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Analysis of effective-medium approximation for a tight-binding model of a liquid metal

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The perturbation expansion for the electronic structure of a tight-binding model of a liquid metal is studied by means of a diagram analysis. The previously developed effective-medium approximation is shown to correspond to the summation of the same terms as occur in Soven's coherent-potential approximation for alloys, within the validity of a generalized Kirkwood superposition approximation for ionic distribution functions. The terms omitted are shown to be of higher order in $1/\bar{z}$, with $\bar{z}$ an effective neighbor number. The results are extended to cover liquid alloys and solid alloys with short-range order and off-diagonal disorder, the latter results agreeing with work of Blackman *et al.* The conclusions apply also to a general model of a liquid metal.

I. INTRODUCTION

Recently we have developed an effective-medium theory[1,2] (EMA) for the electronic structure of liquid metals, based on multiple scattering theory.[3-5] We believe that the EMA is the appropriate generalization of the coherent-potential approximation[6,7] (CPA), which has been so useful for alloys, to the liquid-metal case. We have applied this theory to a tight-binding model[8,9] which has been previously studied by Beeby and Edwards,[10] and Cyrot-Lackmann,[11] and more recently by Ishida and Yonezawa,[12] whose work was based on the work of Matsubara and Toyazawa[13] for the random case appropriate to impurity bands. We found that within the Kirkwood superposition approximation for particle distribution functions, the first and second moments of the spectral function,[8,9] giving the position and width of the quasiparticle resonance, are given correctly by the EMA, and furthermore that it reduces to the CPA in the alloy case.

The above work[1,2] indicated that the present theory is an improvement over several previous attempts[5,12,14] to extend the CPA to correlated liquid metals. For the random liquid metal this and the other theories reduce to the result obtained by Faulkner[15] and Klauder[16] for the general multiple scattering case and by Matsubara and Toyazawa[13] for the tight-binding model. However, it seemed desirable to study further the relationship of the EMA to the CPA and to other theories.

In this paper we shall analyze the EMA for the tight-binding model in greater detail. We shall develop a diagramatic representation[17] for the locator expansion for the one-particle continuum Green's function. This will show clearly which terms are included in the EMA and which are not. In fact we shall find that the structure of the expansion is exactly the same to all orders as that for the CPA. We can also use the diagrams to determine which moments of the density of states are conserved by the theory, and to compare with other results.

The CPA was shown by Schwartz and Siggia[18] to correspond in some sense to an expansion in $1/z$, where z is the number of neighbors in a nearest-neighbor tight-binding model. We shall define an analogous quantity $\bar{z}$ for the liquid-metal case, and shall show that such an expansion applies here also. That is, for certain energies the omitted terms in the self-energy are of order $1/\bar{z}^2$ while those kept are of order 1 and $1/\bar{z}$.

The present formulation and diagram expansion can be used to generalize the CPA to include short-range-order effects. We also formulate the liquid-alloy problem including "off-diagonal disorder," using the ideas of Blackman, Esterling, and Beck[19] and Movaghar, Miller, and Bennemann,[20] and show that it reduces to the result of Blackman *et al.* for the random-alloy case.

In Sec. II we develop the diagram expansion and obtain the EMA. In Sec. III we study several properties of the result: moments, the identification with the alloy case, and the $1/\bar{z}$ expansion. In Sec. IV we discuss the generalization to include short-range order and off-diagonal disorder in solid and liquid alloys. Finally we discuss the implications of our findings in Sec. V.

We have performed numerical calculations for the EMA for several pair distribution functions. These will be reported in a subsequent paper, in which the EMA will be compared primarily with the simpler Ishida-Yonazawa theory.

II. DIAGRAM APPROACH TO TIGHT-BINDING MODEL

We examine here the tight-binding model which we have developed in previous work.[8,9] The Green's function G_t is assumed to be expandable in terms of atomic orbitals, one for each site:

$$G_t(\vec{r},\vec{r}\,')=\sum_{ij}\phi(\vec{r}-\vec{R}_i)G_{ij}\phi(\vec{r}\,'-\vec{R}_j)\,, \qquad (2.1)$$

and G_{ij} is assumed to obey the equation

$$(\omega-H_0)G_{ij}-\sum_{l\neq i}H'(\vec{R}_{il})G_{lj}=\delta_{ij}\,, \qquad (2.2)$$

where

$$H'(\vec{R}_{ij})=H(\vec{R}_{ij})-\omega S(\vec{R}_{ij})\,,$$

with H a transfer integral and S an overlap integral between the atomic functions. For most of what follows we take $H_0=0$ and, for $i\neq j$, $S(R_{ij})=0$; i.e., we consider the case of orthogonal orbitals. We have already discussed some effects of nonorthogonality[9] and we shall examine it further in a subsequent paper.

We consider now the continuum Green's function:

$$G(\vec{R},\vec{R}\,')=\Big\langle\sum_{ij}\rho_i(\vec{R})G_{ij}\rho_j(\vec{R}\,')\Big\rangle\,, \qquad (2.3)$$

where $\rho_i(\vec{R})=\delta(\vec{R}-\vec{R}_i)$ is the density of the ith ion at R, and the average is over all configurations of the system. G has the expansion

$$\begin{aligned}G(\mathrm{R}-\mathrm{R}')={}&\frac{\delta(\vec{R}-\vec{R}\,')}{\omega}\Big\langle\sum_i\rho_i(\vec{R})\Big\rangle\\&+\frac{1}{\omega^2}\Big\langle{\sum_{ij}}'\rho_i(\vec{R})\rho_j(\vec{R}\,')\Big\rangle H(\vec{R}-\vec{R}\,')\\&+\frac{1}{\omega^3}\int\Big\langle{\sum_{ijl}}'\rho_i(\vec{R})\rho_j(\vec{R}\,'')\rho_l(\vec{R}\,')\Big\rangle\\&\times H(\vec{R}-\vec{R}\,'')H(\vec{R}\,''-\vec{R}\,')d\vec{R}\,''+\cdots\,.\end{aligned} \qquad (2.4)$$

Here the prime indicates that neighboring indices are never equal.

For density correlation functions in which no two particles are the same, we write

$$\Big\langle{\sum_{i_1\cdots i_p}}''\rho_{i_1}(\vec{R}_1)\cdots\rho_{i_p}(\vec{R}_p)\Big\rangle=n^p g(\vec{R}_1,\ldots,\vec{R}_p)\,, \qquad (2.5)$$

where g is a p-particle distribution function. The most familiar example is the pair distribution function (PDF) $g(\vec{R},\vec{R}\,')=g(\vec{R}-\vec{R}\,')$. In this article we shall make the assumption that the p-body distribution function can be decomposed into $p(p-1)/2$ PDF's; i.e., we shall use a generalized Kirkwood superposition approximation. This approximation has been discussed at length in terms of the three-body distribution function.[21] It has the happy feature that hard-core exclusions are treated properly. We can represent the various terms in Eq. (2.5), and in particular the various equalities among indices, by diagrams which are essentially those introduced by Cyrot-Lackmann[11] and Ishida and Yonezawa.[12] They are illustrated in Figs. 1(a) and 1(b). Each of p distinct ions is represented by a point, and each of m hopping integrals by a directed line, which follows a continuous sequence from the first point ($\vec{R}$) to the last point ($\vec{R}\,'$). We can think of the sequence of hops as being numbered. Some diagrams are closed—these have a factor $\delta(\vec{R}-\vec{R}\,')$. The point $\vec{R}$ is indicated by an open circle in these graphs to avoid confusion. Each diagram has a factor n^p/ω^{m+1}. There are PDF's connecting each pair of points and we represent these by dashed lines. Some of the PDF's occur with a hopping integral. These chain correlations are indicated by using a dashed line along with a solid line to represent $\tilde{H}(\vec{R})=g(\vec{R})H(\vec{R})$ [Fig. 1(c)]. The remaining PDF's represent out of chain correlations. The diagrams in Fig. 1(a) represent the series

$$\begin{aligned}&\frac{n}{\omega}\delta(\vec{R}-\vec{R}\,')+\frac{n^2}{\omega^2}\tilde{H}(\vec{R}-\vec{R}\,')\\&\quad+\frac{n^2}{\omega^3}\delta(\vec{R}-\vec{R}\,')\int\tilde{H}(\vec{R}-\vec{R}\,'')H(\vec{R}\,''-\vec{R})d\vec{R}\,''\\&\quad+\frac{n^3}{\omega^3}g(\vec{R}-\vec{R}\,')\int\tilde{H}(\vec{R}-\vec{R}\,'')\tilde{H}(\vec{R}\,''-\vec{R}\,')d\vec{R}\,''\\&\quad+\frac{n^3}{\omega^4}\delta(\vec{R}-\vec{R}\,')\int\tilde{H}(\vec{R}-\vec{R}\,'')\tilde{H}(\vec{R}\,''-\vec{R}\,''')\\&\quad\times\tilde{H}(\vec{R}\,'''-\vec{R})d\vec{R}\,''d\vec{R}\,'''\,.\end{aligned} \qquad (2.6)$$

Notice that in the third term we need only one PDF, so we have one $\tilde{H}$ and one H. We next decompose the out-of-chain correlation by letting $g(\vec{R})=1+h(\vec{R})$, with h represented by a dotted line. This is illustrated in Figs. 1(d) and 1(e). The correlation between a pair of points is neglected in the first term on the right-hand side, and the h line in the second term puts in the correlation.

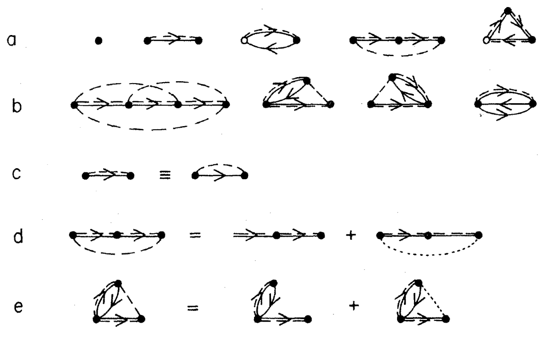

FIG. 1. Diagrams in expansion of $G(\vec{R},\vec{R}\,')$ (see text).

Thus Fig. 1(d) represents

$$\frac{n^3}{\omega^3}\int \tilde{H}(\vec{R}-\vec{R}'')\tilde{H}(\vec{R}''-\vec{R}')d\vec{R}'' + \frac{n^3}{\omega}h(\vec{R}-\vec{R}')\int \tilde{H}(\vec{R}-\vec{R}'')\tilde{H}(\vec{R}''-\vec{R}')d\vec{R}''.$$

The h line corresponds to the multiple-occupancy corrections in the CPA. From now on we regard this decomposition as having been made. However, sometimes we use dashed lines as a shorthand way of drawing several diagrams at once.

We can now make several exact reductions of the diagrams. Consider first the closed diagrams such as appear in Fig. 2(a). Some of these diagrams fall into two or more parts upon removing the point $\vec{R}$. Let us call these unlinked, and those which do not fall apart we shall call linked. Note that the presence of an h line can make a diagram linked. Then we call the sum of the linked parts Σ_d:

$$\Sigma_d=\frac{1}{\omega}\int \tilde{H}(\vec{R}-\vec{R}')H(\vec{R}'-\vec{R})d\vec{R}+\cdots. \qquad (2.7)$$

We omit a factor $(n/\omega^2)\delta(\vec{R}-\vec{R}')$, symbolized by omitting the open circle. [Note, however, that there can be internal locators associated with the point $\vec{R}$, as in the fourth diagram in Fig. 2(b).] The whole series of closed diagrams can be generated by a geometric series in powers of Σ_d, as indicated in Fig. 2(c). The diagonal part of $G(\vec{R},\vec{R}')$ is then $nG_d\,\delta(\vec{R}-\vec{R}')$, where

$$G_d=(\omega-\Sigma_d)^{-1}. \qquad (2.8)$$

Consider now the nondiagonal part of G—the open diagrams. Let us call a diagram reducible if there are attached to a point in the diagram any closed parts which are not connected to any other part of the diagram, even by an h line. Otherwise the diagram is irreducible. For example, the first diagram of Fig. 1(e) is reducible and the second irreducible. In reducible diagrams, the closed parts attached at just one point can be factored off. We can add up a series of diagrams with all possible closed loops attached to, say, the beginning of a diagram, and the sum is the same as the sum of all closed diagrams. This just renormalizes the locator $1/\omega$, i.e., replaces it by $G_d=(\omega-\Sigma_d)^{-1}$ [Fig. 2(a) or 2(c)]. Consider an irreducible diagram. In addition to the initial $1/\omega$ factor, it acquires a factor $1/\omega$ whenever a line goes into an internal point, as in Fig. 2(d), or the end point. Before the line leaves an internal point for other parts, we can add in all closed parts and renormalize this locator. If another line comes into the same point it contributes another factor $1/\omega$ which can also be renormalized [see Fig. 2(e)]. Similarly, final locators can be renormalized, and as indicated above, the initial one. Thus we replace the original perturbation sum by a sum over only irreducible diagrams, and we renormalize all locators. This is indicated by putting circles around all points of an irreducible diagram. In the same manner, in the summation for Σ_d, we include only irreducible Σ parts, and we renormalize all internal locators [the last diagram in Fig. 2(b) is reducible].

Looking again at the open diagrams, we define a node as a point such that when it is removed the diagram falls into two parts, and the sequence of hoppings is broken only once. Thus on the right-hand side of Fig. 1(d) the first diagram has a node while the second does not. Figure 3(a) is ambiguous unless we actually number the hopping sequence, in which case the first diagram has a node and the second does not. We can then write G in a geometric series in terms of a renormalized interaction part $M(\vec{R}-\vec{R}')$, which has no nodes.

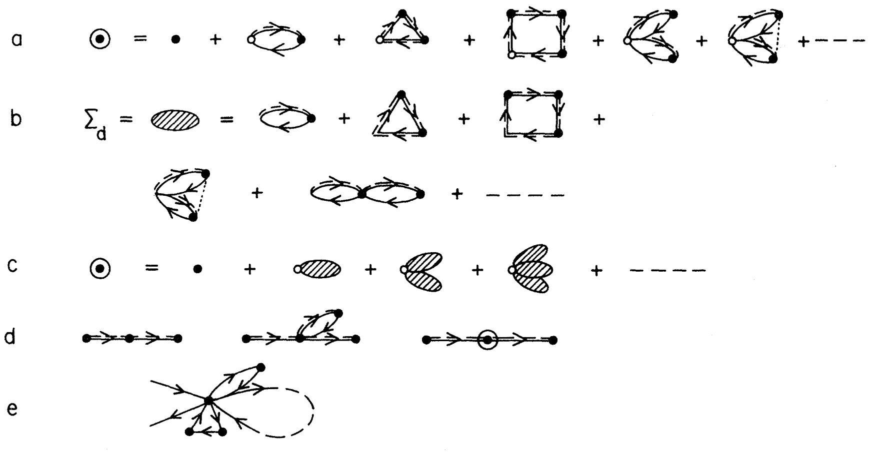

FIG. 2. Renormalization of locators.

This is indicated by a heavy line, and the series for G is shown in Fig. 3(b). If we Fourier transform G, we clearly have

$$G_{\vec{k}} = n(\omega - \Sigma_d - nM_{\vec{k}})^{-1} . \qquad (2.9)$$

The actual diagrams in $M_{\vec{k}}$ will be considered shortly. First let us obtain an exact expression for Σ_d in terms of $G_{\vec{k}}$ and $M_{\vec{k}}$. For after going from site i to site j—the first point—the perturbation sequence back to i is exactly the same as that in the open diagrams of G. Therefore we have exactly, upon Fourier-transforming the convolution product,

$$\Sigma_d = \int H_{\vec{k}} G_{\vec{k}} M_{\vec{k}} \, d\vec{k}/8\pi^3 . \qquad (2.10)$$

This is illustrated in Fig. 3(c).

What remains now is to examine $M_{\vec{k}}$. Figure 3(e) gives the first two orders of contribution of $M_{\vec{k}}$. The first-order term is simply

$$\tilde{H}_{\vec{k}} = \int g(\vec{R}) H(\vec{R}) e^{i\vec{k}\cdot\vec{R}} \, d\vec{R} . \qquad (2.11)$$

The second order is interesting in that it has a similar structure to a contribution to Σ_d. In fact we can add a whole sequence of terms to this, as shown in Fig. 3(f). Let us call this $(1/n)\Sigma_{1\vec{k}}$:

$$\frac{1}{n}\Sigma_{1\vec{k}} = \int h(\vec{k} - \vec{k}') M^2_{\vec{k}'} G_{\vec{k}'} \, d\vec{k}'/8\pi^3 . \qquad (2.12)$$

$\Sigma_{1\vec{k}}$ consists of all interaction diagrams with an h line which when it is removed have at least one node. The attachments here have essentially the same structure of those for Σ_d—the only difference being in counting because Σ_d is closed. The remainder of $M_{\vec{k}}$ we designate Σ_{2k}/n, so that

$$M_{\vec{k}} = \tilde{H}_{\vec{k}} + \frac{1}{n}\Sigma_{1\vec{k}} + \frac{1}{n}\Sigma_{2\vec{k}} . \qquad (2.13)$$

$(1/n)\Sigma_{2\vec{k}}$ corresponds to all $M_{\vec{k}}$ diagrams other than $\tilde{H}_{\vec{k}}$ which have no nodes even on cutting an h line between $\vec{R}$ and $\vec{R}'$. Figure 2(g) gives the contributions to $\Sigma_{2\vec{k}}$ in third order, there being none in the first and second orders. We see that the first term involves repeating scatterings between two sites, and the remainder are analogous but with equality of sites being replaced by correlations between ions. In Sec. III C we shall define an effective number of neighbors $\bar{z}$, i.e., the number of ions interacted with, and show that this type of term is smaller than $H_{\vec{k}}$ by $1/\bar{z}^2$. At any rate, to obtain the EMA we neglect Σ_2. We then have the set of equations

$$G_{\vec{k}} = n(\omega - \Sigma_d - nM_{\vec{k}})^{-1} , \qquad (2.14)$$

$$M_{\vec{k}} = n\tilde{H}_{\vec{k}} + \Sigma_{1\vec{k}} , \qquad (2.15)$$

$$\Sigma_d = \int H_{\vec{k}} G_{\vec{k}} M_{\vec{k}} \, d\vec{k}/8\pi^3 \qquad (2.16a)$$

$$= (\omega - \Sigma_d)^{-1} \int n\tilde{H}_{\vec{k}} (H_k + M_k^2 G_k) \, d\vec{k}/8\pi^3 , \qquad (2.16b)$$

$$\Sigma_{1\vec{k}} = n \int h(\vec{k} - \vec{k}') M^2_{\vec{k}'} G_{\vec{k}'} \, d\vec{k}'/8\pi^3 . \qquad (2.17)$$

If we identify Σ_d with Σ_∞ this is exactly our previous result.[1,2] The second form of Eq. (2.16) is illustrated in Fig. 3(g).

III. ANALYSIS OF EFFECTIVE-MEDIUM-APPROXIMATION RESULT

A. Terms which are included in the EMA; moments

With the diagram construction we can now readily expand the EMA Green's function in powers of the hopping integral and compare with the exact ex-

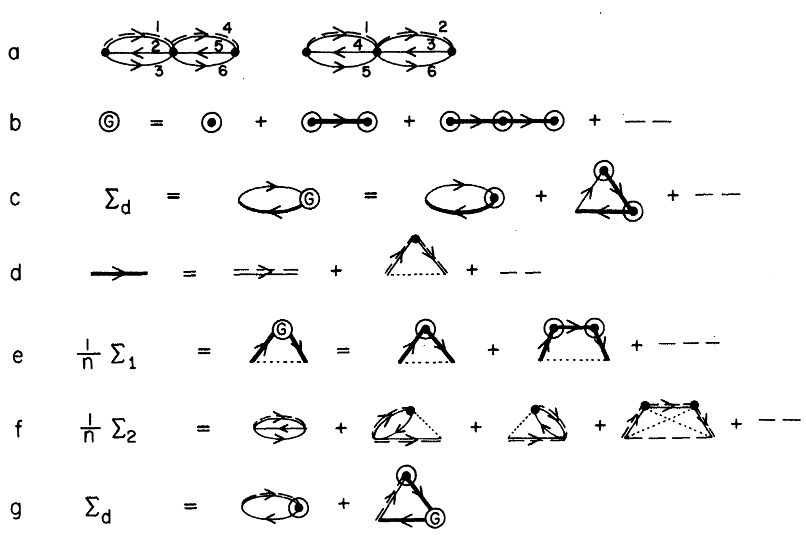

FIG. 3. Renormalization of interactors and locators.

pansion. As noted in our previous work, the coefficient of $\omega^{-(n+1)}$ is the nth moment $\omega_{\vec{k}}^{(n)}$ of the spectral function $(-1/\pi)\operatorname{Im}G_{\vec{k}}$, which for general $\vec{k}$ is a quasiparticle resonance. The coefficients in the $1/\omega$ expansion for the diagonal matrix element G_d are the moments of the density of states per ion. Thus

$$G_{\vec{k}} = \sum_n \omega_{\vec{k}}^{(n)} / \omega^{n+1} , \tag{3.1}$$

$$G_d = \frac{\sum_n \omega^{(n)}}{\omega^{n+1}} = \frac{1}{n} \lim_{k \to \infty} G_{\vec{k}} . \tag{3.2}$$

This applies in particular to the case of orthogonal orbitals. For nonorthogonal orbitals there is no simple expression for the moments.

We summarize the first two orders in $H_{\vec{k}}$ in Fig. 4(a). As noted previously our theory is exact to this order, to within the Kirkwood approximation. The third-order terms which are kept are shown in Fig. 4(b), while those which are not are given in Fig. 4(c). The latter are just the first contribution to Σ_2 [Fig. 3(f)] and correspond to repeated scatterings between two sites, or h lines which cross, or, for the middle two, correlations between different parts of a diagram tied together at a point. These processes are not single-site processes and are not included. The terms which are kept have a basic chain structure (or for diagonal elements, ring structure) with renormalized points and renormalized interaction lines.

In fourth order we have considered only the closed diagrams corresponding to the moments of the density of states. The first three moments of the density of states are given exactly,

$$\omega^{(0)} = 1 , \tag{3.3}$$

$$\omega^{(1)} = 0 , \tag{3.4}$$

$$\omega^{(2)} = n \int \tilde{H}_{\vec{k}} H_{\vec{k}} \, dk / 8\pi^3 , \tag{3.5}$$

$$\omega^{(3)} = n^2 \int \tilde{H}_{\vec{k}}^3 \, dk / 8\pi^3 , \tag{3.6}$$

while approximations begin in the fourth moment, in which the terms in Fig. 4(d) are kept and those in 4(e) are omitted. Again we see a ring structure with renormalized vertices and interaction lines, and with h lines which do not cross. The last diagram in Fig. 4(d) is unlinked and is a contribution to Σ_d^2. The omitted diagrams have a structure similar to those omitted in the third-order open diagrams—arising from the same four diagrams of Σ_2, namely, diagrams with repeated scatterings between two sites, correlations between parts of a diagram tied together by a point and h lines which cross.

Before discussing this further let us consider the alloy and lattice liquid cases.

B. Relation to coherent-potential approximation for the alloy

In our previous article[1] we showed that the single-site arguments leading to the effective-medium approximation also give rise to the CPA when applied to the alloy problem. The proof was actually for the T-matrix expansion. For the locator case the proof is virtually identical and corresponds to Shiba's[22] treatment of the CPA.

Here we will show that our equations go directly over into the CPA for the lattice case and that the diagram expansion is the same as the CPA. Let us first examine the lattice liquid, in which we assume that the ions occupy a fraction x of the sites of a lattice. This corresponds to the split-band limit[7] of the alloy problem and is a simple model of an impurity band. We replace the continuous variable $\vec{R}$ by a discrete variable $\vec{R}$, and this means that we restrict the k integral to one Brillouin zone. The density n becomes the fraction x of occupied sites. The energy function is simply the band energy for the pure solid,

$$\tilde{H}_k = H_{\vec{k}} = \epsilon_{\vec{k}} = \sum_{\vec{R} \neq 0} e^{i\vec{k}\cdot\vec{R}} H_{\vec{R}} , \tag{3.7}$$

where $\vec{R}$ goes over lattice sites, and, assuming that the alloy is random, the pair distribution function $g_{ij} = 1 - \delta_{ij}$ merely excludes multiple occupancy of sites. The superposition approximation is actually exact for the lattice, so that the diagram expansion applies exactly. We have in the EMA

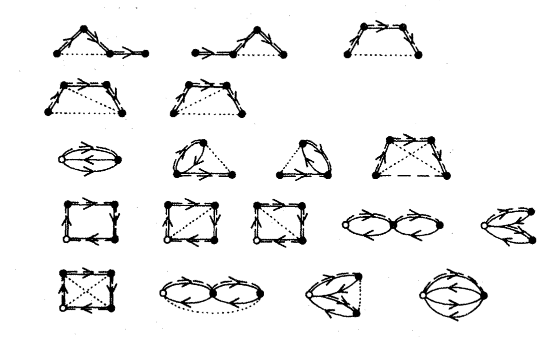

FIG. 4. Diagram expansion of G showing what is included in EMA [(a), (b), and (d)].

$$G_{\vec{k}} = x(\omega - \Sigma_d - xM_{\vec{k}})^{-1}, \tag{3.8}$$

$$\Sigma_d = N^{-1} \sum_{\vec{k}} \epsilon_{\vec{k}} G_{\vec{k}} M_{\vec{k}}, \tag{3.9}$$

$$M_{\vec{k}} = \epsilon_{\vec{k}} + \Sigma_1 / x, \tag{3.10}$$

$$\frac{\Sigma_1}{x} = -N^{-1} \sum_{\vec{k}} M_{\vec{k}}^2 G_{\vec{k}}. \tag{3.11}$$

We have written the $\vec{k}$ integral as a sum, which is the usual notation.

We notice that Σ_1 is a constant for the lattice liquid. If we sum Eq. (3.10) over k, the ϵ_k term cancels from Eq. (3.7), and combining this with Eq. (3.11) we have

$$\frac{1}{N} \sum_{\vec{k}} M_{\vec{k}} (1 + M_{\vec{k}} G_{\vec{k}}) = 0. \tag{3.12}$$

Substituting for $M_{\vec{k}}$ from Eq. (3.8) we find

$$\frac{x}{\omega - \Sigma_d} = \frac{1}{N} \sum_{\vec{k}} G_{\vec{k}} \equiv F. \tag{3.13}$$

Thus the renormalized locator, weighted by the fractional occupation of sites, is the diagonal matrix element of G in a site representation.

To evaluate Σ_1, we have from Eqs. (3.9)–(3.11)

$$\frac{\Sigma_1}{x} + \Sigma_d = N^{-1} \sum_{\vec{k}} \frac{\Sigma_1}{x} M_{\vec{k}} G_{\vec{k}} = 0. \tag{3.14}$$

The last equality results from Eqs. (3.8) and (3.13), because $M_{\vec{k}} G_{\vec{k}} = F^{-1}(G_{\vec{k}} - F)$ is proportional to the off-diagonal part of G in a site representation. Thus the Green's function can be expressed as

$$G_{\vec{k}} = (F^{-1} - G_{\vec{k}} + \Sigma_d)^{-1}, \tag{3.15}$$

with Σ_d determined self-consistently from Eq. (3.13).

To make the result look more familiar we replace $F^{-1} + \Sigma_d$ by $\omega - \Sigma$, and we have

$$G_k = (\omega - \Sigma - \epsilon_k)^{-1}, \tag{3.16}$$

$$\Sigma = -(1 - x)/F, \tag{3.17}$$

which is the split-band limit of the CPA.[7] For $x = 1$, Σ vanishes—this is the pure-solid case.

To show that the result is also the CPA for the random-alloy case, we now can take $x = 1$, but we must perform an average over components. We restore the diagonal energies and replace Eq. (3.13) by

$$F = \langle G_d \rangle = \frac{x}{\omega - \epsilon_A - \Sigma_d} + \frac{1 - x}{\omega - \epsilon_B - \Sigma_d} \tag{3.18}$$

assuming a fraction x of the sites to be occupied by the A atoms and $1 - x$ by B atoms. Equation (3.15) still holds for $G_{\vec{k}}$. The more usual form is again obtained by replacing $F^{-1} + \Sigma_d$ by $\omega - \Sigma$, in which case

$$\Sigma = x\epsilon_A + (1 - x)\epsilon_B - (\epsilon_A - \Sigma)(\epsilon_B - \Sigma)F, \tag{3.19}$$

which is the CPA result.[7]

In diagrammatic derivations of the CPA, Yonezawa[23] and Leath[24] have emphasized the importance of multiple-occupancy corrections. The present diagram representation[17] is actually a compact and convenient one for the locator expansion in the alloy problem—or for that matter the entirely analogous T-matrix expansion. In the present scheme the multiple-occupancy corrections are given by the h lines in the diagrams and what we have found is that these multiple-occupancy corrections can be included by renormalizing the interaction lines. There is a similarity between our approach and that of Blackman, Esterling, and Beck,[19] who use a locator expansion and a functional technique for summing the single-site terms.

The importance of the present section for the liquid-metal case is that we have shown that to all orders the terms in the perturbation expansion included in the EMA are exactly the same as those included for the alloy. Before going on to discuss these results further, we would like to raise one point in interpreting the diagram expansion of the alloy case. We can, as stated earlier, use the same diagram expansion for the alloy as the liquid or lattice liquid. If we go beyond the single-site approximation we have to notice that in $\Sigma_{2\vec{k}}$ there is a dependence on which type of site is at the beginning and end, because internal locators can occur at those sites. We are not allowed to average out this dependence. Σ_2 therefore is really $\Sigma_2^{ss'}$, using the notation of Sec. IV; i.e., it is a 2×2 matrix for the binary alloy, solid or liquid. In Sec. IV we include a species dependence of $H_{\vec{k}}$ and so the machinery for including this dependence in Σ_2 is available.

C. $1/z$ argument

Schwartz and Siggia[18] showed by means of their diagram technique that the CPA represents in some sense an expansion in $1/z$, where z is the number of nearest neighbors. We find it possible to give a similar argument for the liquid metal in the tight-binding model. Actually Matsubara and Toyazawa[13] give an argument to show that their result is a high-density approximation.

We must first define a neighbor number $\overline{z}$. We wish to regard the system as though the hopping integral were a constant $\overline{H}$, and the number of neighbors were $\overline{z}$. If this were the case, then summing H and H^2 over neighbors would give

$$\overline{H}\overline{z} = \int ng(\vec{R}) H(\vec{R}) \, d\vec{R}, \tag{3.20}$$

$$\overline{H}^2 \overline{z} = \int ng(\vec{R}) H^2(\vec{R}) \, d\vec{R}. \tag{3.21}$$

While these relations are exact only for an actual nearest-neighbor model, we can use the two equations to define an effective $\bar{H}$ and $\bar{z}$. $\bar{H}\bar{z}$ gives, incidentally, an estimate of the bandwidth.

Consider now the perturbation expansion. We can compare the $1/\bar{z}$ dependence of the terms in G^{-1}: $n\tilde{H}_k$, Σ_d, Σ_1, and Σ_2. Let us do this for small k. Then $n\tilde{H}_{k=0}=\bar{z}\bar{H}$ by definition. The first term in the expansion for Σ_d is

$$\frac{n}{\omega}\int H^2(\vec{R})g(\vec{R})\,d\vec{R}=\frac{\bar{H}^2\bar{z}}{\omega}\,. \tag{3.22}$$

It is unrealistic to discuss the expansion for arbitrarily small ω (in fact, we can only hope that it converges). We therefore assume $\omega\sim\bar{z}\bar{H}$, i.e., of the order of the bandwidth. Then this contribution to Σ_d is of order $\bar{H}$. Similarly other contributions with a ring structure will contain additional factors of $\bar{H}/\omega$, but as many additional integrals over R, and hence they will be of the same order in $1/\bar{z}$.

The leading term in $\Sigma_{1\vec{k}}$ is

$$\frac{n^2}{\omega}\int e^{i\vec{k}\cdot\vec{R}}h(\vec{R})\tilde{H}(\vec{R}-\vec{R}')\tilde{H}(\vec{R}')\,d\vec{R}\,d\vec{R}'\,. \tag{3.23}$$

Here $nh(\vec{R})$ is finite only near $\vec{R}=0$, and its integral over $\vec{R}$ is of order 1. Therefore, the $\vec{R}$ integral contributes 1 rather than $\bar{z}$. This is then of the same order as Σ_d. The same goes for terms with a chain structure. Σ_{2k}, on the other hand, has for the first term in Fig. 2(g)

$$\frac{n}{\omega^2}\int\tilde{H}(\vec{R})H^2(\vec{R})e^{i\vec{k}\cdot\vec{R}}\,d\vec{R}\sim\frac{\bar{H}^3\bar{z}}{\omega^2}\sim\frac{\bar{H}}{\bar{z}}\,, \tag{3.24}$$

which is of order $(1/\bar{z})^2$ with respect to $n\tilde{H}_k$, and similarly for the other third-order contributions to Σ_2, from the localization of $nh(R)$.

If we made the *Ansatz* that these are the orders in $1/\bar{z}$ of Σ_d, Σ_1, and Σ_2, then $G_d=1/(\omega-\Sigma_d)$ is of order $1/\bar{H}\bar{z}$ and $nM_{\vec{k}}$ of order $\bar{H}\bar{z}$—i.e., the renormalization does not change the leading order. Then the order in $1/\bar{z}$ holds for all terms in the expansion of Σ_d and Σ_1 by virtue of their exact expressions in terms of $M_{\vec{k}}$ and Σ_d. Then the lack of nodes in the expression of Σ_2, even upon cutting an h line, means that all contributions to Σ_2 are of order $(1/\bar{z})^2$ or higher.

Then we see that for frequencies of the order of the bandwidth, the EMA includes all terms of order $1/\bar{z}$ in comparison with the bandwidth, and neglects those of higher order. Thus it is a high-density theory.

The same considerations apply to the lattice liquid, and we should emphasize here that $\bar{z}$ is not the number of nearest neighbors z on the lattice but is weighted by the fraction of occupied sites, i.e., for the lattice the expansion parameter is $1/\bar{z}=1/xz$. For the alloy, in general, Schwartz and Siggia[18] gave evidence that the CPA has an expansion parameter $1/z$. The above analysis offers another derivation of this, but also implies that for energies within an impurity band the CPA is inaccurate for low densities of impurities.

An interesting point is that the $1/\bar{z}$ argument appears to hold even if we include deviations from the Kirkwood approximation. For example, the three-particle distribution function can be written as

$$g(\vec{r},\vec{r}',\vec{r}'')=[1+h(\vec{r},\vec{r}')][1+h(\vec{r},\vec{r}'')]\times[1+h(\vec{r}',\vec{r}'')][1+h_3(\vec{r},\vec{r}',\vec{r}'')]\,, \tag{3.25}$$

where the three-particle correlation function h_3 corrects for the use of the Kirkwood approximation. The factor h_3, however, restricts the range of the three arguments, keeping them close together, and increasing the order in $1/\bar{z}$.

D. Comparisons with other approaches

We have already discussed[1,2] a comparison of our results with the theories of Gyorffy, as modified by Korringa and Mills (GKM),[14] of Schwartz and Ehrenreich [self-consistent approximation (SCA)][5] and of Ishida and Yonezawa (IY).[12] The present representation, however, gives a greater insight into the relationship among the several results. All of the results can be put in the form of Eqs. (2.14) and (2.15) with different expressions for $\Sigma_k=\Sigma_d+\Sigma_{1k}$:

$$\Sigma_{\vec{k}}^{\mathrm{GKM}}=\int[1+nh(\vec{k}-\vec{k}')]H^2_{\vec{k}'}G_{\vec{k}'}\,d\vec{k}'\Big/8\pi^3\,, \tag{3.26}$$

$$\Sigma_{\vec{k}}^{\mathrm{SCA}}=\int[1+nh(\vec{k}-\vec{k}')]H_{\vec{k}'}M_{\vec{k}'}G_{\vec{k}'}\,d\vec{k}\Big/8\pi^3\,, \tag{3.27}$$

$$\Sigma^{\mathrm{IY}}=\int\left(\frac{n\tilde{H}_{\vec{k}}(H_{\vec{k}}-\tilde{H}_{\vec{k}})}{\omega-\Sigma}+\tilde{H}^2_{\vec{k}}G_{\vec{k}}\right)d\vec{k}\Big/8\pi^3\,. \tag{3.28}$$

The SCA result shown here is equivalent to but much simpler than our previous result.[8,9] In the above equations the part depending explicitly on $h(\vec{k}-\vec{k}')$ is Σ_1, and the remainder is Σ_d.

In the SCA, one of the $M_{\vec{k}}$'s in the EMA result for Σ_1 is replaced by $H_{\vec{k}}$, a bare hopping integral. Let us regard this as being the one on the right as shown in Fig. 5(b). Schwartz and Ehrenreich[5] discuss the approximation to the three-body distribution function

$$g(\vec{r},\vec{r}',\vec{r}'')=[1+h(\vec{r},\vec{r}')][1+h(\vec{r},\vec{r}'')+h(\vec{r}',\vec{r}'')] \tag{3.29}$$

In Fig. 5(a) is shown the off-diagonal terms in second order using Eq. (3.27). We see that a term in which two h lines go into the right point from the left is missing (in counting h lines here we include those along the chain). The generalization of Eq. (3.29) to n-body distribution functions discussed by Schwartz and Ehrenreich[5] corresponds to omitting all diagrams with more than one h line going into any point from the left. This clearly leads to Fig. 5(b). Figure 5(c) for Σ_d is the same as the first form of the EMA result, Eq. (2.16a).

Thus the SCA has the same structure as the EMA, but with the generalized Kirkwood approximation replaced by the generalization of Eq. (3.29). As pointed out earlier, the SCA goes over into the CPA for the lattice liquid and also for the alloy. This is consistent with the present result because Eq. (3.29) is equivalent to the Kirkwood approximation for the lattice liquid or random alloy. Thus we can regard the SCA as a coherent-potential approximation but with respect to the Schwartz-Ehrenreich decomposition of the distribution function rather than the Kirkwood. Actually we found this decomposition unphysical for hard spheres, because it changed sign and did not vanish within the excluded volume. As we remarked earlier, the SCA omits some correlation along the chain of scatterings[1, 2] and so the result depends on $H(\vec{R})$ inside an excluded volume.

The GKM result omits more chain correlations than the SCA, and seems to be a CPA with respect to a decomposition of higher-order distribution functions allowing only one h line going into a point from either direction, which is clearly inadequate. The GKM result does not reduce to CPA for the lattice.

The Ishida-Yonezawa theory on the other hand was designed to include all the chain correlations. Their theory is obtained from ours by omitting Σ_1, when Σ_d is expressed by Eq. (2.16b), which explicitly includes the chain correlation. This corresponds in the diagram expansion to omitting all out-of-chain h lines, i.e., out-of-chain correlations. In the alloy case this corresponds to omitting the multiple-occupancy corrections, so that the IY theory is not a CPA. This is a serious omission in the alloy, but we shall find that in the liquid-metal case the omission while important does not lead to drastic errors, at not too high densities. This will be discussed further in Sec. V, and shown through numerical results in a subsequent paper.

In regard to the moment expansion for the density of states, the GKM result has an error in second order in $H(\vec{R})$ while the SCA is correct through second order, and has an error in the third-order term. Both the EMA and IY theories are correct through third order, the EMA including more terms in fourth order than does the IY result.

IV. GENERALIZATIONS

A. Impurity band with short-range order

In discussing the lattice liquid we assumed that $g_{ij} = 1 - \delta_{ij}$, i.e., that there is no correlation between occupation of neighboring sites. It is now very easy to generalize this result to include short-range order by means of a pair distribution function $g_{\vec{R}} = 1 + h_{\vec{R}}$. Equations (3.8) and (3.9) are now replaced by

$$M_{\vec{k}} = \sum_{k} e^{i\vec{k}\cdot\vec{R}} M_{\vec{R}}\,, \tag{4.1}$$

$$M_{\vec{k}} = H_{\vec{R}}\, g_{\vec{R}} + x^{-1}\Sigma_{1\vec{R}}\,, \tag{4.2}$$

$$x^{-1}\Sigma_{1\vec{R}} = h_{\vec{R}} \left(\frac{1}{N} \sum_{\vec{k}} e^{i\vec{k}\cdot\vec{R}} M_{\vec{k}}^{2} G_{\vec{k}} \right). \tag{4.3}$$

One immediate consequence of this analysis is that the second moment of the density of states is given correctly by

$$\omega^{(2)} = x \sum_{\vec{k}} g_{\vec{k}} H_{\vec{R}}^{2}\,. \tag{4.4}$$

Recently Schwartz[25] has considered a lattice model of a liquid with short-range order, and using an analysis based on the T-matrix version of the theory, showed that none of the previous results [QCA (quasicrystalline approximation), GKM, or SCA] gave this moment correctly. The present theory does.

The lattice liquid with short-range order, in fact, goes over into the liquid-metal tight-binding model if we let the size of the unit cell go to zero, while the range of the interaction and the ionic correlation remain finite. Yonezawa and Watabe[17] show in detail how this correspondence comes about. In the same limit the random-lattice liquid goes into the random liquid.

B. Liquid alloys

We now discuss the generalization of our results to the liquid-alloy case. We shall use the 2×2-matrix method developed by Blackman, Esterling and Beck,[19] and ideas of Movaghar, Miller, and Bennemann.[20]

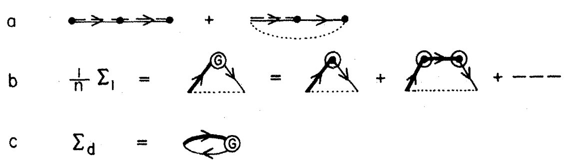

FIG. 5. Diagrams for SCA.

In an A-B alloy we expect that $H_{ii}=\epsilon_i$ will be different for the two components. Also it appears to be unrealistic to assume that the transfer integral H_{ij} is independent of species.

Consider the locator expansion for the Green's function:

$$G_{ij}=\delta_{ij}L_i+(1-\delta_{ij})L_iH_{ij}L_j+\sum_l{}' L_iH_{il}L_lH_{lj}L_j+\cdots, \tag{4.5}$$

where

$$L_i=(\omega-\epsilon_i)^{-1}. \tag{4.6}$$

If we let s go over the species, which could actually be more than 2, we can write

$$L_i=\sum_s \delta_{is}L_s. \tag{4.7}$$

If we also let

$$H_{il}\to H_{il}^{ss'}=H_{ss'}(\vec{R}_i-\vec{R}_l), \tag{4.8}$$

then i and l refer only to the positions of atoms. We can then write

$$G_{ij}=\sum_{ss'} G_{ij}^{ss'}, \tag{4.9}$$

where

$$G_{ij}^{ss'}=\delta_{ij}\,\delta_{is}\,\delta_{ss'}L_s+(1-\delta_{ij})\delta_{is}\,L_sH_{ij}^{ss'}L_{s'}\delta_{js'}+\sum_{ls''}{}'\delta_{is}\,L_sH_{il}^{ss''}\delta_{ls''}L_{s''}H_{lj}^{s''s'}L_{s'}\delta_{js'}+\cdots. \tag{4.10}$$

Then to form the continuum Green's function we introduce partial density functions

$$\rho_i^s(\vec{R})=\delta_{is}\,\delta(\vec{R}-\vec{R}_i) \tag{4.11}$$

and we obtain the result

$$G(\vec{R},\vec{R}')=\sum_{ss'}G_{ss'}(\vec{R},\vec{R}'), \tag{4.12}$$

$$\begin{aligned}G_{ss'}(\vec{R},\vec{R}')&=\Big\langle\sum_{ij}\rho_i^sG_{ij}^{ss'}\rho_j^{s'}\Big\rangle\\&=\delta(\vec{R}-\vec{R}')L_s\,\delta_{ss'}\Big\langle\sum_i\rho_i^s(\vec{R})\Big\rangle\\&\quad+\sum_{ij}{}'\langle\rho_i^s(\vec{R})\rho_j^{s'}(\vec{R}')\rangle L_sH_{ss'}(R-R')L_{s'}\\&\quad+\int\sum_{s''}\Big\langle\sum_{ijl}{}'\rho_i^s(R)\rho_j^{s''}(R'')\rho_l^{s'}(R')\Big\rangle\\&\quad\times L_sH_{ss''}(\vec{R}-\vec{R}'')L_{s''}\\&\quad\times H_{s''s}(\vec{R}''-\vec{R}')L_s'\,d\vec{R}+\cdots.\end{aligned} \tag{4.13}$$

We note that considered as a matrix $H_{ss'}(\vec{R}-\vec{R}')$ is independent of the species at $\vec{R}$ and $\vec{R}'$. This is what enabled Blackman *et al.*[19] to obtain the CPA for alloys with off-diagonal disorder.

We now examine the correlation functions

$$\Big\langle\sum_i\rho_i^s(\vec{R})\Big\rangle=nx_s, \tag{4.14}$$

$$\Big\langle\sum_{ij}{}''\rho_i^s(\vec{R})\rho_j^{s'}(\vec{R}')\Big\rangle=n^2x_sx_{s'}g_{ss'}(\vec{R}-\vec{R}'), \tag{4.15}$$

$$\Big\langle\sum_{ijl}{}''\rho_i^s(\vec{R})\rho_j^{s'}(\vec{R}')\rho_l^{s''}(\vec{R}'')\Big\rangle=n^3x_s\,x_{s'}x_{s''}g_{ss's''}(\vec{R},\vec{R}',\vec{R}''), \tag{4.16}$$

etc., where x_s is the fractional concentration of species and the double prime means no two indices are equal. This gives a species-dependent n-body distribution function. To obtain the EMA in this case, we introduce a Kirkwood factorization of the n-body distribution function for $n>2$:

$$g_{ss's''}(\vec{R},\vec{R}',\vec{R}'')=g_{ss'}(\vec{R}-\vec{R}')g_{ss''}(\vec{R}-\vec{R}'')\times g_{s's''}(\vec{R}'-\vec{R}''). \tag{4.17}$$

Then we can follow virtually the same procedure as before to obtain the generalization of Eqs. (2.14)–(2.17):

$$G_{\vec{k}}^{ss'}=n\tilde{L}_s\Big(\delta_{ss'}+\sum_{s''}M_{\vec{k}}^{ss''}G_{\vec{k}}^{s''s'}\Big), \tag{4.18}$$

$$\tilde{L}_s=x_s(\omega-\epsilon_s-\Sigma_d^s)^{-1}, \tag{4.19}$$

$$\begin{aligned}\Sigma_d^s&=\int(H_{\vec{k}}G_{\vec{k}}M_{\vec{k}})_{ss}\,d\vec{k}/8\pi^3\\&=\int[\tilde{H}_{\vec{k}}\tilde{L}(H_{\vec{k}}+M_{\vec{k}}G_{\vec{k}}M_{\vec{k}})]_{ss}\,d\vec{k}/8\pi^3,\end{aligned} \tag{4.20}$$

$$\tilde{H}_{\vec{k}}^{ss'}=\int H_{ss'}(\vec{R})g_{ss'}(\vec{R})e^{i\vec{k}\cdot\vec{R}}\,d\vec{R}, \tag{4.21}$$

$$M_{\vec{k}}^{ss'}=\tilde{H}_{\vec{k}}^{ss'}+n^{-1}\Sigma_{1\vec{k}}^{ss'}, \tag{4.22}$$

$$n^{-1}\Sigma_{1\vec{k}}^{ss'}=\int h^{ss'}(\vec{k}-\vec{k}')[M_{\vec{k}'}G_{\vec{k}'}M_{\vec{k}'}]_{ss'}\,d\vec{k}'/8\pi^3. \tag{4.23}$$

Here we have used matrix multiplication in Eqs. (4.20) and (4.23).

These equations include, in addition to diagonal and off-diagonal disorder in the Hamiltonian matrix elements, differences in pair distribution functions for different species which have been found to be important in considering conductivity in liquid alloys.[26]

C. Off-diagonal disorder in alloys

We wish to show now that these results reduce to the Blackman *et al.*[19] theory for the random-alloy case. Actually Eqs. (4.18)–(4.23) apply directly to an alloy with short-range order, if we make the $\vec{k}$ integral go over one Brillouin zone, let $n=1$, and change the $\vec{R}$ integral in Eq. (4.21) to a sum. So, what we have is a generalization of the CPA to include short-range order and off-diagonal disorder.

Specializing to the random-alloy case, we have $h^{ss'}(\vec{k}-\vec{k}')=-1$, and by an argument analogous to that leading to Eqs. (3.13) and (3.14), we have

$$N^{-1}\sum_{\vec{k}} G_{\vec{k}}^{ss'}=\delta_{ss'}\tilde{L}_s \tag{4.24}$$

and

$$\Sigma_d^s=-\Sigma_1^{ss}. \tag{4.25}$$

We have thus a 2×2 matrix Σ_1 to determine, We can write the inverse of $G_{\vec{k}}^{ss'}$ as

$$[G_{\vec{k}}^{-1}]_{ss'}=\tilde{L}_s^{-1}\delta_{ss'}-\Sigma_1^{ss'}-H_k^{ss'}, \tag{4.26}$$

with

$$\tilde{L}_s=x_s(\omega-\epsilon_s+\Sigma_1^{ss})^{-1}. \tag{4.27}$$

Then the three independent components of Σ_1 can be determined from Eqs. (4.24), (4.26), and (4.27). Finally $G_{\vec{k}}=\sum_{ss'}G_{\vec{k}}^{ss'}$ is the total Green's function. This is precisely the result of Blackman *et al.*,[19] which was shown by Bass and Leath[27] to give the correct low-density limit.

To recover the diagonally disordered alloy result, for which $H_{\vec{k}}^{ss'}$ is independent of s and s', we assume that $\Sigma_1^{ss'}$ is also independent of s and s'. Then we can show by summing Eq. (4.18) over s and s'

$$G_{\vec{k}}^{-1}=\left(\sum_s \tilde{L}_s\right)^{-1}-\Sigma_1-H_{\vec{k}}, \tag{4.28}$$

which with Eq. (4.19) and $\Sigma_1=-\Sigma_d$ is the same as Eqs. (3.15) and (3.18).

V. DISCUSSION

In this article we have demonstrated a close correspondence between the effective-medium approximation for the liquid metal and the coherent-potential approximation for a lattice model of a liquid, and also for the alloy. We have used a similar technique to obtain formal results for liquid alloys and for alloys with off-diagonal disorder and short-range order.

It is important to emphasize that while the present formalism was developed for the tight-binding model the conclusions apply equally well to the general multiple scattering version of the EMA and other approximations.

We have found that the result of extending the CPA to structurally disordered materials is intimately connected with how the higher-order distribution functions are approximated, so that different CPA extensions can be constructed corresponding to different decompositions of the distribution functions. The Kirkwood approximation appears to be reasonable for liquid metals. A question arises as to whether a CPA-like theory can be constructed which would include three-body correlations, such as are important in tetrahedrally coordinated systems. Our remarks at the end of Sec. III C suggest that such correlations are of higher order in $1/\bar{z}$ than CPA-like terms. However, in insisting upon keeping chain correlations we are already including certain higher-order terms in $1/\bar{z}$. So the question as to whether such a CPA-like theory can be derived, or whether some kind of cluster approximation would be necessary for such a system, seems to be an open one at the moment.

In a subsequent paper of this work we shall describe calculations based on the present results for several pair distribution functions and for the most part compare our results with those of Ishida and Yonezawa. Preliminary results have already been published.[2] We find that for $\bar{z}$ not too large, the two results are not drastically different. This is encouraging in that calculations for more realistic systems are more feasible with the IY theory. Further interesting properties and the analytic behavior of the solutions will be described in the above-mentioned paper.

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