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Self-Consistent Average Green's Function in Random Lattices: A Generalized Coherent-Potential Approximation (n) and Its Diagrammatic Equivalents*

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We describe a simple generalization of the coherent-potential approximation that is *exactly* equivalent to the self-contained cumulant expansions and the self-consistent diagrammatic-resummation techniques. A detailed analysis of these different methods for the pair case is given.

I. INTRODUCTION

Much of the recent work in disordered-model alloy problems has been concerned with the calculation of the average Green's functions. Since this calculation can be done exactly for only one special model,[1] attempts have been made to develop a systematic scheme which can be used to obtain a sequence of improving approximations. Notable among these techniques are the cumulant expansions of Yonezawa and Matsubara,[2] the corrected or self-contained cumulant expansions of Yonezawa,[3] and, paralleling this latter development, the diagrammatic expansion of Leath[4] and Leath and Goodman.[5] A rather different approach is suggested by the coherent-potential approximation (CPA) of Soven[6] for electronic states, the self-consistent method of Taylor[7] for vibrational excitations, and the treatment of excitons by Onondera and Toyozawa,[8] all of which are formally identical and can be considered as good first approximations.

The diagrammatic (or corrected-cumulant) approaches are appealing in the sense that one can "visualize" the approximations that are made and they can, in principle, be used to obtain a sequence of improving results. In practice, however, the solution of the counting problem has proved very elusive and so far only the lowest-order or so-called "single-site" approximation has been correctly obtained and applied. Thus although previous attempts have been made to calculate the next-order or "pair" approximation, these calculations have been either incomplete or have contained significant errors.[9,10] We will make additional comments on these last two calculations later in an attempt to relate them to the present development.

The CPA calculation has been shown to be exactly equivalent to the single-site corrected-cumulant approximation mentioned above.[4] However, it is not obvious how one would generalize the method in the "best" possible way—formal generalizations of course exist,[11,12] but none of the approximation schemes that have been developed[13] have actually led to a generalization that has the (simple) equivalence to the corrected-cumulant or diagrammatic expansions possessed by the elementary CPA.

What we show below is that there does exist a generalization of CPA such that CPA (n) is exactly equivalent to the n-site corrected-cumulant or diagrammatic approximation. This generalization is quite straighforward in any order but for simplicity we restrict ourselves mainly to CPA (2) or the pair approximation. It is also of interest to note that the method outlined below can be easily extended to obtain a systematic sequence of approximations for the average two-particle Green's function.

A very convenient model system, which we use as the basis for our discussion, is described in Sec. II. Although some extensions of this model are obviously possible without substantially modifying our generalization of the CPA, we have not made any detailed analysis to determine exactly what aspects of the CPA (n) are specifically model dependent. In Sec. III we outline the cumulant and corrected-cumulant techniques of Matsubara and Yonezawa[2,3] and then in Sec. IV we review the diagrammatic summation technique of Leath[4] and use it to derive

the corrected-cumulant approximation for pairs. Our derivation is slightly different from the original pair calculation in Aiyer *et al.*[10] and may appear somewhat more involved; however, it shows up more clearly the details of the interrelationship between the single-site and pair approximations. In Sec. V we describe a generalization of CPA to CPA (n) and use it to rederive the results of the diagrammatic expansion for pairs. For the reader who is not interested in the details of the diagrammatic resummations, we note here that the justification of CPA (n) depends only on some rather general properties of the diagrammatic expansions so that Sec. V can be read independently of Sec. IV. Section VI contains a brief description of an extension of this method to calculations of the average two-particle Green's function.

II. MODEL

The random-model system we will use as the basis for our analysis is described by the standard lattice Hamiltonian with diagonal (in coordinate representation) disorder. That is,

$$H=\sum_{i\neq j} W_{ij}a_i^\dagger a_j+\sum_i \epsilon_i a_i^\dagger a_i \equiv W+\epsilon\ , \tag{1}$$

where the sums are over lattice sites, W_{ij} is translationally invariant, and ϵ_i is a random variable. The particular form of the distribution of levels ϵ_i is not important but to make the connection with previous studies we will specialize to the case of a binary alloy where

$$\begin{aligned}\epsilon_i &= v \quad \text{with probability } c\\ &= 0 \quad \text{with probability } 1-c\ .\end{aligned} \tag{2}$$

With the definitions

$$g=(E-W)^{-1}\ ,\quad G=(E-H)^{-1}\ , \tag{3}$$

the perturbation expansion for $\langle G\rangle$ is given by

$$\langle G_{ij}\rangle = g_{ij}+\sum_k g_{ik}g_{kj}\langle\epsilon_k\rangle+\sum_k\sum_l g_{ik}g_{kl}g_{lj}\langle\epsilon_k\epsilon_l\rangle+\cdots . \tag{4}$$

A few rather trivial comments might be made. First, the ensemble averaging restores translational invariance so that $\langle G\rangle$ is diagonal in momentum representation. Second, and this is the point that has made the study of disordered systems so difficult, one must be careful in distinguishing various combinations of site index labels. Thus, for example,

$$\begin{aligned}\langle\epsilon_k\epsilon_l\rangle &= c^2v^2\ , \quad k\neq l\\ &= cv^2\ , \quad k=l\end{aligned} \tag{5}$$

so that the second-order term in (4) must really be written as two separate terms containing restricted summations.

III. CUMULANT AND CORRECTED CUMULANT EXPANSION

The essence of the cumulant expansion is very simple. The ensemble averaging procedure introduces restricted summations in the perturbation expansion of $\langle G\rangle$ and these restrictions must be removed if we wish to write a Dyson equation

$$\langle G\rangle = g+g\Sigma\langle G\rangle\ , \tag{6}$$

which will be an algebraic equation in momentum space and in which the self-energy Σ is considered a functional of the exact $\langle G\rangle$ rather than the unperturbed g. The removal of the restrictions can be achieved by rearranging the perturbation series and assigning to each diagram a weight function that is simply related to various cumulant averages of the random potential ϵ_i. This rearrangement yields a self-energy which is shown schematically in Fig. 1; explicit expressions for the cumulant functions $P_s\equiv P_s(c)$ can be found in Yonezawa and Matsubara.[2]

Although the representation for Σ as given in Fig. 1 is exact, in practice one is still faced with the problem of choosing from this infinite series that class of diagrams which one believes to be the most important or in some sense "self-contained." For example, one might choose that class of terms that refers only to scattering off a single site. Since in the rearrangement of the series in terms of cumulant averages we have removed *all* site index restrictions, this class of single-site terms is not just the sequence

$$P_1v+P_2v^2\langle G_{ii}\rangle+P_3v^3\langle G_{ii}\rangle^2+\cdots + P_{n+1}v^{n+1}\langle G_{ii}\rangle^n+\cdots\ ,$$

but rather (again refer to Fig. 1)

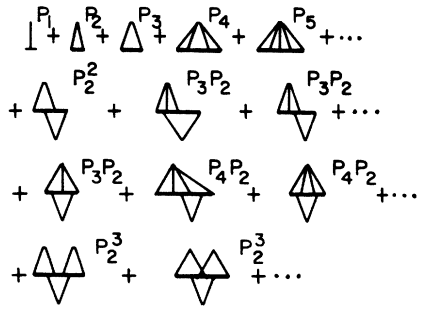

FIG. 1. Schematic representation of the exact $\Sigma\{\langle G\rangle\}$. The weight associated with each term is a simple product function of the cumulants $P_s(c)$. Each vertical line represents a potential v (i.e., no t-matrix resummations have been performed); the internal lines are the full propagators $\langle G_{ij}\rangle$. It follows from the definition of the cumulant averages that there are *no* site index restrictions in this series. Thus, for example, the term labeled P_2^2 represents both a pair term $P_2^2v^4\langle G_{ij}\rangle^3$, $i\neq j$, and a single-site term $P_2^2v^4\langle G_{ii}\rangle^3$.

$$\Sigma_{ii}^{(1)} = P_1 v + P_2 v^2 \langle G_{ii} \rangle + P_3 v^3 \langle G_{ii} \rangle^2 + (P_4 + P_2^2) v^4 \langle G_{ii} \rangle^3 + (P_5 + 5P_3 P_2) v^5 \langle G_{ii} \rangle^4 + (P_6 + 9P_4 P_2 + 7P_3^2 + 4P_2^3) v^6 \langle G_{ii} \rangle^5 + \cdots$$

$$\equiv Q_1 v + Q_2 v^2 \langle G_{ii} \rangle + Q_3 v^3 \langle G_{ii} \rangle^2 + \cdots + Q_{n+1} v^{n+1} \langle G_{ii} \rangle^n + \cdots , \quad (7)$$

where again, explicit expressions for the corrected cumulants $Q_s \equiv Q_s(c)$ can be found in Yonezawa.[3]

This and other higher-order self-contained approximations are derived by simply rearranging the series for Σ such that site labels on any one diagram are all different. The self-energy Σ has then been separated explicitly into terms that refer to single sites, pairs, triplets, etc. The first few weight factors that one obtains after this new arrangement are shown in Fig. 2. Note that the expression for Σ with the site index restrictions is *not* obtained from the cumulant expansion with the simple replacement $P_n \to Q_n$. In particular, whereas the weight associated with each diagram in Fig. 1 is always a simple product function of the P's (e.g., $P_4 P_2$), the weight associated with the diagrams in Fig. 2 can be more complicated (e.g., $Q_4 Q_2 + Q_2^3$). This is a rather crucial point since it means that the pair series, for example, cannot be generated from the single-site series by any very simple combinatorial analysis. In their generalization to pairs, Yonezawa and Homma[9] considered just these leading product terms obtained by the replacement $P \to Q$ [Eq. (7) in Ref. 9] and thus although their approximation is correct through order v^5 and c^2 it is certainly not a complete representation of the pair scattering.

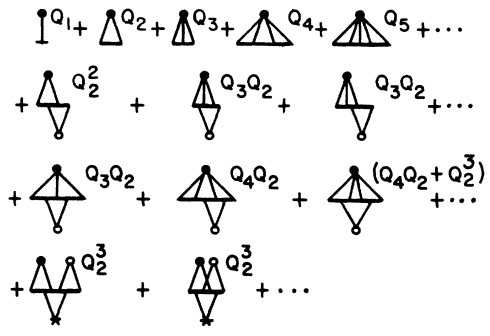

FIG. 2. Schematic representation of $\Sigma\{\langle G \rangle\}$ in terms of single-site series, pair series, triplet series, etc. The site index labels on any one diagram are all different. To distinguish scattering sites we have used the following symbols: single site—closed circle, pairs—closed and open circles, triplets—closed and open circles and asterisk. The weights associated with each term cannot always be represented as a single product function of the corrected cumulants $Q_s(c)$.

We will show below that the different series for Σ shown in Fig. 2 can be summed and yield closed expressions for Σ in terms of $\langle G \rangle$ in coordinate representation. Thus, for example, the single-site series yields an expression for $\Sigma_{ii}^{(1)}$ in terms of $\langle G_{ii} \rangle$. The pair series yields the diagonal and off-diagonal matrix elements $\Sigma_{ii}^{(2)}(j)$ and $\Sigma_{ij}^{(2)}$ as functions of $\langle G_{ii} \rangle = \langle G_{jj} \rangle$ and $\langle G_{ij} \rangle = \langle G_{ji} \rangle$ for every pair separation $R_{ij} \neq 0$. On the other hand, (6) can be conveniently solved in momentum representation so that one must go back and forth from coordinate to momentum representation according to

$$\Sigma_{\vec{p}} = \Sigma_{ii}^{(1)} + \sum_j{}' \Sigma_{ii}^{(2)}(j) + \sum_j{}' \sum_k{}' \frac{1}{2!} \Sigma_{ii}^{(3)}(j,k) + \cdots + \sum_j{}' e^{i\vec{p}\cdot\vec{R}_{ij}} [\Sigma_{ij}^{(2)} + \sum_k{}' \Sigma_{ij}^{(3)}(k) + \cdots] \quad (8)$$

and

$$\langle G_{ij} \rangle = \int \frac{d^3p}{(2\pi)^3} \frac{e^{-i\vec{p}\cdot\vec{R}_{ij}}}{g_{\vec{p}}^{-1} - \Sigma_{\vec{p}}} , \quad (6')$$

where the primes on the lattice sums indicate that no two indices be the same.

IV. DIAGRAMMATIC EXPANSION

Although the above rearrangement of the perturbation series in terms of cumulants and its subsequent rearrangement in terms of the corrected cumulants is exact, it has not been found possible to adapt it to obtain closed expressions for the various cluster approximations to Σ. We therefore turn to another method which one can use to derive the corrected cumulants more directly.

We note that to obtain a particular approximation for Σ we must subtract *all* possible terms involving lower-order approximations to Σ which when iterated in the Dyson equation *or* used to renormalize the internal propagators would correspond to an overcounting. A particularly convenient way of arranging these subtractions is due to Leath[4]; such an arrangement for the single-site approximation $\Sigma_{ii}^{(1)}$ is shown in Fig. 3. Note that in this arrangement only the site i is involved explicitly, so that pair and higher-order cluster terms such as $\Sigma_{ij}^{(2)}$ $(R_{ij} \neq 0)$ do not appear except implicitly in the propagator $\langle G_{ii} \rangle$. It is for this reason that one can call the single-site approximation self-contained and can obtain a closed expression for $\Sigma_{ii}^{(1)}$ independently of any knowledge of higher-cluster approximations.

The rows in Fig. 3 are identities involving the corrected cumulants and can be used to rederive expressions for them. However, this is not necessary for our purpose since we can sum the various columns directly. The first column or left-hand side of the equation is of course just $\Sigma_{ii}^{(1)}\{\langle G_{ii} \rangle\}$; if instead we transpose it to the right-hand side and combine it with the last column, we get $-\Sigma_{ii}^{(1)}\{\Gamma\}$,

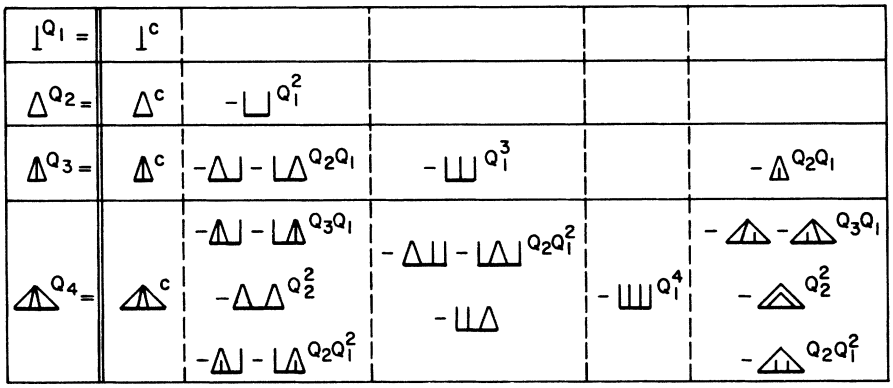

FIG. 3. Rearrangement of the single-site series $\Sigma_{ii}^{(1)}\{\langle G\rangle\}$. The first column on the right is the "bare" single-site t matrix; the remaining columns are corrections. Each row is an identity in the corrected-cumulant functions.

that is, all internal lines have been renormalized according to the transcription $\langle G_{ii}\rangle \to \Gamma$ where[14]

$$\Gamma \equiv \langle G_{ii}\rangle + \langle G_{ii}\rangle \Sigma_{ii}^{(1)}\{\Gamma\} + \langle G_{ii}\rangle\langle G_{ii}\rangle \Sigma_{ii}^{(1)}\{\Gamma\}\langle G_{ii}\rangle \Sigma_{ii}^{(1)}\{\Gamma\}\langle G_{ii}\rangle + \cdots = \langle G_{ii}\rangle (1 - \Sigma_{ii}^{(1)}\{\Gamma\}\langle G_{ii}\rangle)^{-1} \tag{9a}$$

or

$$\langle G_{ii}\rangle = \Gamma(1 + \Sigma_{ii}^{(1)}\{\Gamma\}\Gamma)^{-1} . \tag{9b}$$

All the other columns, except for the first column on the right-hand side, also involve the self-energy with renormalized propagators, that is, they sum to

$$-\Sigma_{ii}^{(1)}\{\Gamma\}\langle G_{ii}\rangle\Sigma_{ii}^{(1)}\{\Gamma\} - \Sigma_{ii}^{(1)}\{\Gamma\}\langle G_{ii}\rangle\Sigma_{ii}^{(1)}\{\Gamma\}\langle G_{ii}\rangle\Sigma_{ii}^{(1)}\{\Gamma\} - \cdots .$$

Finally, the one remaining column is just the concentration c times the single-site t matrix

$$c\tau\{\langle G_{ii}\rangle\} \equiv cv(1 - \langle G_{ii}\rangle v)^{-1} , \tag{10}$$

so that Fig. 3 can be represented by the equation

$$0 = c\tau\{\langle G_{ii}\rangle\} - \Sigma_{ii}^{(1)}\{\Gamma\}(1 - \langle G_{ii}\rangle\Sigma_{ii}^{(1)}\{\Gamma\})^{-1} . \tag{11}$$

If we substitute the expression (9b) for $\langle G_{ii}\rangle$ into (11), we get

$$\Sigma_{ii}^{(1)}\{\Gamma\} = cv(1 - v\Gamma + \Sigma_{ii}^{(1)}\{\Gamma\}\Gamma)^{-1} , \tag{12}$$

which, with the dummy variable replacement $\Gamma \to \langle G_{ii}\rangle$, yields

$$\Sigma_{ii}^{(1)} \equiv \Sigma_{ii}^{(1)}\{\langle G_{ii}\rangle\} = cv[1 - (v - \Sigma_{ii}^{(1)})\langle G_{ii}\rangle]^{-1} . \tag{13}$$

To extend these arguments to the pair approximation, it is convenient to introduce a matrix notation similar to that discussed in Aiyer *et al.*[10] We define (for each possible pair i, j)

$$\langle \underline{G}\rangle \equiv \begin{pmatrix} \langle G_{ii}\rangle & \langle G_{ij}\rangle \\ \langle G_{ji}\rangle & \langle G_{jj}\rangle \end{pmatrix} , \quad \underline{\Sigma}^{(1)} = \begin{pmatrix} \Sigma_{ii}^{(1)} & 0 \\ 0 & \Sigma_{jj}^{(1)} \end{pmatrix} ,$$

$$\underline{\Sigma}^{(2)} = \begin{pmatrix} \Sigma_{ii}^{(2)}(j) & \Sigma_{ij}^{(2)} \\ \Sigma_{ji}^{(2)} & \Sigma_{jj}^{(2)}(i) \end{pmatrix} , \tag{14}$$

and

$$\underline{\Sigma} = \underline{\Sigma}^{(1)} + \underline{\Sigma}^{(2)} ,$$

where by symmetry $\langle G_{ii}\rangle = \langle G_{jj}\rangle$, $\langle G_{ij}\rangle = \langle G_{ji}\rangle$, $\Sigma_{ii} = \Sigma_{jj}$, and $\Sigma_{ij} = \Sigma_{ji}$. We will also use the definitions

$$\underline{\Gamma} = \langle \underline{G}\rangle (1 - \underline{\Sigma}\{\underline{\Gamma}\}\langle \underline{G}\rangle)^{-1} , \tag{15a}$$

or

$$\langle \underline{G}\rangle = \underline{\Gamma}(1 + \underline{\Sigma}\{\underline{\Gamma}\}\underline{\Gamma})^{-1} , \tag{15b}$$

which are simple extensions of the single-site expressions to the 2×2 $\{i, j\}$ subspace. Finally, we will find it convenient to separate $\langle \underline{G}\rangle$ and $\underline{\Gamma}$ into purely diagonal and nondiagonal parts, i.e.,

$$\langle \underline{G}\rangle = \langle \underline{G}_d\rangle + \langle \underline{G}_n\rangle , \quad \underline{\Gamma} = \underline{\Gamma}_d + \underline{\Gamma}_n . \tag{16}$$

The expansion for the off-diagonal matrix element $\Sigma_{ij}^{(2)}$ is shown in Fig. 4; the subtractions and arrangements of these pair terms is the same as that given in Aiyer *et al.*[10] except that we have tried to be more explicit in displaying exactly which scatterings occur off the two different sites i and j. In analogy with the single-site series, we would like to obtain closed expressions for the sums of the various columns; however, the corrections to the bare-pair terms alone involve a restricted set of scattering diagrams and cannot be conveniently summed. For example, one of the subtractions to the bare lowest-order pair graph is the term (see box, Fig. 4)

$$-Q_1^4 v^4 \langle G_{ij}\rangle\langle C_{ji}\rangle\langle G_{ij}\rangle ,$$

corresponding to propagation in the definite sequence $i \to j \to i \to j$. Now the removal of the restrictions in the intermediate sites can by systematical-

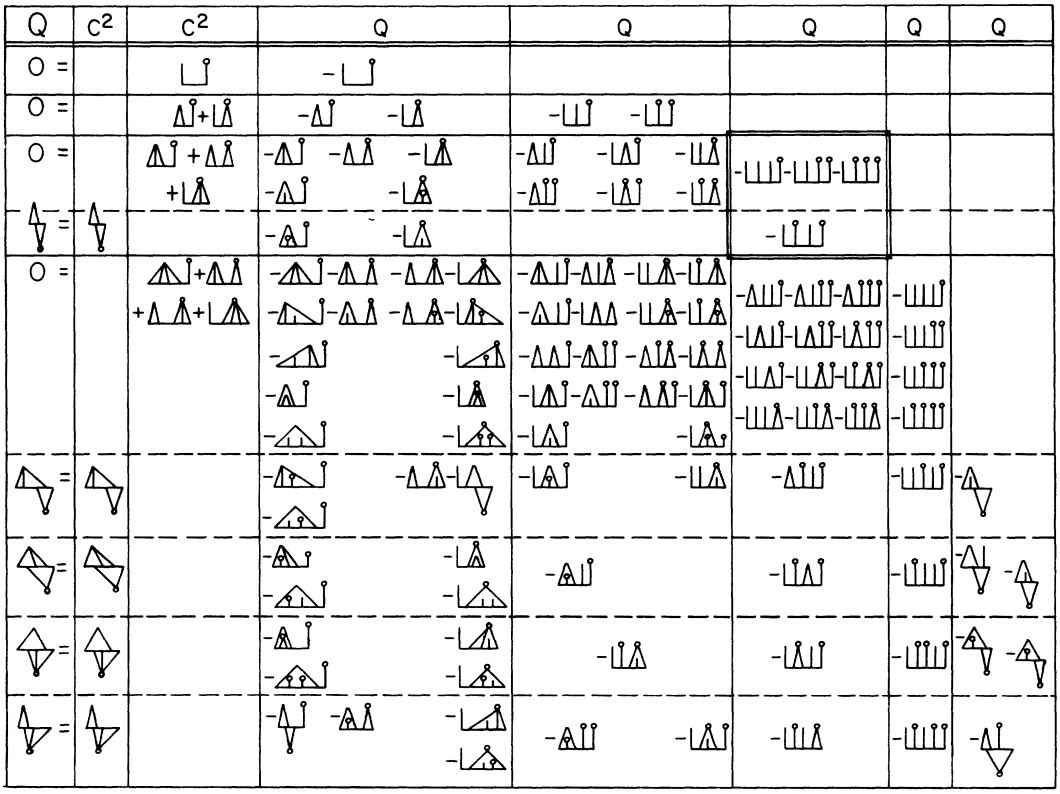

FIG. 4. Rearrangement of the pair series $\Sigma_{ij}^{(2)}\{\langle G\rangle\}$. The unmarked vertices are the site i, the vertices marked 0 are j. The first column on the right is the bare two-site t matrix, the second column is the product of two single-site t matrices; both are weighted by c^2. The rest of the columns labeled Q are weighted with the appropriate corrected-cumulant functions. Note that the single-site identities, when added to the pair terms, guarantee that *all* possible scatterings off *both* i and j occur in the correction terms. Boxed area is described in text.

ly achieved by adding in certain single-site identities which are simply rearrangements of the terms in Fig. 3. These identities have been included in Fig. 4 and on returning to the example given above we note that to the pair-correction term

$$-Q_1^4 v^4 \langle G_{ij}\rangle \langle G_{ji}\rangle \langle G_{ij}\rangle$$

the identities have added the three terms

$$-Q_1^4 v^4 [\langle G_{ij}\rangle \langle C_{jj}\rangle \langle G_{jj}\rangle + \langle G_{ii}\rangle \langle G_{ij}\rangle \langle G_{jj}\rangle + \langle G_{ii}\rangle \langle G_{ii}\rangle \langle C_{ij}\rangle] .$$

Thus this term can be neatly represented as the off-diagonal element of the matrix:

$$-Q_1^4 v^4 \langle \underline{G}\rangle \langle \underline{G}\rangle \langle \underline{G}\rangle .$$

Note also that just as in the single-site problem the internal lines are renormalized—except that now the renormalization involves *all* possible scatterings off *both* sites i and j. The renormalization is formally the same and simply requires the replacement of the matrix $\langle \underline{G}\rangle$ by the matrix $\underline{\Gamma}$.

The left-hand side of Fig. 4 sums to $\Sigma_{ij}{}^{(2)}\{\langle \underline{G}\rangle\}$ but just as in the single-site case we will transpose this to the right-hand side and combine it with the last column to obtain $-\Sigma_{ij}{}^{(2)}\{\underline{\Gamma}\}$. Furthermore, since $\underline{\Sigma}^{(1)}$ is diagonal, we note that up to pairs this is just the off-diagonal element of $-\underline{\Sigma}\{\underline{\Gamma}\}$. The remaining columns corresponding to corrections to the bare terms involve higher powers of $\underline{\Sigma}\{\underline{\Gamma}\}$, i.e., they are the off-diagonal matrix elements of the series

$$-\underline{\Sigma}\{\underline{\Gamma}\}\langle \underline{G}\rangle \underline{\Sigma}\{\underline{\Gamma}\} - \underline{\Sigma}\{\underline{\Gamma}\}\langle \underline{G}\rangle \underline{\Sigma}\{\underline{\Gamma}\}\langle \underline{G}\rangle \underline{\Sigma}\{\underline{\Gamma}\} - \cdots .$$

Finally, the bare-pair terms (the first column on the right-hand side of Fig. 4) yield the series

$$c^2[\tau^4\{\langle G_{ii}\rangle\}\langle G_{ij}\rangle^3 + \tau^6\{\langle G_{ii}\rangle\}\langle C_{ij}\rangle^5 + \tau^8\{\langle G_{ii}\rangle\}\langle G_{ij}\rangle^7 + \cdots] ,$$

and the bare single-site terms which have been added as part of the identities sum to

$$c^2\tau^2\{\langle G_{ii}\rangle\}\langle G_{ij}\rangle ,$$

where we have used the definition (10) for $\tau\{\langle C_{ii}\rangle\}$. Since the off-diagonal matrix element of $\langle \underline{G}_n\rangle^{2m}$ is

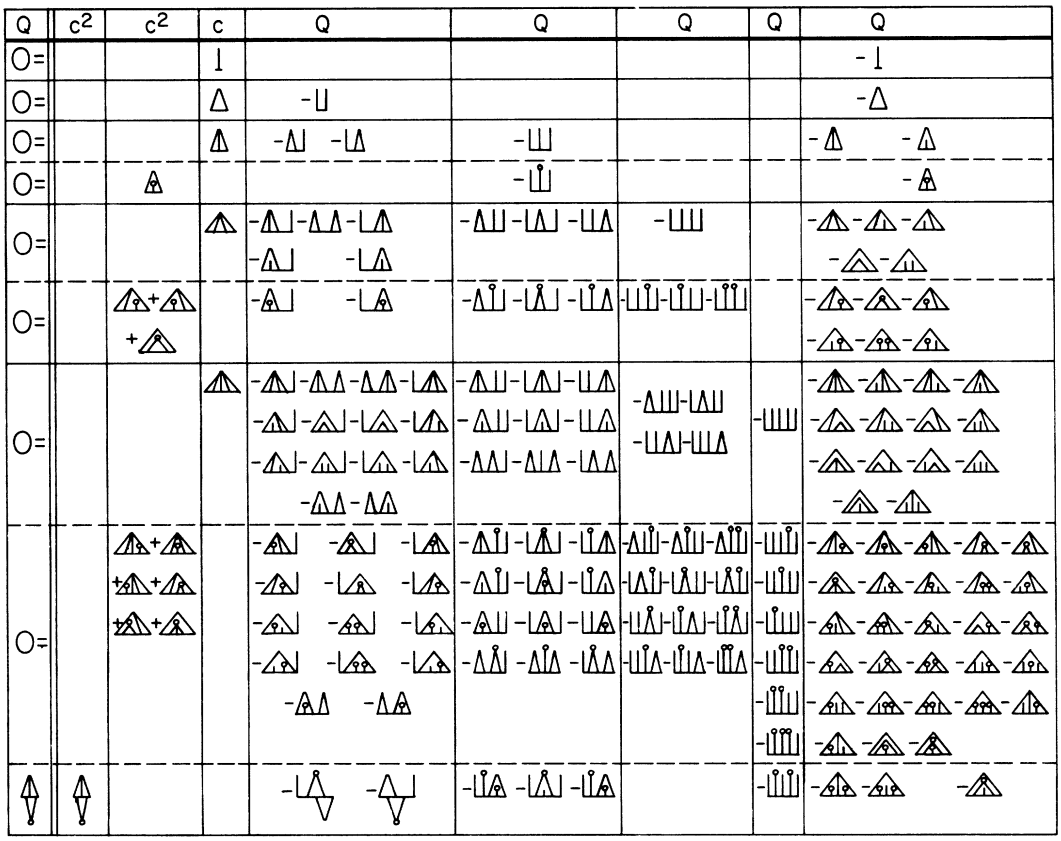

FIG. 5. Rearrangement for the diagonal pair term $\Sigma_{ii}^{(2)}\{\langle G\rangle\}$. The markings are as in Fig. 4. Note that now two types of identities have been added to allow for *all* possible scatterings off i and j in the correction terms.

zero and of $\langle \underline{G}_n \rangle^{2m+1}$ is $\langle C_{ij} \rangle^{2m+1}$, the bare terms can be represented concisely as the off-diagonal matrix element of

$$c^2[\tau^2\{\langle G_{ii}\rangle\}\langle \underline{G}_n\rangle + \tau^3\{\langle G_{ii}\rangle\}\langle \underline{G}_n\rangle^2 + \tau^4\{\langle G_{ii}\rangle\}\langle \underline{G}_n\rangle^3 + \cdots],$$

and thus Fig. 4 is given by

$$c^2\tau^2\{\langle G_{ii}\rangle\}\langle \underline{G}_n\rangle(1-\tau\{\langle G_{ii}\rangle\}\langle \underline{G}_n\rangle)^{-1}\big|_{\text{off diag}} = \underline{\Sigma}\{\underline{\Gamma}\}(1-\langle \underline{G}\rangle\underline{\Sigma}\{\underline{\Gamma}\})^{-1}\big|_{\text{off diag}} . \tag{17}$$

The diagonal matrix element $\Sigma_{ii}^{(2)}(j)$ together with the appropriate identities is shown in Fig. 5. We can again transpose the left-hand side and combine it with the correction terms on the right to obtain the diagonal matrix element of

$$-\underline{\Sigma}\{\underline{\Gamma}\}(1-\langle \underline{G}\rangle\underline{\Sigma}\{\underline{\Gamma}\})^{-1} .$$

The remaining bare terms are the pair series

$$c^2[\tau^5\{\langle G_{ii}\rangle\}\langle G_{ij}\rangle^4 + \tau^7\{\langle G_{ii}\rangle\}\langle G_{ij}\rangle^6 + \cdots)]$$

and the single-site terms

$$c^2\tau^3\{\langle G_{ii}\rangle\}\langle G_{ij}\rangle^2 + c\tau\{\langle G_{ii}\rangle\} .$$

These can be written as the diagonal matrix element of

$$c\tau\{\langle G_{ii}\rangle\} + c^2[\tau^3\{\langle G_{ii}\rangle\}\langle \underline{G}_n\rangle^2 + \tau^4\{\langle G_{ii}\rangle\}\langle \underline{G}_n\rangle^3 + \tau^5\{\langle G_{ii}\rangle\}\langle \underline{G}_n\rangle^4 + \cdots]$$

so that Fig. 5 is given by

$$c\tau\{\langle G_{ii}\rangle\} + c^2\tau^3\{\langle G_{ii}\rangle\}\langle \underline{G}_n\rangle^2(1-\tau\{\langle G_{ii}\rangle\}\langle \underline{G}_n\rangle)^{-1}\big|_{\text{diag}} = \underline{\Sigma}\{\underline{\Gamma}\}(1-\langle \underline{G}\rangle\underline{\Sigma}\{\underline{\Gamma}\})^{-1}\big|_{\text{diag}} . \tag{18}$$

Now $c\tau\{\langle G_{ii}\rangle\}$ is purely diagonal and $c^2\tau^2\{\langle G_{ii}\rangle\} \times \langle \underline{G}_n \rangle$ is purely off diagonal, so that we can combine (17) and (18) into the single matrix equation

$$\underline{\tau}^{(2)}\{\langle \underline{G}\rangle\} = \underline{\Sigma}\{\underline{\Gamma}\}(1 - \langle \underline{G}\rangle \underline{\Sigma}\{\underline{\Gamma}\})^{-1}\,, \tag{19}$$

where

$$\underline{\tau}^{(2)}\{\langle \underline{G}\rangle\} \equiv c\tau\{\langle G_{ii}\rangle\} + c^2\tau^2\{\langle G_{ii}\rangle\}\{\langle \underline{G}_n\rangle(1 - \tau\{\langle G_{ii}\rangle\}\{\langle \underline{G}_n\rangle)^{-1}\,. \tag{20}$$

Equation (19) can be written

$$\underline{\Sigma}\{\underline{\Gamma}\} = \underline{\tau}^{(2)}\{\langle \underline{G}\rangle\}(1 + \langle \underline{G}\rangle \underline{\tau}^{(2)}\{\langle \underline{G}\rangle\})^{-1}\,, \tag{21}$$

and to obtain $\underline{\Sigma}\{\langle \underline{G}\rangle\}$ we substitute (15b) for $\langle \underline{G}\rangle$ into (21) and then make the dummy variable replacement $\underline{\Gamma} \to \langle \underline{G}\rangle$, i.e.,

$$\underline{\Sigma} \equiv \underline{\Sigma}\{\langle \underline{G}\rangle\} = \underline{\tau}^{(2)}\{\underline{\Gamma}'\}(1 + \underline{\Gamma}'\,\underline{\tau}^{(2)}\{\underline{\Gamma}'\})^{-1}, \tag{22}$$

where[15]

$$\underline{\Gamma}' \equiv \langle \underline{G}\rangle(1 + \underline{\Sigma}\langle \underline{G}\rangle)^{-1}\,. \tag{23}$$

Other forms for $\underline{\Sigma}$ are possible; we can, for example, put it in the form of Eq. (63) of Ref. 10, except that $\underline{\eta}_2$ is now correctly given by

$$\underline{\eta}_2 = \tau^3\{\underline{\Gamma}'_d\}(\underline{\Gamma}'_n)^2(1 - \tau\{\underline{\Gamma}'_d\}\underline{\Gamma}'_n)^{-1} \tag{24}$$

rather than by Eq. (64) of Ref. 10.

One remark about the pair theory that was not sufficiently stressed in Alyer *et al.*[10] should be made here. Note that since the momentum representation for Σ involves $\Sigma^{(1)}$ and $\Sigma^{(2)}$ differently [cf. Eq. (8)], we must solve *both* (22) for $\underline{\Sigma}$ and (13) for $\Sigma^{(1)}$ to obtain $\underline{\Sigma}^{(2)} = \underline{\Sigma} - \underline{\Sigma}^{(1)}$. In principle (22) has to be solved for all pair separations R_{ij}; however, since $\Sigma_{ij}^{(2)}$ decays asymptotically as $\langle G_{ij}\rangle^3$, we can expect only small R_{ij} to contribute significantly except possibly at isolated energies near band edges.

V. CPA (n)

The diagrammatic derivation given in Sec. IV is quite involved, and, although in principle it could be extended to higher-order clusters, in practice the labor would be prohibitive. However, the structure of the various approximations suggests an alternative derivation which completely eliminates the need for a diagrammatic expansion and leads directly to a generalization of the CPA which we describe below.

We begin by noting that the approximations considered above are self-contained in the sense that the single-site corrections involve only single-site terms and not pairs, the pair corrections involve only single-sites and pairs and not triplets, and so on. Furthermore, the single-site rearrangement (Fig. 3) involves only the site i explicitly; the pair rearrangement (Figs. 4 and 5) involves explicitly only the sites i and j. That is to say, the expansion depicted in Figs. 3, 4, and 5 are purely "kinematic" expansions in that they represent identities between certain cumulant functions which correctly account for the fluctuations in the site energy levels. In these identities the internal propagators appear only incidentally as dummy variables so that each diagram simply defines a unique fuctional $\underline{\Sigma}\{\underline{x}\}$ and all the "dynamics" (by which we mean the effect of the rest of the lattice outside the cluster) is accounted for by setting $\underline{x} = \langle \underline{G}\rangle$.

Note also that the only approximation that one makes in the entire calculation is in truncating the series (8) for $\Sigma_{\mathfrak{F}}$. Thus if we formally restrict ourselves to a finite system, the series (8) becomes a finite series and the system of equations represented by the Dyson equation

$$\langle \underline{G}\rangle = \underline{g} + \underline{g}\,\underline{\Sigma}\langle \underline{G}\rangle \tag{25}$$

and the diagrammatic equations for

$$\underline{\Sigma} = \underline{\Sigma}\{\langle \underline{G}\rangle\}$$

become exact. Furthermore, in this finite system we can calculate $\langle \underline{G}\rangle$ in terms of $\underline{g}$ algebraically so that we can use (25) to define $\underline{\Sigma}\{\langle \underline{G}\rangle\}$; this enables us to calculate this functional *independently* of the diagrammatic summations.

The above remarks are best illustrated by example. Consider a one-site problem in which the exact G is given by the algebraic equation

$$G = g + g\epsilon_i g + g\epsilon_i g\epsilon_i g + \cdots = g(1 - \epsilon_i g)^{-1} \tag{26}$$

and the average G is simply

$$\langle G\rangle = \langle g(1 - \epsilon_i g)^{-1}\rangle. \tag{27}$$

Now (25) is the equation

$$g = \langle G\rangle(1 + \Sigma\langle G\rangle)^{-1}, \tag{28}$$

which if we substitute into (27) yields

$$\langle G\rangle = \langle \langle G\rangle[1 - (\epsilon_i - \Sigma)\langle G\rangle]^{-1}\rangle$$

or

$$\langle t\rangle = 0 \tag{29}$$

where

$$t \equiv (\epsilon_i - \Sigma)[1 - (\epsilon_i - \Sigma)\langle G\rangle]^{-1}\,. \tag{30}$$

This is the standard CPA result; for a system in which ϵ_i is v and 0 with probability c and $1 - c$, respectively, (29) becomes

$$\Sigma = cv[1 - (v - \Sigma)\langle G\rangle]^{-1}\,. \tag{31}$$

If we now put in the correct dynamics by interpreting the single-site $\langle G\rangle$ in (31) as the crystal $\langle G_{ii}\rangle$ we get exactly (13) for $\Sigma_{ii}^{(1)}$.

The extension to pairs is straightforward. We define

$$\underline{\epsilon} = \begin{pmatrix} \epsilon_i & 0 \\ 0 & \epsilon_j \end{pmatrix} \tag{32}$$

and use the definitions (14) for $\underline{\Sigma}$ and $\langle \underline{G} \rangle$. Then the arguments leading to (29) and (30) can be carried over with the simple replacement of all the numbers by their matrix analogs. We get

$$\langle \underline{t} \rangle = 0 , \tag{33}$$

where

$$\underline{t} = (\underline{\epsilon} - \underline{\Sigma})[1 - (\underline{\epsilon} - \underline{\Sigma})\langle \underline{G} \rangle]^{-1} \tag{34}$$

as the defining equation for $\underline{\Sigma}\{\langle \underline{G} \rangle\}$.

Equations (33) and (34) can be reduced exactly to the form (22) as follows: We rewrite the condition on the average t-matrix by multiplying (33) by $\langle \underline{G} \rangle$ and by adding 1 to both sides to get

$$1 = \langle [1 - (\underline{\epsilon} - \underline{\Sigma})\langle \underline{G} \rangle]^{-1} \rangle$$

$$= \langle (1 + \underline{\Sigma}\langle \underline{G} \rangle)^{-1} (1 - \underline{\epsilon}\,\underline{\Gamma}')^{-1} \rangle , \tag{35}$$

where we have used the definition (23) for $\underline{\Gamma}'$. The only fluctuations occur in the last factor on the right so that we rewrite (35) as

$$1 + \underline{\Sigma}\langle \underline{G} \rangle = \langle (1 - \underline{\epsilon}\,\underline{\Gamma}')^{-1} \rangle . \tag{36}$$

Now $\underline{\epsilon}$ is given by

$$\begin{pmatrix} v & 0 \\ 0 & v \end{pmatrix}, \quad \begin{pmatrix} v & 0 \\ 0 & 0 \end{pmatrix}, \quad \begin{pmatrix} 0 & 0 \\ 0 & v \end{pmatrix}, \quad \text{and} \quad \begin{pmatrix} 0 & 0 \\ 0 & 0 \end{pmatrix} ,$$

with probabilities c^2, $c(1-c)$, $c(1-c)$, and $(1-c)^2$, respectively. The first and last terms contribute

$$c^2(1 - v\underline{\Gamma}')^{-1} + (1-c)^2$$

to the average in (36). The remaining terms contribute

$$c(1-c)\left[1 + \begin{pmatrix} v & 0 \\ 0 & 0 \end{pmatrix}\underline{\Gamma}' + \begin{pmatrix} v & 0 \\ 0 & 0 \end{pmatrix}\underline{\Gamma}'\begin{pmatrix} v & 0 \\ 0 & 0 \end{pmatrix}\underline{\Gamma}' + \cdots \right.$$

$$\left. + 1 + \begin{pmatrix} 0 & 0 \\ 0 & v \end{pmatrix}\underline{\Gamma}' + \begin{pmatrix} 0 & 0 \\ 0 & v \end{pmatrix}\underline{\Gamma}'\begin{pmatrix} 0 & 0 \\ 0 & v \end{pmatrix}\underline{\Gamma}' + \cdots \right]$$

$$= c(1-c)\,[2 + v(1 - v\underline{\Gamma}_d')^{-1}\underline{\Gamma}'] ,$$

so that (36) becomes

$$1 + \underline{\Sigma}\langle \underline{G} \rangle = c^2(1 - v\underline{\Gamma}')^{-1} + (1-c)^2 + c(1-c)\,[2 + v(1 - v\underline{\Gamma}_d')^{-1}\underline{\Gamma}'] \tag{37}$$

or

$$\underline{\Sigma}\langle \underline{G} \rangle = c^2 v\underline{\Gamma}'\,(1 - v\underline{\Gamma}')^{-1} + c(1-c)v\,(1 - v\underline{\Gamma}_d')^{-1}\underline{\Gamma}'$$

If we now eliminate v in favor of τ and $\langle \underline{G} \rangle$ in favor of $\underline{\Gamma}'$ according to

$$v = \tau(1 + \underline{\Gamma}_d'\tau)^{-1} , \quad \langle \underline{G} \rangle = \underline{\Gamma}'(1 - \underline{\Sigma}\underline{\Gamma}')^{-1} , \tag{38}$$

we obtain

$$\underline{\Sigma}(1 - \underline{\Gamma}'\underline{\Sigma})^{-1} = c\tau + c^2\tau^2\underline{\Gamma}_n'(1 - \tau\underline{\Gamma}_n')^{-1} = \underline{\tau}^{(2)}\{\underline{\Gamma}'\}$$

or

$$\underline{\Sigma} = \underline{\tau}^{(2)}\{\underline{\Gamma}'\}(1 + \underline{\Gamma}'\underline{\tau}^{(2)}\{\underline{\Gamma}'\})^{-1} ,$$

which is (22). This completes our proof of the equivalence of the generalization of CPA to the diagrammatic techniques.

The extension of the CPA to larger clusters is fairly obvious and again is best discussed in terms of an example. For the triplet case we define $\underline{\Sigma}$ as a 3×3 matrix which consists of a triplet cluster and all possible pair and singlet clusters. That is, we define

$$\underline{\Sigma}^{(1)} = \begin{pmatrix} \Sigma_{ii}^{(1)} & 0 & 0 \\ 0 & \Sigma_{jj}^{(1)} & 0 \\ 0 & 0 & \Sigma_{kk}^{(1)} \end{pmatrix} , \quad \underline{\Sigma}^{(2)} = \begin{pmatrix} \Sigma_{ii}{}^{(2)}(j) + \Sigma_{ii}{}^{(2)}(k) & \Sigma_{ij}{}^{(2)} & \Sigma_{ik}{}^{(2)} \\ \Sigma_{ji}{}^{(2)} & \Sigma_{jj}{}^{(2)}(i) + \Sigma_{jj}{}^{(2)}(k) & \Sigma_{jk}{}^{(2)} \\ \Sigma_{ki}{}^{(2)} & \Sigma_{kj}{}^{(2)} & \Sigma_{kk}{}^{(2)}(i) + \Sigma_{kk}{}^{(2)}(j) \end{pmatrix} ,$$

and

$$\underline{\Sigma}^{(3)} = \begin{pmatrix} \Sigma_{ii}{}^{(3)}(j,k) & \Sigma_{ij}{}^{(3)}(k) & \Sigma_{ik}{}^{(3)}(j) \\ \Sigma_{ji}{}^{(3)}(k) & \Sigma_{jj}{}^{(3)}(i,k) & \Sigma_{jk}{}^{(3)}(i) \\ \Sigma_{ki}{}^{(3)}(j) & \Sigma_{kj}{}^{(3)}(i) & \Sigma_{kk}{}^{(3)}(i,j) \end{pmatrix} ,$$

Then, with the definitions

$$\underline{\Sigma} = \underline{\Sigma}^{(1)} + \underline{\Sigma}^{(2)} + \underline{\Sigma}^{(3)}$$

and

$$\underline{\epsilon} = \begin{pmatrix} \epsilon_i & 0 & 0 \\ 0 & \epsilon_j & 0 \\ 0 & 0 & \epsilon_k \end{pmatrix} , \quad \langle \underline{G} \rangle = \begin{pmatrix} \langle G_{ii} \rangle & \langle G_{ij} \rangle & \langle G_{ik} \rangle \\ \langle G_{ji} \rangle & \langle C_{jj} \rangle & \langle G_{jk} \rangle \\ \langle G_{ki} \rangle & \langle G_{kj} \rangle & \langle G_{kk} \rangle \end{pmatrix} ,$$

the CPA (3) again reads

$$\langle \underline{t} \rangle = \langle\langle (\underline{\epsilon} - \underline{\Sigma})[1 - (\underline{\epsilon} - \underline{\Sigma})\langle \underline{G} \rangle]^{-1} \rangle = 0 . \tag{39}$$

Note that we must satisfy the lower-order CPA conditions also so as to be able to separate $\underline{\Sigma}$ into its

$\underline{\Sigma}^{(1)}$, $\underline{\Sigma}^{(2)}$, and $\underline{\Sigma}^{(3)}$ parts for use in the series (8). General arguments can be given to justify the above generalization; we have also explicitly checked this particular form using the binary random-model system considered above.

One rather important comment regarding CPA (n) should be made here. We note that if we consider the disorder problem as a power series in v or c, then the first corrections to CPA are of order v^4 or c^2; the corrections to CPA (2) are of order v^6 or c^3; to CPA (3), v^8 or c^4; and so on. Now the increased accuracy in going from CPA to CPA (2) could only be achieved by going from the diagonal $\Sigma^{(1)}$ to the *completely off-diagonal* (in coordinate representation) $\Sigma^{(2)}$. What makes the method described above practical is that we do *not* deal anywhere with infinite (i.e., large) matrices. We can calculate *each* off-diagonal element of $\Sigma^{(2)}$ *separately* in a 2×2 subspace [cf. Eq. (22)].

It is exactly this point that can be expected to limit the usefulness of other generalizations of CPA. If one tries to overcome these difficulties by requiring only partial self-consistency, then of course, the accuracy of the method is lost. An explicit example of this can be seen in the work of Capek.[13] If one makes a perturbation expansion of his two-center approximation, one finds that the terms of order v^4 are not correctly counted.

VI. TWO-PARTICLE GREEN'S FUNCTION

We now turn to a discussion of one further generalization of the CPA which enables us to calculate the average two-particle Green's function $\langle G(E_1)\otimes G(E_2)\rangle$. Although our model Hamiltonian (1) describes noninteracting excitations, the averaging procedure introduces an effective interaction which can be described by an irreducible scattering kernel $I\{\langle G(E_1)\rangle, \langle G(E_2)\rangle\}$ that is related to the two-particle Green's function via

$$\langle G(E_1)\otimes G(E_2)\rangle = \langle G(E_1)\rangle\otimes\langle G(E_2)\rangle \times[1+I\{\langle G(E_1)\rangle, \langle G(E_2)\rangle\}\langle G(E_1)\otimes G(E_2)\rangle] . \quad (40)$$

A diagrammatic representation of I is shown in Fig. 6 and, just as for the self-energy, we would like to obtain single-site, two-site, etc, approximations.

The single-site approximation has been obtained previously; Velicky[16] has shown that $I^{(1)}$ is given by the solution of the algebraic equation

$$\langle t(E_1)t(E_2)\rangle = I^{(1)}[1-\langle G(E_1)\rangle\langle G(E_2)\rangle I^{(1)}]^{-1} , \quad (41)$$

where $t(E)$ is given by (30), and $\langle G(E)\rangle = \langle G_{ii}\rangle$. To obtain $I^{(2)}$ we define $\underline{I}=\underline{I}^{(1)}+\underline{I}^{(2)}$, where now $\underline{I}$ is a 16-component tensor in the coordinate subspace $\{i,j\}$. The generalization of (41) is

$$\langle \underline{t}(E_1)\otimes\underline{t}(E_2)\rangle = \underline{I}[1-\langle\underline{G}(E_1)\rangle\otimes\langle\underline{G}(E_2)\rangle\underline{I}]^{-1} , \quad (42)$$

where $\underline{t}(E)$ is given by (34) and $\langle\underline{G}(E)\rangle$ by (14). Equation (42) can be verified by arguments similar to those leading to CPA (2) or by checking directly with the diagrammatic expansion shown in Fig. 6. However, even given $\underline{I}$ as in (42), since the solution of (40) is nontrivial [i.e., (40) is an integral equation in momentum space] we will not pursue this development further.

VII. CONCLUSIONS AND SUMMARY

We have interpreted the corrected-cumulant or self-contained approximation for pairs and higher-order clusters and shown how to derive explicit expressions for the weight factors associated with each term in the diagrammatic expansion of the self-energy. We have then related this method to the diagrammatic expansion of Leath[4] and have clarified (and corrected) the self-consistent pair treatment of Aiyer *et al.*[10] The essential point here is that one cannot arbitrarily separate pair scatterings from single-site scatterings—to consistently sum up pair effects one must also allow for all possible single-site scatterings in the intermediate states. We have achieved this self-consistency by adding in certain single-site scattering relations as identities into the equations for the pair terms before we perform the diagrammatic resummations.

The main point of the above discussion, however, has been to show that all these rather complicated diagrammatic techniques can be very concisely represented by a simple CPA-like algebraic condition. The CPA (2) condition for pairs, for example, requires that an average two-center t matrix be zero for every pair of sites in the system independently of all the rest. Thus one never deals with anything more complicated than a simple 2×2 matrix. Another important point is that one must simultaneously satisfy the lower-order single-site CPA condition to consistently separate

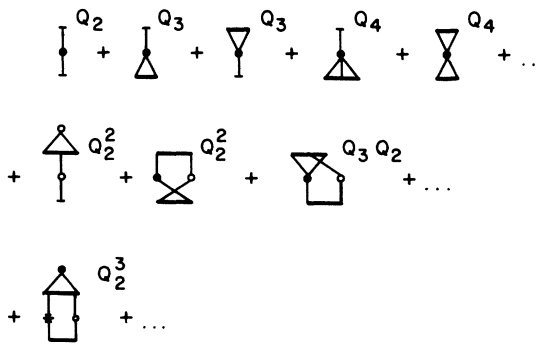

FIG. 6. Representation of $I\{\langle G(E_1)\rangle, \langle G(E_2)\rangle\}$ as an expansion in single-site terms, pairs, triplets, etc.

pair and single-site effects. In general, if we wish to go to the nth cluster approximation we must simultaneously satisfy all CPA (m), $m \leq n$, conditions.

Finally, we have shown that this method can be easily extended to evaluate average two-particle Green's functions.

Note added in proof. The recent work of Cyrot-Lackmann and Ducastelle [Phys. Rev. Letters 27, 429 (1971)] is different from the diagrammatic expansion given above. In particular, a perturbation expansion of their equation (26) shows that beginning at order v^6 and c^3, their self-energy contains terms which correspond to *removing* pair renormalizations of the internal lines in $\Sigma^{(1)}$. The net result is that the $\langle \underline{G}_{ii} \rangle$ which appears in $\Sigma_{ii}^{(1)}$ is not the fully renormalized $\langle \underline{G} \rangle$ given by the solution of the Dyson equation (i.e., Eq. 6′ with Σ containing *both* single site and pair terms). There are other differences beginning at order v^8 and c^4 which do not appear to have any such simple explanation. A detailed comparison of the two methods has been made by Ducastelle. We wish to express our gratitude to Dr. Ducastelle for communicating these results to us prior to their publication.

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[15]Note the different signs in Eqs. (23) and (15a). Also the self-energy in (23) is $\underline{\Sigma} \equiv \underline{\Sigma}\{\langle \underline{G} \rangle\}$; (15) involves $\underline{\Sigma}\{\underline{\Gamma}\}$.

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Electronic States in a Disordered Binary Alloy

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The electronic structure of a disordered binary alloy is discussed by using the method of Matsubara and Yonezawa. The self-energy is evaluated in a first-order approximation. The theory is applied to a model alloy where the host is assumed to possess a semicircular density of states. We also calculate the density of states for α-brass, by using the available density-of-states curve for copper.

I. INTRODUCTION

The behavior of electrons in disordered materials raises very complex problems, and recently this has been the subject of intensive investigations from many points of view. There have been several attempts to formulate a theory for alloys across the whole range of concentrations of solute atoms. Initially a number of simple but crude models were proposed.[1-3] The rigid-band approximation[1] is the earliest model and is based on a perturbative approach. In this approximation it is assumed that the constant energy surfaces and the density-of-states curve of the solvent remain unchanged on alloying, the only effect of the addition of solute atoms being, if its valency is greater than that of the solvent, to add electrons to the band, thus swelling the Fermi surface and filling the density-of-states curve to a higher energy.[2] Sometimes the virtual crystal approximation (VCA)[3] is used to interpret experimental results. In the VCA one approximates a disordered alloy by an equivalent ordered alloy wherein every site is assigned a potential equal to the concentration-weighted aver-