldsymbol{R}_{1} \quad j=\boldsymbol{R}_{1}+\boldsymbol{e}_{1} \quad \boldsymbol{h}=\boldsymbol{R}_{2} \quad \boldsymbol{k}=\boldsymbol{R}_{2}+\boldsymbol{e}_{2}  \tag{A1.16}\\
& \boldsymbol{R}_{12}=\boldsymbol{R}_{1}-\boldsymbol{R}_{2}=l \boldsymbol{e}_{x}+m \boldsymbol{e}_{y}+n e_{z},
\end{align*}
$$

where each vector $e_{1}, e_{2}$ is a unit vector parallel to one of the coordinate axes, we introduce the following notation

$$
\begin{equation*}
\gamma_{i}^{h}=\frac{1}{2} I(3 ; l, m, n ; 1) \equiv \gamma(l m n) \quad \Gamma_{i j, h k} \equiv \Gamma\left(l m n \xi_{1} \xi_{2}\right) \tag{A1.17}
\end{equation*}
$$

where $\xi_{i}=1,2,3$ according to whether $\boldsymbol{e}_{i}=\boldsymbol{e}_{x}, \boldsymbol{e}_{y}, \boldsymbol{e}_{z}$.
The values of $\xi_{1}$ and $\xi_{2}$ thus determine the directions of the two bonds, ( $i j$ ) and ( $h k$ ), each of which is taken to point in the positive direction along one of the coordinate axes. The integers $l, m, n$ determine the vector $\boldsymbol{R}_{12}$ which points from the origin of $(h k)$ to the origin of $(i j)$.

In practice, we only need to calculate two types of matrix elements
$\Gamma(l m n 11)=2 \gamma(l m n)-\gamma(l-1 m n)-\gamma(l+1 m n)$
$\Gamma(l m n 21)=\gamma(l m n)-\gamma(l-1 m n)-\gamma(l m+1 n)+\gamma(l-1 m+1 n)$,
and these need only be calculated for $l, m, n \geqslant 0$, because all other matrix elements can be found from the following equations:

$$
\begin{align*}
& \Gamma(l m n 33)=\Gamma(m n l 22)=\Gamma(n l m 11) \\
& \Gamma(l m n 31)=\Gamma(l n m 21)=\Gamma(m \ln 32) \\
& \Gamma(l m n 21)=\Gamma(-l-m-n 12) \\
& \Gamma(l m n 11)=\Gamma(l n m 11)=\Gamma(|l||m||n| 11) \\
& \Gamma(l m n 21)=\Gamma(l m|n| 21) \\
& \Gamma(-l m n 21)=-\Gamma(l+1 m n 21) \\
& \Gamma(l-m n 21)=-\Gamma(l m-1 n 21) \tag{A1.19}
\end{align*}
$$

These equations are, in turn, easily obtained from (A1.18) and from

$$
\begin{equation*}
\gamma(l m n)=\gamma(|l||m||n|) . \tag{A1.20}
\end{equation*}
$$

In this way the following series were obtained

$$
\begin{align*}
& \Gamma(l m n 11)=\sum_{k=0}^{\infty} \sum_{r=-\infty}^{2 k} V(k r) \\
& \times \frac{5 k+2(l+1)(p-2 r)-6 l(l+1)-\frac{1}{6}(p-2 r)(p-2 r+1)}{(p+6 k-2 r)(l+k+1)}  \tag{A1.21}\\
& \Gamma(l m n 21)=\sum_{k=0}^{\infty} \sum_{r=-\infty}^{2 k} V(k r) \\
& \times\left(\frac{p-2 r-6 l}{p+6 k-2 r}-\frac{(m+n+4 k-2 r+1)(p-2 r-6 l+1)}{6(m+2 k-r+1)(m+n+2 k-r+1)}\right), \tag{A1.22}
\end{align*}
$$

where

$$
\begin{align*}
& V(k r)=\frac{1 y^{p}+1+6 k-2 r}{(m+n+4 k-2 r)!(p+6 k-2 r)!} \\
& \times \frac{(l+k)!(2 k-r)!(m+2 k-r)!(n+2 k-r)!(m+n+2 k-r)!}{k=l+m+n, \quad m, n \geqslant 0, \quad l \geqslant 1 ;} \tag{A1.23}
\end{align*}
$$

and
$\Gamma(0 m n 11)=\sum_{k=0}^{\infty} \sum_{r=-\infty}^{2 k} V(k r) \frac{2 r-m-n+5}{3(k+1)}$
$\Gamma(0 m n 21)=\sum_{k=0}^{\infty} \sum_{r=-\infty}^{2 k} \frac{V(k r)}{6(k+1)}$
$\times\left(2 r-m-n+5+\frac{(m+n-2 r-4)(m+n+6 k-2 r+1)(m+n+4 k-2 r+1)}{6(m+2 k-r+1)(m+n+2 k-r+1)}\right)$
where

$$
\begin{equation*}
m, n \geqslant 0 \tag{A1.25}
\end{equation*}
$$

and where $V(k r)$ is again given by (A1.23) but with $l=0$ and $p=m+n$.
In order to get an idea of the convergence properties of these double series, consider for example equation (A1.22). Using Stirling's approximation, we find that the general term of that series has the following forms of asymptotic behaviour

$$
\begin{array}{ll}
\left(\frac{1}{3}\right)^{2 k} \sqrt{ } k & \text { for } r=2 k \gtrdot p \\
\left(\frac{2}{3}\right)^{\mid 2 r}(1 /|2 r|) & \text { for }|r| \gg 3 k \gg p  \tag{A1.27}\\
-\frac{\sqrt{ } 6}{288 \pi^{2} k^{3}}\left(1-\frac{r^{2}}{3 k}+\mathrm{O}(r \mid k)\right) & \text { for } k \gtrdot r^{2} .
\end{array}
$$

We see that the slowest asymptotic decrease occurs in a region along the $k$-axis whose width in terms of $r$ is

$$
\begin{equation*}
\Delta r \approx \sqrt{ }(3 k) . \tag{A1.28}
\end{equation*}
$$

Thus, if all the terms in such a region are summed up to $k_{\text {max }}$, the number of terms will be $\sim 2 \sqrt{ } 3 k_{\text {max }}^{3 / 2}$. When (A1.22) is summed only over $r$ for large $k$, the result will be of order $2 \sqrt{ }(3 k) /\left(10^{3} k^{3}\right) \simeq 3.5 \times 10^{-3} k^{-5 / 2}$ (the $10^{-3}$ factor comes from the small coefficient in the last line of (A1.27)). Therefore the last term in the subsequent sum on $k$ will be $\sim 3.5 \times 10^{-3} k_{\max }^{-5 / 2}$, while the absolute error will be $\sim 3.5 \times 10^{-3} k_{\max }^{-3 / 2}$. Thus, if we take $k_{\text {max }}=100$, we have altogether to sum over about 3500 terms for every matrix element $\Gamma_{a b}$, and we can expect to obtain it with an absolute accuracy of $3 \times 10^{-6}$.

Before closing this Appendix, we mention some exact properties of the $\Gamma$-matrices that are useful in providing us with an independent means of checking the accuracy of the numerical calculations. One is the fact that the diagonal element $\Gamma_{a a}=\frac{1}{3}$ (equation (A1.9)), from which we deduce

$$
\begin{equation*}
\Gamma(00011)=\frac{1}{3} . \tag{A1.29}
\end{equation*}
$$

The second is the idempotency of $\Gamma$ (equation (A1.8)), from which it follows, in particular, that

$$
\begin{equation*}
\sum_{1} \Gamma_{01}^{2}=\Gamma_{00}=\frac{1}{3} . \tag{A1.30}
\end{equation*}
$$

The last property is the fact that

$$
\begin{equation*}
\Gamma(l l l 11)=0, \quad \text { for } l \neq 0 \tag{A1.31}
\end{equation*}
$$

This follows from the equation (see (A1.7))

$$
\begin{align*}
\Gamma(l l l 11)=\int_{-\pi}^{\pi} & \frac{\mathrm{d} x \mathrm{~d} y \mathrm{~d} z}{(2 \pi)^{3}} \frac{\sin ^{2} \frac{1}{2} z \cos l(x+y+z)}{\sin ^{2} \frac{1}{2} x+\sin ^{2} \frac{1}{2} y+\sin ^{2} \frac{1}{2} z} \\
& =\frac{1}{3} \int_{-\pi}^{\pi} \frac{\mathrm{d} x \mathrm{~d} y \mathrm{~d} z}{(2 \pi)^{3}} \cos l(x+y+z)=\frac{1}{3} \delta_{10} . \tag{A1.32}
\end{align*}
$$

## Appendix 2

In this Appendix we give the decomposition of the $n=5$ and $n=6$ correlation functions of $\theta_{a}$, which are needed in any attempt to extend the expansion of (3.3) and (3.5) up to terms of order $u^{5}$ and $u^{6}$, respectively.

$$
\begin{align*}
\left\langle\theta_{0} \theta_{1} \ldots \theta_{4}\right\rangle= & p^{5}+p^{4}(1-p)\left(10 \text { pairs } \delta_{01}, \text { etc }\right) \\
& +p^{3}(1-p)(1-2 p)\left(10 \text { triplets } \delta_{012}, \text { etc }\right) \\
& +p^{3}(1-p)^{2}\left(15 \text { products } \delta_{01} \delta_{23}, \text { etc }\right) \\
& +p^{2}(1-p)\left(1-6 p+6 p^{2}\right)\left(5 \text { quartets } \delta_{0123}, \text { etc }\right) \\
& +p^{2}(1-p)^{2}(1-2 p)\left(10 \text { products } \delta_{01} \delta_{234}, \text { etc }\right) \\
& +p(1-p)(1-2 p)\left(1-12 p+12 p^{2}\right) \delta_{01234} \tag{A2.1}
\end{align*}
$$

$$
\begin{align*}
\left\langle\theta_{0} \theta_{1} \ldots \theta_{5}\right\rangle= & p^{6}+p^{5}(1-p)(15 \text { pairs })+p^{4}(1-p)(1-2 p)(20 \text { triplets }) \\
& +p^{4}(1-p)^{2}\left(45 \text { products } \delta_{01} \delta_{23}, \text { etc }\right) \\
& +p^{3}(1-p)\left(1-6 p+6 p^{2}\right)(15 \text { quartets }) \\
& +p^{3}(1-p)^{2}(1-2 p)\left(60 \text { products } \delta_{01} \delta_{234}, \text { etc }\right) \\
& +p^{3}(1-p)^{3}\left(15 \text { products } \delta_{01} \delta_{23} \delta_{45}, \text { etc }\right) \\
& +p^{2}(1-p)^{2}(1-2 p)^{2}\left(10 \text { products } \delta_{012} \delta_{345}, \text { etc }\right) \\
& +p^{2}(1-p)^{2}\left(1-6 p+6 p^{2}\right)\left(15 \text { products } \delta_{0123} \delta_{45}, \text { etc }\right) \\
& +p^{2}(1-p)(1-2 p)\left(1-12 p+12 p^{2}\right)(6 \text { quintets }) \\
& +p(1-p)\left[1-30 p(1-p)(1-2 p)^{2}\right] \delta_{012345 .} \tag{A2.2}
\end{align*}
$$

## Appendix 3

In this Appendix we give some analytical expressions for the functions used to expand $\langle f(u)\rangle$ in a power series up to order $u^{7}$.

$$
\begin{align*}
u \theta_{0}(u)=u p+ & (1 / 3) p(1-p) u^{2}+\left(1 / 3^{2}\right) p(1-p)(1+p) u^{3} \\
& +\left(1 / 3^{3}\right) p(1-p)\left(1+4 p-p^{2}\right) u^{4} \\
& +\left(1 / 3^{4}\right) p(1-p)(1+p)\left(1+8 p-5 p^{2}\right) u^{5} \\
& +\left(1 / 3^{5}\right) p(1-p)\left(1+16 p+26 p^{2}-24 p^{3}-3 p^{4}\right) u^{6} \\
& +\left(1 / 3^{6}\right) p(1-p)(1+p)\left(1+24 p+66 p^{2}-96 p^{3}+21 p^{4}\right) u^{7} \\
& +\mathrm{O}\left(u^{8}\right)  \tag{A3.1}\\
& \begin{aligned}
&\left\langle\delta \kappa^{2}\right\rangle=u^{2}(1-p) p\left[1+\frac{2}{3}(1+p) u+\frac{1}{9}\left(3+10 p-p^{2}\right) u^{2}\right. \\
&\left.+\frac{4}{27}\left(1+7 p+3 p^{2}-3 p^{3}-3 p^{4}\right) u^{3}+\mathrm{O}\left(u^{4}\right)\right] \\
&\left\langle\delta \kappa^{3}\right\rangle=u^{3}(1-p) p(1-2 p)\left[1+(1+p) u+\frac{1}{9}\left(5+14 p+p^{2}\right) u^{2}\right. \\
&+\left.\frac{10}{27}\left(1+6 p+3 p^{2}-2 p^{3}\right) u^{3}+\mathrm{O}\left(u^{4}\right)\right] \\
&\left\langle\delta \kappa^{4}\right\rangle=u^{4}(1-p) p\left(3 p^{2}-3 p+1\right)+\mathrm{O}\left(u^{5}\right) \\
&\langle f(u)\rangle-u \theta_{o}(u) \\
& \hline 1-u \theta_{0}(u)=A\left\langle\delta \kappa^{2}\right\rangle^{2}+B\left\langle\delta \kappa^{2}\right\rangle\left\langle\delta \kappa^{3}\right\rangle+C\left\langle\delta \kappa^{3}\right\rangle^{2}+D\left\langle\delta \kappa^{2}\right\rangle^{3} \\
&+E\left\langle\delta \kappa^{4}\right\rangle\left\langle\delta \kappa^{3}\right\rangle+F\left\langle\delta \kappa^{2}\right\rangle^{2}\left\langle\delta \kappa^{3}\right\rangle+\mathrm{O}\left(u^{8}\right) \\
& A=-0.2824 \times 10^{-2} \quad B=0.3254 \times 10^{-2} \\
& C=-0.5387 \times 10^{-4} \quad D=0.8478 \times 10^{-3} \\
& E=0.5748 \times 10^{-4} \quad F=0.6210 \times 10^{-3} .
\end{aligned}
\end{align*}
$$

By using equations (A3.1)-(A3.5) we can expand $\langle f(u)\rangle$ in a power series as follows:

$$
\begin{align*}
\langle f(u)\rangle=u p+ & (1 / 3) p(1-p) u^{2}+\left(1 / 3^{2}\right) p(1-p)(1+p) u^{3} \\
& +\left(1 / 3^{3}\right) p(1-p)\left[J_{2}(p)+p(1-p) H_{0}(p)\right] u^{4} \\
& +\left(1 / 3^{4}\right) p(1-p)\left[J_{3}(p)+p(1-p) H_{1}(p)\right] u^{5} \\
& +\left(1 / 3^{5}\right) p(1-p)\left[J_{4}(p)+p(1-p) H_{2}(p)\right] u^{6} \\
& +\left(1 / 3^{6}\right) p(1-p)\left[J_{5}(p)+p(1-p) H_{3}(p)\right] u^{7}+O\left(u^{8}\right) \tag{A3.6}
\end{align*}
$$

where $\left(1 / 3^{n-1}\right) p(1-p) J_{n-2}(p)$ is the coefficient of $u^{n}$ from equation (A3.1), while $H_{n}(p)$ are given by:

$$
\begin{align*}
& H_{0}(p) \equiv A^{\prime} \\
& H_{1}(p) \equiv K(p)+3 A^{\prime} p \\
& H_{2}(p) \equiv L(p)+3\left(K(p)+A^{\prime}\right) p+3 A^{\prime} p^{2} \\
& H_{3}(p) \equiv M(p)+3\left(L(p)+K(p)+A^{\prime}\right)+3 K(p) p^{2}+3 A^{\prime} p^{3} \\
& A^{\prime} \equiv 3^{3} A \\
& K(p) \equiv 3^{3}[(4 A+3 B)+(4 A-6 B) p] \\
& L(p) \equiv 3^{3}[(10 A+15 B+9 C)+(28 A-15 B-36 C+9 D) p \\
& \left.+(2 A-30 B+36 C-9 D) p^{2}\right] \\
& M(p) \equiv 3^{3}[(20 A+42 B+54 C+27 E)+3(36 A+8 B-52 C+18 D \\
& -45 E+9 F) p+3(20 A-66 B+81 E-27 F) p^{2} \\
& \left.+2(-14 A-18 B+108 C-27 D-81 E+27 F) p^{3}\right] \tag{A3.7}
\end{align*}
$$

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[^1]:    $\dagger$ Since this sum is actually independent of both the position and the orientation of the bond 0 , one can sum over 0, 2 instead of over 1,2, and then use (A1.8) to obtain

    $$
    \sum_{0} \hat{\Gamma}_{20} \hat{\Gamma}_{01}=\Gamma_{21}-2 \Gamma_{00} \Gamma_{21}=\frac{1}{3} \Gamma_{21} .
    $$

