

Displacement Correlations and Frequency Spectra for Mass-Disordered Lattices. II*

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The full cluster expansion for the phonon Green's function of a binary isotopic disordered alloy is derived for the case of a reference lattice of atomic mass intermediate between that of the two constituents. This result is extended to an alloy which is disordered except for specified atoms which occupy a small number of distinguished lattice sites. The latter Green's functions determine the displacement correlations of atoms in or near a small cluster of impurities in an alloy. The one- and two-vertex self-energies are calculated formally to all orders in the concentration, and it is shown that the disease of spurious poles, reported earlier, persists to the two-vertex self-energy and is a general feature of infinite partial summations when the cumulants of the full cluster expansion are used. The approximation of Elliott and Taylor, which does not have spurious poles, is discussed in this context and is used to evaluate the one-vertex self-energy for a reference lattice of intermediate atomic mass.

I. INTRODUCTION

IN this work we continue the discussion of the perturbation expansion of the vibrational frequency spectrum and related Green's functions of a mass-disordered alloy. In Sec. II, the restriction against multiple occupancy of each atomic site by atoms is handled in a much simpler way than previously,^{1,2} so that it can be seen that there is no difficulty in defining the expansion about a reference lattice of arbitrary atomic mass. The same vertex factors, or cumulants, are obtained as for the solvent-atom reference lattice.

An extension of these arguments in Sec. III leads to the formulation of the perturbation expansion of the Green's functions which are needed for calculating the frequency spectrum or displacement correlations in the neighborhood of defect atoms in an alloy. The fact that certain sites are distinguished as occupied by specific types of atoms modifies the multiple-occupancy vertex factors of the original expansion.

In Sec. IV the complete one- and two-vertex self-energy partial sums are evaluated. The disease of spurious poles, noted in I for the one-vertex self-energy, is seen to persist in the two-vertex self-energy and is a general feature of partial summations using the cumulants of the *full* perturbation expansion. The spurious poles are not present in the one-vertex self-energy ex-

pression obtained by Elliott and Taylor.³ Their procedure can be regarded as the first step using cumulants that correspond to a restricted part of the perturbation expansion. It is used in Sec. V to evaluate the one-vertex self-energy for a reference lattice of arbitrary mass.

II. PERTURBATION EXPANSION USING A REFERENCE LATTICE OF ARBITRARY ATOMIC MASS

We consider a lattice occupied by two chemically identical types of atoms, *A* and *B*, which differ only in their mass. When the concentration of neither species is small, it is useful to consider a perfect reference lattice of intermediate atomic mass M_r , as the unperturbed lattice. This perturbation expansion was first attempted by Takeno,⁴ who was unable to identify the general terms involved in the rather complicated expansion. It turns out that the complete expansion has almost the same form as in Langer's original theory⁵ which used $M_r = M_A$.

Our first approach to this problem used two kinds of interaction lines, one for the deviation of M_A from M_r , and the other for the deviation of M_B from M_r . An elaborate inductive argument resulted in the appearance of the same multiple-occupancy polynomial vertex factors $P_n(c)$ derived in Refs. 1 and 2, where c is the concentration of *B* atoms.

This stimulated a look for the common features in the expansions. Matsubara and Yonezawa² and Maradudin⁶ had pointed out that the $P_n(c)$ are cumu-

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¹ P. L. Leath and B. Goodman, *Phys. Rev.* **148**, 968 (1966), hereafter referred to as I.

² F. Yonezawa and T. Matsubara, *Progr. Theoret. Phys.* (Kyoto) **34**, 871 (1965); **35**, 357 (1966); **35**, 759 (1966).

³ R. J. Elliott and D. W. Taylor, *Proc. Roy. Soc. (London)* **296**, 161 (1967).

⁴ S. Takeno, *Progr. Theoret. Phys.* (Kyoto) **28**, 33 (1962).

⁵ J. S. Langer, *J. Math. Phys.* **2**, 584 (1961).

⁶ A. A. Maradudin, Extended Aarhus Summer School Lectures, 1963 (unpublished).

lants of the indicator function for the presence of, say, a B atom. This function takes on the value unity with probability c and zero with probability $1-c$. The two-valuedness obtains regardless of the reference lattice, so that similar statistical properties are to be expected. Furthermore, with an arbitrary M_r , the expansion will be formally symmetrical in *each order* with respect to the A and B atoms. If M_r is taken to be a symmetrical function of $\{M_B, c\}$ and $\{M_A, 1-c\}$ such that it becomes M_A or M_B for c equal to zero or 1, respectively, then an approximation which is applicable for small c should also be applicable for small $1-c$. This does not necessarily mean that the approximation will be accurate for intermediate concentrations.

Use of the position representation instead of the k representation allows the configuration average for a completely disordered system to be carried out in terms of the simplest cumulant properties and our resulting development is more compact than that given by Yonezawa and Matsubara.² The extension to ordered systems is direct in principle, but since the cumulants of any order involve correlation functions up to that order, any application will require truncating the hierarchy of correlation functions.⁷

The retarded displacement Green's function is defined by¹

$$D(n\alpha, m\beta, t-t') \equiv (i\hbar)^{-1} \langle [u(n\alpha, t), u(m\beta, t')] \rangle_T \times \theta(t-t'), \quad (1)$$

where $u(n\alpha, t)$ is the Cartesian displacement α of atom n at time t , $\theta(t) \equiv (1 \text{ for } t > 0, 0 \text{ for } t < 0)$, and the subscript T denotes a thermal average. It gives the displacement correlations $\langle uu \rangle$ discussed in I. For a harmonic system, its Fourier time transform $\mathbf{D}(\omega)$ satisfies the equation of motion

$$(\mathbf{M}\omega^2 - \mathbf{V})\mathbf{D}(\omega) = \mathbf{I}, \quad (2)$$

where \mathbf{V} is the force-constant matrix and \mathbf{M} is the diagonal mass matrix with elements $M(l\alpha, m\beta) = \delta_{l\alpha, m\beta} M(l)$. Equation (2) may be rearranged for a reference mass M_r to obtain

$$(\mathbf{M}_r\omega^2 - \mathbf{V})\mathbf{D}(\omega) = \mathbf{I} + \mathbf{u}\mathbf{D}(\omega). \quad (3)$$

The perturbation matrix \mathbf{u} is diagonal with the diagonal element

$$\mu(l) = \mu_A \Delta_A(l) + \mu_B \Delta_B(l) \quad (4)$$

at the site l , where $\Delta_A(l)$ is the indicator function which is 1 or zero depending upon whether there is an atom of type A at site l , and

$$\mu_A \equiv (M_r - M_A)\omega^2, \quad \mu_B \equiv (M_r - M_B)\omega^2. \quad (5)$$

Equation (3) may be rewritten as

$$\mathbf{D} = \mathbf{d} + \mathbf{d}\mathbf{u}\mathbf{D}, \quad (6)$$

⁷ A treatment of the vibrations of a dilute alloy with short-range order has been given by W. M. Hartmann, Phys. Rev.

where \mathbf{d} is the Green's function for the reference lattice

$$\mathbf{d}(\omega) = (\mathbf{M}_r\omega^2 - \mathbf{V})^{-1}. \quad (7)$$

Iterating and averaging over configurations of the two types of atoms on the lattice, we obtain

$$\langle \mathbf{D} \rangle = \mathbf{d} + \mathbf{d}\langle \mathbf{u} \rangle \mathbf{d} + \mathbf{d}\langle \mathbf{u}\mathbf{d}\mathbf{u} \rangle \mathbf{d} + \dots \quad (8)$$

The s th-order term in this expansion involves the configuration averages of the μ -products

$$\langle \mu(l_1)\mu(l_2)\dots\mu(l_s) \rangle. \quad (9)$$

This average may be factored into the product of averages in which each factor contains the μ 's for a cluster of sites in which the occupation of one site is dependent on the occupation of others in that cluster but is independent of the occupation of other clusters. The l sums in Eq. (8) can be carried out independently for each factor as long as the associated clusters remain separated. When clusters interact the product of their factors must be replaced by a new factor or, alternatively, a term must be added as a higher-order correlation correction to the product. The correlation corrections of increasing order are thus defined inductively as in the Ursell-Mayer expansion of the partition function of an imperfect gas.

The result of the above procedure is to represent Eq. (9) as the sum over all possible combinations of products of correlation functions,

$$\langle \mu(l_1)\mu(l_2)\dots\mu(l_s) \rangle = \sum_{\text{partitions}} \kappa[\mu(l_1)\dots]\kappa[\mu(l_i)]\dots\kappa[\mu(l_j)\dots], \quad (10)$$

where $\kappa\{\mu(l)\mu(l')\dots\mu[l^{(r-1)}]\}$ is an r th-order correlation function of the r μ 's which vanishes when any subset of its arguments is independent of the others. Once the form of the functions κ is known for every r , the sums over the l 's in (8) can be performed *without restrictions* between factors. Equation (10) is a particular case of the decomposition of the average of a product of random variables X_i into multivariate cumulants,⁸

$$\langle X_1 X_2 \dots X_s \rangle = \sum_{\text{partitions}} \kappa(X_1 \dots) \kappa(X_i \dots) \dots \kappa(X_j \dots). \quad (11)$$

Equation (11) defines the cumulants recursively. One can solve for them in terms of the product moments

172, 677 (1968). In this work the higher-order correlation functions are approximated by products of pair correlation functions.

⁸ The cumulants of a single random variable X are defined by

$$\langle \exp \alpha X \rangle \equiv \exp \left(\sum_{r=1}^{\infty} \frac{\alpha^r \kappa_r(X)}{r!} \right).$$

In our case, for $\langle X^n \rangle = \langle [\Delta_B(l)]^n \rangle = c$, the exponent is simply

$$g(\alpha; c) = \sum_{r=1}^{\infty} \alpha^r \frac{P_r(c)}{r!} = \ln(1 - c + ce^\alpha),$$

which was originally derived in Ref. 2.

$\langle X_{i_1} \cdots X_{i_r} \rangle$, for $i_1 < i_2 < \cdots < i_r \leq s$, as follows:

$$\begin{aligned} & \kappa(X_1, X_2, \cdots, X_s) \\ &= \sum_{m=1}^s (-1)^{m-1} (m-1)! \sum_{\substack{\text{partitions} \\ \text{into } m \text{ parts}}} \langle X_1 \cdots \rangle \\ & \quad \times \langle X_i \cdots \rangle \cdots \langle X_j \cdots \rangle. \end{aligned} \quad (12)$$

The properties of multivariate cumulants are reviewed by Meeron⁹ and Kubo.¹⁰ Equations (10)–(12) have been written as if all the random variables are distinct; if, say, $X_i = X_k$, they may still be treated as distinct random variables which are perfectly correlated. This avoids the more complicated formulas in Appendix A of Ref. 9 and Ref. 2 which result when Eq. (11) contains powers higher than the first of the random variables, i.e., when site indices coincide on the left side of Eq. (10). We now restrict ourselves to the case of a completely disordered alloy so that $\mu(l)$ and $\mu(l')$ are independent if $l \neq l'$. Since a cumulant product vanishes if any subset of its variables is independent of the others,⁹ we may write

$$\kappa[\mu(l)\mu(l') \cdots \mu(l^{(r-1)})] = \delta(l' \cdots l^{(r-1)}) \kappa_r[\mu(l)], \quad (13)$$

where $\delta(l' \cdots l^{(r-1)})$ is unity when all the l 's are the same and is zero otherwise.

In order to find the cumulants $\kappa_r[\mu(l)]$ of the random variable μ , we rewrite Eq. (4) in the form

$$\mu(l) = \mu_A + (\mu_B - \mu_A) \Delta_B(l), \quad (14)$$

so that it differs by the additive constant μ_A from the type of random perturbation considered by Langer.^{1,2,5} The first-order cumulant becomes

$$\kappa_1(\mu) = \langle \mu \rangle = \mu_A + (\mu_B - \mu_A)c = (M_r - \langle M \rangle)\omega^2, \quad (15)$$

where

$$\langle M \rangle = (1-c)M_A + cM_B, \quad (16a)$$

and

$$\mu_B - \mu_A = (M_A - M_B)\omega^2. \quad (16b)$$

The higher-order cumulants $\kappa_r(\mu)$, which depend on the fluctuations of the random variable μ about its average, are unchanged by the additive term in Eq. (14). Thus, for $r > 1$,

$$\kappa_r(\mu) = (\mu_A - \mu_B)^r P_r(c), \quad (17)$$

which by (16b) is independent of the choice of M_r , and where

$$P_r(c) = \kappa_r(\Delta_B) \quad (18)$$

is the cumulant of the indicator function and was given in closed form in I as a polynomial of degree r in c with the coefficients of c^m containing $S(r, m)$, the Stirling number of the second kind. A very simple derivation of the $P_r(c)$ follows immediately from Eq. (12) and the direct connection of the Stirling numbers with the

cumulants. Recall that $\kappa_r(\Delta_B)$ in Eq. (18) means $\kappa(\Delta_B, \Delta_B, \cdots, \Delta_B)$, with r "temporarily distinct" Δ_B 's, which by Eq. (12) is a sum over all partitions of the Δ_B 's into m averages $\langle \Delta_B \Delta_B \cdots \Delta_B \rangle \langle \Delta_B \cdots \rangle \cdots \langle \Delta_B \cdots \rangle$. Since

$$\langle (\Delta_B(l))^n \rangle = \langle \Delta_B(l) \rangle^n = c, \quad (19)$$

Equation (12) becomes

$$P_r(c) = \sum_{\substack{\text{partitions} \\ \text{into } m \text{ parts}}} (-1)^{m-1} (m-1)! c^m, \quad (20)$$

$$P_r(c) = \sum_{m=1}^r (-1)^{m-1} (m-1)! c^m S(r, m),$$

since $S(r, m)$ is the number of ways of partitioning a set of order r into m nonempty subsets.¹¹

The diagram representation in I of the expansion of $\langle \mathbf{D} \rangle$ now applies with the modifications that (a) vertices with single interaction lines carry the factor $(1-c)\mu_A + c\mu_B$; (b) in vertices with $m > 1$ interaction lines $\mu_B - \mu_A$ appears as the interaction strength of each line; and (c) the propagation lines are \mathbf{d} .

The resulting Dyson equation is

$$\langle \mathbf{D} \rangle = \mathbf{d} + \mathbf{d} \mathbf{\Sigma} \langle \mathbf{D} \rangle, \quad (21)$$

where $\mathbf{\Sigma}$ is the self-energy. The formal solution of this equation is

$$\langle \mathbf{D}(\omega) \rangle = \{ M_r \omega^2 [\mathbf{I} - \mathbf{\Pi}(\omega)] - \mathbf{V} \}^{-1}, \quad (22)$$

where

$$\mathbf{\Pi}(\omega) = (M_r \omega^2)^{-1} \mathbf{\Sigma}(\omega).$$

We note that, for fixed M_r , the vertex elements (15) and (17) are symmetric with respect to interchange of A and B labels. This follows from the identity

$$P_r(1-c) = (-1)^r P_r(c) \quad \text{for } r > 1, \quad (23)$$

which follows from Ref. 8, or more directly from the fact that, for $r > 1$,

$$\kappa_r(\Delta_B) = \kappa_r(1 - \Delta_A) = \kappa_r(-\Delta_A) = (-1)^r \kappa_r(\Delta_A), \quad (24)$$

where the second equality comes from the fact that the cumulants of greater than first order are unaffected by a constant shift in the random variable. Thus the expansion as defined in rules (a)–(c) above is symmetric with respect to A and B in each order.

If only single-interaction lines are kept, $\mathbf{\Sigma}$ is diagonal with the diagonal element $\langle \mu \rangle$ such that

$$\begin{aligned} \langle \mathbf{D}(\omega) \rangle &= \{ [M_r \omega^2 + (\langle M \rangle - M_r) \omega^2] \mathbf{I} - \mathbf{V} \}^{-1} \\ &= \mathbf{d}^{\langle M \rangle}(\omega), \end{aligned} \quad (25)$$

the Green's function for the mean lattice.

That the one-vertex diagrams are equivalent to using the reference lattice of mean atomic mass is

⁹ E. Meeron, J. Chem. Phys. 27, 1238 (1957).

¹⁰ R. Kubo, J. Phys. Soc. Japan 17, 1100 (1962).

¹¹ This closed form of the cumulant appears in calculations in binary alloys, in spin- $\frac{1}{2}$ systems, and whenever the stochastic variable is limited to two values.

further manifested by Eq. (15) where κ_1 vanishes for $M_r = \langle M \rangle$ and the perturbation expansion containing no one-vertex diagrams starts with $(\mu_B - \mu_A)^2$.

III. PERTURBATION EXPANSION INCLUDING DISTINGUISHED SITES

Measurements involving the interaction with radiation generally distinguish between atomic species in an alloy. Examples include defect-induced optical absorption, nuclear γ -ray emission and absorption, and neutron scattering. In the case of nuclear γ -ray emission the impurity is the emitting atom and the " $n=m$ = impurity" elements of the Green's functions are of main interest. It is also of interest to calculate the behavior of impurity modes in the vicinity of an impurity or a cluster of impurities.

The perturbation development of Sec. II can be adopted to the treatment of such *distinguished-site* Green's functions, that is, Green's functions for when the atomic species at some particular sites are known. The case will be considered in detail where the origin atom is distinguished, but generalization to more than one distinguished site will be evident. For simplicity, only the argument for the displacement Green's function and for the use of the host lattice as reference lattice is given.

Let $\langle \mathbf{D}^0(\omega) \rangle$ denote the displacement Green's function for the alloy with a distinguished atom at the origin. It is evaluated by the expansion (8) as before except that there are new values for the moments $\langle \mu(l_1) \cdots \mu(l_s) \rangle$. It is clear that $\langle \mathbf{D}^0 \rangle$ is not translationally invariant.

With $M_r = M_A$, Eq. (4) becomes

$$\mu(l) = \mu_B \Delta_B(l). \quad (26)$$

Again we assume no short-range order, so that sites l and $l' \neq l$ are occupied independently. The cumulants of $\Delta_B(l)$ still satisfy Eq. (13) but $\kappa_r[\Delta_B(l)]$ now depends upon the site l .

Let each site l be occupied by a B atom with probability c for $l \neq 0$ and probability c_0 for $l=0$, so that

$$\langle \Delta_B(l) \rangle = c + b \delta_{l0}, \quad (27)$$

where $b = c_0 - c$. From Eqs. (12), (20), and (26) it follows that

$$\kappa_r[\Delta_B(l)] = \sum_{m=1}^r (-1)^{m-1} (m-1)! \langle \Delta_B(l) \rangle^m S(r, m), \quad (28a)$$

$$\kappa_r[\Delta_B(l)] = P_r(c) + [P_r(b+c) - P_r(c)] \delta_{l0}. \quad (28b)$$

The first term on the left, $P_r(c)$, contributes at all sites and is taken into account by the same diagrams (of Sec. II) for the completely disordered alloy. The second term represents the extra scattering of the phonon by the origin atom.

The moments $\langle \mu(l_1) \cdots \mu(l_s) \rangle$ are still evaluated according to Eq. (10) and, as in Sec. II, each product on the right side of (10) corresponds to the vertex factors of some diagram. According to (28b) each vertex can be divided into two parts, the second of which carries the factor $\delta_{l0}[P_r(b+c) - P_r(c)]$ and gives an extra diagram. The new vertex can be represented by an open circle as in Fig. 1. Because of the δ_{l0} , all of the j open-circle vertices in a diagram can be collected together into a single vertex with the factor

$$\delta_{l0}[P_{n_1}(b+c) - P_{n_1}(c)][P_{n_2}(b+c) - P_{n_2}(c)] \cdots [P_{n_j}(b+c) - P_{n_j}(c)]. \quad (29)$$

Then all the resultant diagrams (coming from the various assignments of interaction lines to the original open-circle vertices) that now have the same topological structure can be collected together into a diagram with a single open-circle vertex of order r and value

$$P_r(b, c) \delta_{l0} = \delta_{l0} \sum_{\text{partitions}} [P_{n_1}(b+c) - P_{n_1}(c)] \times [P_{n_2}(b+c) - P_{n_2}(c)] \cdots [P_{n_j}(b+c) - P_{n_j}(c)]. \quad (30)$$

Examples of these extra diagrams are shown in Fig. 1(a) and are obtained from the diagrams of Sec. II by replacing each open-circle vertex by Eq. (30).

Since $P_r(b, c)$ measures the total *extra* scattering at the distinguished site it is proportional to the *extra* probability b that a B atom is there. This may be seen by comparing the μ moments with and without b . Doing the average of any $f(\mu)$ for the distinguished site last gives $c_0 f(\mu_B) + (1-c_0) f(\mu_A)$ versus $c f(\mu_B) + (1-c) f(\mu_A)$ and the difference is proportional to b . Since each factor $P_n(b+c) - P_n(c)$ in the summand of (30) is a polynomial in b beginning with the first power, it must be that all terms cancel out except for the linear term of

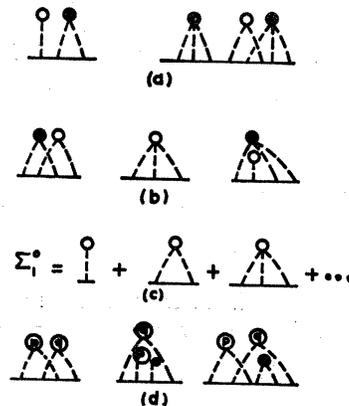


FIG. 1. (a) Some diagrams occurring in the expansion of $\langle \mathbf{D}^0 \rangle$ with scattering by the distinguished site; (b) some irreducible parts contributing to Σ_0 ; (c) the one-vertex distinguished site self-energy; and (d) some irreducible parts with scattering by two distinguished sites p and q contributing to $\Sigma^{2\mathcal{Q}}$.

the trivial partition into one, so that

$$P_r(b,c) = b - P_r(c) = \frac{b}{c(1-c)} P_{r+1}(c), \quad (31)$$

where the first equality follows from Eq. (20) and the second follows from the relation⁸

$$P_n(c) = (d/d\alpha)^n \ln(1-c+ce^\alpha) \Big|_{\alpha=0}. \quad (32)$$

The first few values of $P_r(b,c)$ are given in Table I.

Since a diagram contains at most one open-circle vertex with the factor (31), $\langle \mathbf{D}^0 \rangle$ is related to the Green's function $\langle \mathbf{D} \rangle$ of the disordered alloy without a distinguished site by the relation

$$\langle \mathbf{D}^0 \rangle = \langle \mathbf{D} \rangle + \langle \mathbf{D} \rangle \Sigma^0 \langle \mathbf{D} \rangle, \quad (33)$$

where Σ^0 is the sum of all irreducible parts, such as those in Fig. 1(b), which contain an open-circle vertex.

As a check, consider an isolated B atom in the pure A crystal so that $c=0$ and $b=1$. Then $P_r(b,c) = b=1$ and $\langle \mathbf{D} \rangle = \mathbf{d}_A$, the A lattice Green's function. The only contributions to Σ^0 are the one-vertex diagrams of Fig.

TABLE I. Distinguished site vertex factors $P_r(b,c)$ for $r \leq 6$.

| |
|---|
| $P_1(b,c) = b$ |
| $P_2(b,c) = b(1-c)$ |
| $P_3(b,c) = b(1-6c+6c^2)$ |
| $P_4(b,c) = b(1-14c+36c^2-24c^3)$ |
| $P_5(b,c) = b(1-30c+150c^2-240c^3+120c^4)$ |
| $P_6(b,c) = b(1-62c+540c^2-1560c^3+1800c^4-720c^5)$ |

1(c), so that

$$\Sigma^0 = \sum_{r=1}^{\infty} \mu_B^r d_0^{r-1} P_r(1,0) = \mu / (1 - \mu d_0^A), \quad (34)$$

where $d_0^A = d_A(0x, 0x)$. Then Eq. (33) reproduces the usual Green's function for a single impurity.

The extension to cases where there are more than one distinguished site is straightforward. For example, if sites p and $q \neq p$ have extra probabilities b_p and b_q , respectively, the extra diagrams will contain an open-circle vertex for either or both sites with the corresponding factors (31). The extension of Eq. (33) is more complicated;

$$\langle \mathbf{D}^{pq} \rangle = \langle \mathbf{D} \rangle + \langle \mathbf{D} \rangle (\Sigma^p + \Sigma^q + \Sigma^{pq}) \langle \mathbf{D} \rangle + \langle \mathbf{D} \rangle \Sigma^p \times \langle \mathbf{D} \rangle \Sigma^q \langle \mathbf{D} \rangle + \langle \mathbf{D} \rangle \Sigma^q \langle \mathbf{D} \rangle \Sigma^p \langle \mathbf{D} \rangle, \quad (35)$$

where Σ^{pq} is the sum of all irreducible parts containing both a p and q open-circle vertex such as shown in Fig. 1(d).

The special matrix elements $\langle D^p(p,m) \rangle$ and $\langle D^{pq}(p,q) \rangle$, for which one or both sites coincides with distinguished sites, have been evaluated by Elliott and Taylor³ using a different method. These matrix elements appear directly in expressions where the two atomic species

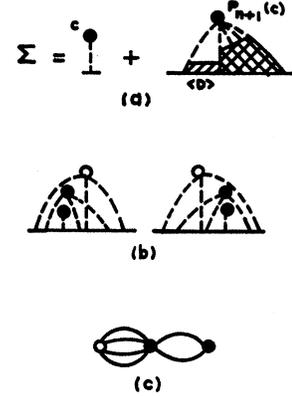


FIG. 2. (a) An analysis of the self-energy Σ to explain the form of Σ^0 ; (b) two diagrams which are represented by (c) a single diagram in the notation of Dzyub (Ref. 12).

interact differently with radiations but they do not apply, for example, to the displacement correlations among atoms in the neighborhood of a defect (distinguished site) nor to clusters of defects. The relationship with the distinguished-site expansion of the approach of Elliott and Taylor is shown below and is instructive when it comes to considering approximations. They note that the configuration average of Eq. (6) connects $\langle \mathbf{D} \rangle$ with $\langle \mathbf{D}^p \rangle$, namely, (for $M_r = M_A$)

$$\langle D(l,m) \rangle = d_A(l,m) + \mu_B \sum_p d_A(l,p) \langle \Delta_B(p) D(p,m) \rangle. \quad (36)$$

But

$$\begin{aligned} \langle \Delta_B(p) D(p,m) \rangle &= \langle \Delta_B(p) \rangle \langle D^p(p,m) \rangle \\ &= c \langle D^p(p,m) \rangle, \end{aligned} \quad (37)$$

where the second equality assumes no long-range order and $\langle \mathbf{D}^p \rangle$, the average of \mathbf{D} conditional on there being a B atom at site p , requires $b=1-c$ in Eq. (31). Solving Eq. (36) for $\langle D^p(p,m) \rangle$ and using Eq. (21), one obtains

$$\begin{aligned} \langle D^p(p,m) \rangle &= (c\mu_B)^{-1} [\mathbf{d}_A^{-1} \langle \mathbf{D} \rangle - \mathbf{I}]_{(p,m)} \\ &= (c\mu_B)^{-1} [\Sigma \langle \mathbf{D} \rangle]_{(p,m)} \end{aligned} \quad (38)$$

as a relation between the exact Green's functions (which holds even in the case of short-range order). But $\Sigma(p,n)$ is of the form

$$\Sigma(p,n) = c\mu_B \delta_{pn} + (\text{parts with at least two interaction lines}). \quad (39)$$

Consideration of Fig. 2(a) shows that, after division by $c\mu_B$ [since an $(r+1)st$ -order first vertex in Σ at the site l has the factor $\mu_B^r P_{r+1}(c)/c = \mu_B^r b P_{r+1}(c)/c(1-c)$], Σ is related to Σ^p by

$$(\mu_B c)^{-1} \Sigma(p,n) = \delta_{pn} + [\langle \mathbf{D} \rangle \Sigma^p]_{(p,n)}, \quad (40)$$

which, when put into Eq. (38), gives

$$\langle D^p(p,m) \rangle = \langle D(p,m) \rangle + \sum_{l,n} \langle D(p,l) \rangle \Sigma^p(l,n) \langle D(n,m) \rangle,$$

which agrees with Eq. (33). This consistency relation (40) may not hold for approximate forms of Σ and Σ^p . For example, use of the form Eq. (53) of Sec. V, as was done in Ref. 3, is equivalent to replacing the $\langle \mathbf{D} \rangle$ in

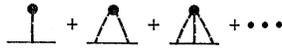


FIG. 3. The one-vertex self-energy.

Fig. 2(a) and in Eq. (40) by \mathbf{d}_A (which means neglecting all scatterings prior to the interaction with the particular defect). A self-consistent approximation in which \mathbf{d}_A lines are replaced by $\langle \mathbf{D} \rangle$ lines will satisfy Eq. (40). We shall not repeat the argument of Elliott and Taylor³ for expressing $\langle D^{pq}(p, q) \rangle$ in terms of $\langle \mathbf{D} \rangle$ but shall note only that the relation

$$\langle D^{pp}(p, p) \rangle = \langle D^p(p, p) \rangle \quad (41)$$

is not satisfied when the approximation (53) is used.^{11a} Since Eq. (35) applies only when $p \neq q$, there is no question about Eq. (41) here.

Dzyub¹² has calculated the neutron scattering cross section to second order in concentration which includes all two-vertex diagrams in $\langle \mathbf{D}^0 \rangle$. His calculation is the same as ours in this order. To extend it further would require something like the factors $P_r(c)$. In addition, his three-vertex and higher-order diagrams must be multiplied by appropriate multiplicity factors. For example, the two diagrams shown in Fig. 2(b) correspond to the same diagram, Fig. 2(c), in his notation.

IV. PARTIAL SUMMATIONS

The use of cumulants in the vertex factors in Secs. II and III permits each vertex index to be summed over all sites independently of other vertices so that the rigorous Dyson equation (21) and similar equations (22) and (35) can be written, as was first emphasized by Langer.⁵ Equation (21) effects a partial summation in terms of the self-energy, the series for which can be arranged, following Langer, in terms of partial sums

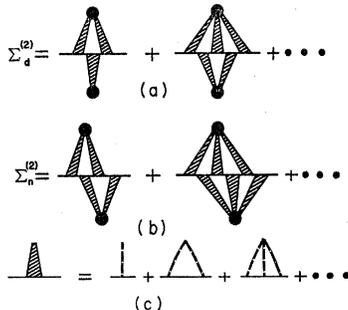


FIG. 4. The (a) diagonal and (b) nondiagonal two-vertex self-energy, where (c) the cross-hatched legs are one-impurity t matrices.

^{11a} Note added in proof. It has been pointed out to us by Dr. R. J. Elliott that (41) is satisfied by Taylor's self-consistent calculation of Ref. 17, as this analysis plus the connection established by Ref. 18 would indicate. Indeed, Eq. (41) can be used to derive Taylor's result.

¹² I. P. Dzyub, *Fiz. Tverd. Tela* **6**, 1866 (1964); **6**, 3691 (1964) [English transl.; *Soviet Phys.—Solid State* **6**, 1469 (1964); **6**, 2955 (1965)].

$$\Sigma^{(n)}, \quad \Sigma = \Sigma^{(1)} + \Sigma^{(2)} + \Sigma^{(3)} + \dots \quad (42)$$

in increasing order of the number n of interlocking vertices representing the interference of scattering from a cluster of the corresponding number of atomic sites. The contributions to $\Sigma^{(1)}$ and $\Sigma^{(2)}$ are shown in Figs. 3 and 4, respectively. In Fig. 3, the vertices, after the first, have the polynomial factors $P_2(c)$, $P_3(c)$, etc. The series for $\Sigma^{(1)}$ was summed in closed form in I for the case $M_r = M_A$. For M_r , it has the form $\Sigma^{(1)}(n\alpha, m\beta) = \Sigma^{(1)} \delta_{n\alpha, m\beta}$, where

$$\Sigma^{(1)} = \sum_{r=1}^{\infty} \kappa_r(\mu) d_0^{r-1}, \quad (43a)$$

$$\Sigma^{(1)} = \mu_A + \mu_{BAC} \sum_{p=1}^{\infty} (p-1)! (-c\mu_{BA}d_0)^{p-1} [(1-\mu_{BA}d_0) \times (1-2\mu_{BA}d_0) \dots (1-p\mu_{BA}d_0)]^{-1}, \quad (43b)$$

or

$$\Sigma^{(1)} = \mu_A + \frac{\mu_{BAC}}{1-\mu_{BA}d_0} {}_2F_1\left(1, 1; 2 - \frac{1}{\mu_{BA}d_0}; c\right), \quad (43c)$$

where $d_0 = d(n\alpha, n\alpha)$ and $\mu_{BA} = \mu_B - \mu_A$.

Yonezawa and Matsubara² have also derived an expression [their Eq. (44)] for the one-vertex part in the form of an integral based on the generating function for $P_r(c)$ in Ref. 8. This integral can be reduced to a standard representation of the hypergeometric function above. The series form shows the analytic properties clearly.

There is a sequence of poles in $\Sigma^{(1)}$ at

$$1 - m\mu_{BA}d_0(\omega) = 0, \quad m = 1, 2, \dots \quad (44)$$

Near each pole there is an ω interval within which the denominator of $\langle \mathbf{D}(\omega) \rangle$ in (22) has a zero eigenvalue so that $\langle \rho_D(\omega) \rangle \neq 0$, where $\rho_D(\omega)$ is the weighted frequency spectrum which is proportional to $\text{Im}[\mathbf{D}(\omega + i\epsilon)]$. The first pole ($m=1$) is the eigenfrequency condition for an isolated impurity. The poles for $m=2, 3, \dots$ are the eigenfrequency conditions for m superimposed perturbations on a single site and can occur at frequencies higher than the maximum frequency of a lattice entirely of the lighter atoms.¹ These spurious poles result from an overcounting implicit in the partial summation $\Sigma^{(1)}$.

More evidence for overcounting is seen in the two-vertex summation. This may be calculated in two parts,

$$\Sigma^{(2)} = \Sigma_d^{(2)} + \Sigma_n^{(2)}, \quad (45)$$

as shown in Figs. 4(a) and 4(b), respectively. As a matrix in configuration space, $\Sigma_d^{(2)}$ is diagonal with elements corresponding to the upper of the two sites while $\Sigma_n^{(2)}$ begins and ends on different sites.¹³ Each

¹³ Strictly speaking, $\Sigma_n^{(2)}$ has a diagonal part also, corresponding to the coincidence of the two lattice points. The cumulants allow and require independent summation over all vertex sites.

cross-hatched leg shown in Figs. 4(a) and 4(b) represent the sum over all interaction lines to the same vertex as shown in Fig. 4(c). The nondiagonal part $\Sigma_n^{(2)}$ introduces a mixing of the polarizations of the normal modes of the perfect crystal with a corresponding branch and directional \mathbf{k} dependence of the phonon linewidths and frequency shifts.

In the Appendix it is shown that

$$\Sigma_n^{(2)}(l,m) = d(l,m)^3 \sum_{p=2}^{\infty} (-1)^p \left(\frac{c}{1-c} \right)^p \times \sum_{s=1}^{p-1} \frac{t_s^2 t_{p-s}^2}{s(p-s)[1-t_s t_{p-s} d(l,m)^2]} \quad (46a)$$

and

$$\Sigma_d^{(2)}(l,m) = \delta_{l,m} \sum_{p=2}^{\infty} (-1)^p \left(\frac{c}{1-c} \right)^p \sum_{s=1}^{p-1} \frac{t_s t_{p-s}^2}{(p-s)} \times \sum_k \frac{d(l,k)^2}{1-t_s t_{p-s} d(l,k)^2}, \quad (46b)$$

This is the normal mode condition for two mass impurities $\Delta M_s = s(M_A - M_B)$ at site R_l and $\Delta M_{p-s} = (p-s)(M_A - M_B)$ at site R_k in the M_r lattice. For $p=2$ the only term in Eq. (46) is $s=p-s=1$ corresponding to the physical case of an impurity $\Delta M = M_A - M_B$ at the two sites R_l and R_k and condition (48) gives the frequencies of the optical and acoustical modes of vibration for the two impurities. The terms for $p>2$ correspond to p impurities superimposed onto two lattice sites in all ways and give rise to new spurious poles for $m>1$. The coefficient of these spurious terms are of order c^3 and higher.

The lowest terms in Eq. (45), of order c^2 , are

$$\Sigma_n^{(2)}(l,m) = \frac{c^2 d(l,m)^3 t_1^4}{1-t_1^2 d(l,m)^2} + O(c^3) \quad (49a)$$

and

$$\Sigma_d^{(2)}(l,m) = \delta_{l,m} c^2 \sum_k \frac{d(l,k)^2 t_1^3}{1-t_1^2 d(l,k)^2} + O(c^3), \quad (49b)$$

and are of the form first given by Langer for the case $M_r = M_A$.⁵ From the previous discussion it is evident that the $k=l=m$ terms of Eq. (49) correspond, at their pole, to a spurious overlap of two mass impurities. The singular part of this diagonal term of (49) cancels the first spurious pole ($m=2$) of $\Sigma^{(1)}$ in Eq. (43b) as was shown by Langer. It seems likely that the poles of $\Sigma^{(3)}$ in which two of the three vertices coincide will cancel the spurious two-site poles of $\Sigma^{(2)}$ for $p=3$, while the $m=3$ pole of $\Sigma^{(1)}$ together with the $k=l=m$ term

where

$$t_s = \frac{s\mu_{BA}}{1-s\mu_{BA}d_0}, \quad s=1,2,\dots \quad (47)$$

is the scattering matrix (diagonal) for an isolated site with s superimposed perturbations, and $d(l,m)$ is still a 3×3 matrix in α and β .

The expressions (46) are again much more transparent than the multiple-integral form derived by Yonezawa and Matsubara² [Eq. (3.14) of the third paper], but they are still complicated to evaluate numerically and this was not done.

The poles of $\Sigma^{(2)}$ occur at frequencies where

$$(1-t_s t_{p-s} d(k,l)^2)$$

has a zero eigenvalue for some s , $p-s$, l , and k . After some rearrangement using Eqs. (5) and (47), this eigenvalue condition can be shown to be equivalent, if the sites l and k do not coincide, to the vanishing of the 6×6 determinant

$$\begin{vmatrix} 1-s(M_A-M_B)\omega^2 d(l,l) & -s(M_A-M_B)\omega^2 d(l,k) \\ -(p-s)(M_A-M_B)\omega^2 d(k,l) & 1-(p-s)(M_A-M_B)\omega^2 d(k,k) \end{vmatrix} = 0. \quad (48)$$

in c^3 of $\Sigma^{(2)}$ will cancel with the triple-coincidence term in $\Sigma^{(3)}$.

V. DISCUSSION

The appearance in each order of $\Sigma^{(n)}$ of spurious poles which are eventually cancelled by terms in other orders is inherent with the use in a partial summation of the cumulants defined by the complete expansion. When a restricted summation is made, appropriately restricted cumulant corrections for the coincidence of the diagram elements should be used. These cumulants will change as more terms are included in the expansion. We do not know if such a procedure can be developed *rigorously* but the $\Sigma^{(1)}$ approximation given by Elliott and Taylor³ and recently extended to $\Sigma^{(2)}$ diagrams¹⁴ may be regarded as a first step in such a scheme.

Their $\Sigma^{(1)}$ approximation is a partial summation of $\langle \mathbf{D} \rangle$ in Eq. (8) starting from labeled diagrams (i.e., before summing over l_1, l_2, \dots) containing irreducible parts with one vertex only. However, in summing over site labels they correct for the coincidence of successive scattering sites but not for other coincidences. This partial sum $\langle \mathbf{D}^{(1)} \rangle$ now contains only one-vertex irreducible parts (even in the corrections) and the latter define a $\Sigma^{(1)}$ exactly.

The connection with cumulants is illustrated by an example. Let us consider the contribution to the third-order vertex shown in Fig. 5(a), for the case $M_r = M_A$. In order to obtain the contribution $\kappa_3(\mu)$ to this vertex

¹⁴ R. N. Aiyer, R. J. Elliott, J. A. Krumhansl, and P. L. Leath (to be published).



FIG. 5. (a) A third-order vertex and (b) diagrams whose vertex confluence determines $P_3(c)$.

in I we subtracted from $c\mu_B^3$ the contribution of all diagrams coming from distinct ways that the diagram could be broken apart as shown in Fig. 5(b). The result of this procedure is

$$\begin{aligned}\kappa_3(\mu) &= \mu_B^3 \{c - [P_1(c)]^3 - 3P_1(c)P_2(c)\} \\ &= \mu_B^3 (c - 3c^2 + 2c^3).\end{aligned}\quad (50)$$

However, the diagram on the extreme right in Fig. 5(b) contains a two-vertex irreducible part. Thus, for example, if only one-vertex parts are put into the self-energy in a partial summation of the diagrams, this diagram does not appear explicitly although there is a correction for it in Eq. (49). This kind of overcorrection leads to spurious poles. Elliott and Taylor³ leave out such corrections and would obtain as the contribution κ_3' to the third-order vertex

$$\begin{aligned}\kappa_3'(\mu) &= \mu_B^3 \{c - [P_1(c)]^3 - 2P_1(c)P_2(c)\} \\ &= \mu_B^3 c(1-c)^2.\end{aligned}\quad (51)$$

The general vertex factor found by this procedure is

$$\kappa_n'(\mu) = \mu_B^n c(1-c)^{n-1}.\quad (52)$$

This result, using Eq. (43a), gives

$$\Sigma_{BT}^{(1)} - \mu_B c / [1 - (1-c)\mu_B d_0],\quad (53)$$

the result obtained by Elliott and Taylor. The spurious poles are missing, which indicates that their presence was indeed related to the overcounting. However κ_n' given by this method is not a true cumulant of the restricted summation if cumulants are defined as in Ref. 8 and thereby are related to the moments by Eq. (12). The reason that these relationships are not satisfied by κ_n' is due to the fact that many diagrams unavoidably appear in any partial summation even if they are not included explicitly. For example, the last diagram in Fig. 5(b) appears in the "one-vertex" partial summation $\langle \mathbf{D}^{(1)} \rangle$ with weight c^3 . It appears in the summation over internal indices of the first diagram in Fig. 5(b) when the first and last site coincide. This correction would be properly made by any true cumulant. The undercorrection is, however, of higher order in c than the overcorrection caused by using the cumulants of the full expansion and does not seem to lead to spurious poles.

As a further example of the method, we calculate the one-vertex self-energy $\Sigma^{(1)}$ for the arbitrary reference mass M_r . The bare one-vertex self-energy, Fig. 3, with no corrections is

$$\sigma_1 = (1-c)\mu_A / (1-\mu_A d_0) + c\mu_B / (1-\mu_B d_0),\quad (54)$$

which is the mean t matrix for scattering at a site. This term can be obtained from Eq. (43b) by neglecting all correction terms [those of $O(c^n)$ for $n \geq 2$, and those of $O(\mu_A^n \mu_B^m)$ for both $n, m \geq 1$]. The corrections to this term come from all ways that the diagrams in Fig. 3 can be broken apart such that only one-vertex irreducible parts make up the resulting diagrams. The total corrections to $\Sigma^{(1)}$ from breaking into two such parts can be summed to

$$\sigma_2 = -\Sigma^{(1)} d_0 \Sigma^{(1)}.\quad (55)$$

The corrections from three parts is

$$\sigma_3 = -\Sigma^{(1)} d_0 \Sigma^{(1)} d_0 \Sigma^{(1)},\quad (56)$$

and so forth, where $\Sigma^{(1)}$ is the fully corrected self-energy. The result for $\Sigma^{(1)} = \sum_{i=1}^{\infty} \sigma_i$ is

$$\Sigma^{(1)} = \sigma_1 - (\Sigma^{(1)} d_0 \Sigma^{(1)} + \Sigma^{(1)} d_0 \Sigma^{(1)} d_0 \Sigma^{(1)} + \dots),\quad (57)$$

which can be solved with the result

$$\Sigma^{(1)} = \sigma_1 / (1 + d_0 \sigma_1).\quad (58)$$

Upon substituting for σ_1 from Eq. (50), one obtains

$$\Sigma^{(1)} = \frac{(1-c)\mu_A + c\mu_B - \mu_A \mu_B d_0}{1 - [c\mu_A + (1-c)\mu_B] d_0},\quad (59)$$

which is formally symmetric with respect to interchange of A and B atom types and reduces to Eq. (53) when $\mu_A = 0$, or $M_r = M_A$. The vertex factors κ_n' obtained by expressing (59) in the form (43a) are

$$\begin{aligned}\kappa_1'(\mu) &= (1-c)\mu_A + c\mu_B, \\ \kappa_n'(\mu) &= c(1-c)(\mu_A - \mu_B)^2 [c\mu_A + (1-c)\mu_B]^{n-2},\end{aligned}\quad (60)$$

for $n > 2$ as compared with Eq. (17). For $M_r = M_A$, this reduces to Eq. (52). For $M_r = (1-c)M_A + cM_B = \langle M \rangle$, however, Eq. (60) reduces to

$$\kappa_n'(\mu) = c(1-c)(1-2c)^{n-2}(\mu_A - \mu_B)^n.\quad (61)$$

In summary, we can say that the two procedures agree to the same order as that of the uncorrected diagrams that are put into the partial summation but that the higher-order terms which are put in only approximately (by both procedures) lead to spurious poles in the full cumulant expansion but do not in Elliott and Taylor's approximation.

Finally, we note the importance of reducing the effect of over- or undercounting in self-consistent partial summations where many more diagrams are included. Self-consistent calculations based on the uncorrected self-energy insertion σ_1 on all internal d lines give exaggerated broadening of impurity-mode bands in three-dimensional systems¹⁵ similar to the results of Davies and Langer in one dimension.¹⁶ Recent self-consistent

¹⁵ P. L. Leath, Ph.D. thesis, University of Missouri, 1966 (unpublished).

¹⁶ R. W. Davies and J. S. Langer, Phys. Rev. **131**, 163 (1963).

calculations by Taylor, which were based on the use of Eq. (53) in a multiple-scattering formalism, have given much improved results for three dimensions.¹⁷ It has been shown¹⁸ that the form of $\Sigma_{s.c.}^{(1)}$ involved can be obtained by an application of the arguments leading to Eq. (58). Self-consistency is required to get a sensible result for the frequency spectrum of a distinguished atom starting from (33). Expressions like Fig. 1(c) for Σ_1^0 have isolated poles in ω and not branch cuts, so that the contribution of Σ^0 tends to be in δ -function peaks rather than in broadened bands. Bands result from the corresponding approximation to Σ in $\langle \mathbf{D}(\omega) \rangle$ because Σ appears in the denominator. Another advantage of self-consistency was mentioned below Eq. (39).

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APPENDIX

In the nondiagonal two-vertex self-energy $\Sigma_n^{(2)}$ shown in Fig. 4(a), the diagram rules lead to

$$\begin{aligned} \Sigma_n^{(2)}(l,m) = & \sum_{n=2}^{\infty} \sum_{i_1, i_2, \dots, i_N; j_1, \dots, j_N > 0} (\mu_B - \mu_A)^{2+j} \\ & \times P_i(c) P_j(c) d_0^{i_1-1} d(l,m) d_0^{j_1-1} \\ & \times d(m,l) \cdots d(l,m) d_0^{j_n-1}, \quad (\text{A1}) \end{aligned}$$

where N is the number of cross-hatched legs, and i and j satisfy

$$i = \sum_{k=1}^N i_k, \quad j = \sum_{k=1}^N j_k.$$

The d factors are 3×3 matrices in Cartesian indices, d_0 is a constant matrix, and $d(m,l) = d(l,m)$ with the assumed symmetry; thus we can collect like terms in

(A1) to obtain

$$\begin{aligned} \Sigma_n^{(2)}(l,m) = & \sum_{N=2}^{\infty} d(l,m)^{2N-1} (d_0)^{-2N} \\ & \times \{A_N[(\mu_B - \mu_A) d_0, c]\}^2, \quad (\text{A2}) \end{aligned}$$

where

$$A_N(X, c) = \sum_{j_1, j_2, \dots, j_N=1}^{\infty} X^j P_j(c). \quad (\text{A3})$$

However, Eq. (32) can be rewritten as

$$P_j(c) = \frac{d^j}{dy^j} \left\{ \ln \left[1 + (\text{expy}) \frac{c}{1-c} \right] \right\} \Big|_{y=0}. \quad (\text{A4})$$

Thus A_N becomes

$$\begin{aligned} A_N(X, C) &= \left(\sum_{j_1, j_2, \dots, j_N=1}^{\infty} X^j \frac{d^j}{dy^j} \right) \ln \left(1 + \frac{c}{1-c} \text{expy} \right) \Big|_{y=0} \quad (\text{A5a}) \\ &= \left\{ \prod_{k=1}^N \left[\frac{1}{1-X(d/dy)} - 1 \right] \right\} \\ & \quad \times \ln \left(1 + \frac{c}{1-c} \text{expy} \right) \Big|_{y=0} \quad (\text{A5b}) \end{aligned}$$

$$\begin{aligned} &= \left(\frac{X(d/dy)}{1-X(d/dy)} \right)^N \sum_{s=1}^{\infty} \frac{(-1)^{s-1}}{s} \left(\frac{c}{1-c} \right)^s \\ & \quad \times \text{expsy} \Big|_{y=0} \quad (\text{A5c}) \end{aligned}$$

$$= \sum_{s=1}^{\infty} \frac{(-1)^{s-1}}{s} \left(\frac{c}{1-c} \right)^s \left(\frac{Xs}{1-Xs} \right)^N. \quad (\text{A5d})$$

Inserting (A5d) into (A2) and interchanging orders of summation, we obtain

$$\begin{aligned} \Sigma_n^{(2)}(l,m) = & \sum_{s,r=1}^{\infty} \frac{(-1)^{s+r}}{sr} \left(\frac{c}{1-c} \right)^{s+r} \frac{1}{d(l,m)} \\ & \times \sum_{N=2}^{\infty} [t_{s,t,d}(l,m)^2]^N, \quad (\text{A6}) \end{aligned}$$

which is equivalent to (46a).

The diagonal part $\Sigma_d^{(2)}$ [Fig. 4(b)] can be evaluated similarly with the change that the variable inner vertex k has $N-1$ legs when the vertex $l=m$ has N legs, so that Eq. (46b) is the result.

¹⁷ D. W. Taylor, Phys. Rev. 156, 1017 (1967).

¹⁸ P. L. Leath, Phys. Rev. 171, 725 (1968).