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Self-Consistent Cluster Theory of Disordered Alloys*

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Several techniques for extending the single-site coherent-potential approximation (CPA) to account for particular local configurations of atoms are evaluated. It is shown that if one attempts to define a site-diagonal medium by requiring consistency between the Green's function evaluated at the center of the cluster and the external medium, one may obtain unphysical results. If, however, one requires consistency between a site at the boundary and the medium, one can obtain (at least in one dimension) a site-diagonal medium which reproduces the cellular CPA exactly.

I. INTRODUCTION

The most important recent advance in the theory of disordered alloys has been the introduction of the coherent-potential approximation[1,2] (CPA) and its development to treat (at least some) actual physical systems.[3–6] The CPA is in essence a weak scattering theory which works best when the electronic mean free path is long.[7] Its great advantage over other weak scattering theories is that it is a self-consistent theory which is exact in all of the weak-scattering limits. Thus the CPA for a substitutional binary alloy is exact in the limit of vanishing concentration of either constituent and in the limit in which the difference between the two constituent atoms becomes small.

When the concentration of both constituents is high and the difference between the constituent atomic potentials is large, or when the energy of interest lies in an impurity band the mean free path will be short. In this regime the CPA still yields a fairly accurate representation of the gross features of the density of states,[8] however it completely misses any structure associated with local clusters of atoms. In addition the "band edges" are given incorrectly. These points are illustrated in Figs. 1(a)–1(d) in which the CPA density of states for a model one-dimensional substitutional binary alloy is compared with the exact density of states (histogram) obtained from the Schmidt integral-equation technique.[9]

The purpose of this paper is to develop a theory which encompasses the strong-scattering short-mean-free-path limit as well as the regime adequately treated by the CPA. In our earlier work[10] we emphasized the fact that the density of states of a disordered system is a local property, i.e., the average density of states per unit volume at point $\vec{r}$, depends only upon the configurations of atoms which lie within a mean free path or so of $\vec{r}$. (Similar conclusions have been reached by Matsuda and co-workers.[11]) This locality property means that a properly performed cluster calculation is exact in the limit of short-mean free path.

In the following our aim will be to develop a theory which treats a local cluster of atoms exactly and the more removed regions of the system in an approximate but self-consistent fashion. Such a theory should be exact in all of the weak scattering limits (as is the CPA) because it is self-consistent and should be exact in the strong scattering limit as well since the cluster size will then be greater than the electronic-mean free path. In addition, the ability to treat clusters will allow us to introduce off-diagonal disorder and short-range atomic correlations within the cluster in a straightforward way.

In this paper we shall focus our attention mainly upon the popular two level tight binding model. The Hamiltonian is defined in terms of localized atomic orbitals $|i\rangle$. The orbital $|i\rangle$ will be localized on site i. The Hamiltonian consists of two terms, H_0 which is diagonal on this basis but disordered and W which is off diagonal:

$$H=H_0+W, \tag{1.1}$$

$$H_0=\sum_i E_i|i\rangle\langle i|, \tag{1.2}$$

$$W=\sum_{j\neq i} W_{ij}|i\rangle\langle i|. \tag{1.3}$$

E_i may be E_A with probability C_A or E_B with probability C_B. W_{ij} is the interaction matrix element between sites i and j. We shall usually take W_{ij} to be zero unless i and j are nearest neighbors and to be a constant W_0 independent of E_i and E_j when i and j are nearest neighbors.

The remainder of the paper is arranged as follows: In Sec. II we shall briefly review the coherent potential approximation. We shall also describe what appears to us to be in principle the simplest self-consistent cluster approximation, the cellular CPA.[12] The cellular CPA (CCPA) applies the CPA formalism not to a single site but to a cluster or cell of sites. Although simple in principle the CCPA has the *appearance* of being impractical for actual calculations.

In Sec. III we shall describe an approximation

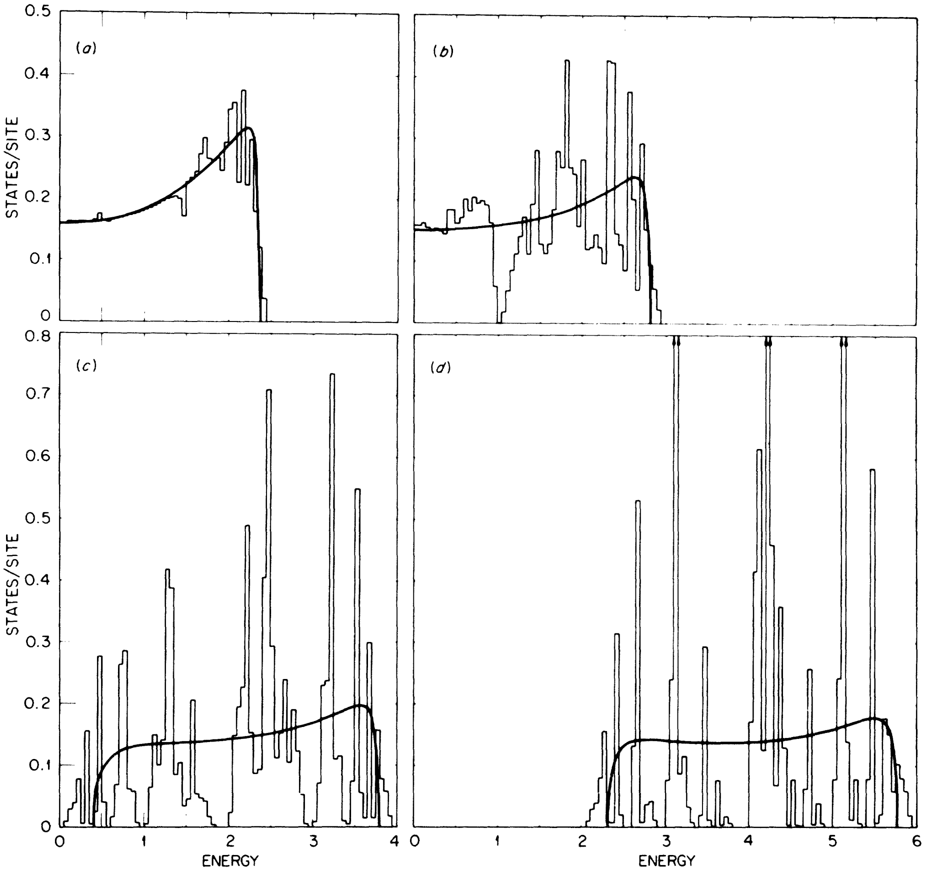

FIG. 1. Density of states from the CPA compared with the exact density of states (histogram). All four calculations are for $C_A = C_B = 0.5$ and $W_0 = 1.0$. The strength of the scattering between (a) and (d) is increased by increasing the difference "between" the atoms $E_A - E_B$. $E_A = -E_B = 0.5$ (a), 1.0 (b), 2.0 (c), 4.0 (d). The curves are symmetric about $E = 0$.

which we call the self-consistent central site approximation. We proposed this approximation originally[13] to avoid some of the computational difficulties associated with the CCPA. It has also been proposed by Capek,[14] by Brouers *et al.*[15] and by Tsukada.[16] Although the self-consistent central-site approximation (SCCS) can yield quite reasonable density-of-states curves there are problems in the strong scattering regime—the density of states may not be a single valued function of energy or for certain values of the energy the density of states may be undefined.[17] We shall explain the origin of these problems.

In Sec. IV we shall discuss the self-consistent boundary-site approximation (SCBS). We first considered this approximation to be a means of avoiding the difficulties inherent in the self-consistent central site approximation. To our surprise when we applied the SCBS approximation to a one-dimensional model binary alloy it proved to be identical to the CCPA, although requiring no more computational effort than the very simple SCCS approximation. Although the equivalence of the SCBS and CCPA is probably exact only in one dimension, we believe the SCBS to be a useful approximation in three dimensions as well.

II. CPA AND CCPA

In this section we shall describe the coherent-potential approximation and the cellular-coherent-potential approximation in terms of our model Hamiltonian (1.1).

We desire to calculate the density of states $\rho(E)$. This may be obtained from the Green's function in the usual way:

$$G(z) = (z - H)^{-1}, \tag{2.1}$$

$$\rho(E) = -\operatorname{Im}[\operatorname{Tr} G(E + i0)]/(\pi N). \tag{2.2}$$

N in Eq. (2.2) is the number of sites in the system. Alternatively, since the system is homogeneous on the average we may obtain the density of states from a single diagonal element of the configurationally averaged Green's function:

$$\hat{\rho}(i, E) = -(1/\pi)\operatorname{Im}\langle i|G(E + i0)|i\rangle, \tag{2.3}$$

$$\rho(E) = \langle\hat{\rho}(i, E)\rangle_{\text{av}}. \tag{2.4}$$

The CPA replaces the configurationally averaged Green's function $\langle G\rangle_{\text{av}}$ with the Green's function for an effective periodic medium:

$$\langle G\rangle_{\text{av}} \simeq \overline{G} = (z - \overline{H})^{-1}, \tag{2.5}$$

$$\overline{H}=\sum_i \sigma|i\rangle\langle i|+W. \tag{2.6}$$

The effective medium described by σ is determined by setting the average scattering $\langle \bar{t}_i\rangle_{\mathrm{av}}$ off a single site immersed in the medium equal to zero:

$$\bar{t}_{A(B)}=(E_{A(B)}-\sigma)(1+\langle 0|\overline{G}|0\rangle\,\bar{t}_{A(B)}), \tag{2.7}$$

$$\langle \bar{t}\rangle_{\mathrm{av}}=C_A\bar{t}_A+C_B\bar{t}_B=0. \tag{2.8}$$

Since the Green's function for a system with σ on all sites except the origin is given by $\tilde{G}_{A(B)}$, where

$$\tilde{G}_{A(B)}=\overline{G}+\overline{G}\,|0\rangle\,\bar{t}_{A(B)}\langle 0|\overline{G}, \tag{2.9}$$

and since $\bar{t}$ is a 1×1 matrix, (2.8) is equivalent to

$$\langle\langle 0|\tilde{G}|0\rangle\rangle_{\mathrm{av}}=C_A\langle 0|\tilde{G}_A|0\rangle+C_B\langle 0|\tilde{G}_B|0\rangle=\langle 0|\overline{G}|0\rangle. \tag{2.10}$$

Figure 1 compares the CPA density of states with the exact density of states for a one-dimensional form of our model Hamiltonian. The parameters for the calculation are $C_A=C_B=0.5$, $W_0=1.0$, and $E_A=-E_B=0.5$ (a), 1.0 (b), 2.0 (c), and 4.0 (d). Since the curves are all symmetric about $E=0$, only the $E>0$ part is shown. As can be seen from Fig. 1, the density of states obtains more structure as $\delta\equiv(E_A-E_B)/2W_0$ increases. This structure, which can be associated with local clusters of atoms which have particular configurations, is outside the scope of the single-site CPA. Although this structure is more pronounced in one dimension than in three it is evident from numerical calculations[18,19] that it persists in three dimensions, especially for energies in the impurity band.

Probably the most obvious way to include these effects in a self-consistent theory is to apply the CPA formalism to a cell containing several sites rather than to a single site.[12,16] One first divides the lattice into identical cells each containing several sites and then applies the CPA equation (2.8) or (2.10) to the cell rather than to a single site. The configurational average will now be over all of the configurations of the cell. The t matrix $\bar{t}$ will now be an $n\times n$ matrix where n is the number of sites in the cell. The coherent potential σ will also be replaced by an $n\times n$ matrix.

For simplicity of exposition we shall write out the CCPA equations for a one-dimensional tight-binding model although clearly the principle is much more general. We rewrite the Hamiltonian (1.1) as

$$H=\sum_\alpha |\alpha\}\,\mathcal{E}_\alpha\,|\alpha\}+W, \tag{2.11}$$

where $|\alpha\}$ is a column vector consisting of n of the orbitals $|i\rangle$,

$$\{\alpha|=(\langle n\alpha+1|,\ \ldots,\ \langle n(\alpha+1)|). \tag{2.12}$$

The diagonal matrix $\mathcal{E}_\alpha$ contains the energies of orbitals $n\alpha+1$ through $n\alpha+n$:

$$\mathcal{E}_\alpha=\begin{bmatrix} E_{n\alpha+1} & & & & \\ & E_{n\alpha+2} & & & \\ & & \cdot & & \\ & & & \cdot & \\ & & & & E_{n\alpha+n}\end{bmatrix}. \tag{2.13}$$

$\overline{H}$ corresponding to Eq. (2.6) in the single-site CPA will have the following form for the CCPA:

$$\overline{H}=\sum_\alpha |\alpha\}\,\Sigma\,\{\alpha|+W, \tag{2.14}$$

where Σ is the $n\times n$ matrix

$$\Sigma=\begin{bmatrix} \sigma_{11} & \sigma_{12} & \cdots & \sigma_{1n} \\ \sigma_{21} & \sigma_{22} & \cdots & \sigma_{2n} \\ \cdot & & & \\ \cdot & & & \\ \cdot & & & \\ \sigma_{n1} & \sigma_{n2} & \cdots & \sigma_{nn}\end{bmatrix}. \tag{2.15}$$

There are some simplifications in Σ due to symmetry, e.g., $\sigma_{11}=\sigma_{nn}$, $\sigma_{12}=\sigma_{21}$, etc., but there are still many elements which must be solved for self-consistently.

The t matrix that describes the scattering off an n-site cluster with the set of orbital energies $\{E_\alpha\}=\{E_{\alpha n+1},\ldots,E_{\alpha n+n}\}$ in the periodic medium described by Hamiltonian $\overline{H}$ and Green's function $\overline{G}=(z-\overline{H})^{-1}$ is

$$\bar{t}_\alpha=(\mathcal{E}_\alpha-\Sigma)(1+\overline{G}_{\alpha\alpha}\bar{t}_\alpha). \tag{2.16}$$

The Green's function for the system with the medium everywhere except cell α is

$$\tilde{G}=\overline{G}+\overline{G}|\alpha\}\,\bar{t}_\alpha\,\{\alpha|\overline{G}. \tag{2.17}$$

Thus the CPA conditions (2.8) and (2.10) become

$$\langle \bar{t}_\alpha\rangle_{\mathrm{av}}=0, \tag{2.18}$$

where the average is over $\{E_\alpha\}$ and

$$\langle\{\alpha|\tilde{G}|\alpha\}\rangle_{\mathrm{av}}=\{\alpha|\overline{G}|\alpha\}. \tag{2.19}$$

These equations appear to be quite complicated and difficult to solve without further approximations. For the one-dimensional nearest-neighbor tight-binding model, however, it turns out that the exact solution of Eq. (2.19) is quite easy. We shall discuss this further in Sec. IV, where we show that the matrix Σ (2.15), may be replaced as far as its effect on cell α is concerned by a simple scalar.

Results of three-, five-, and seven-site CCPA calculations are shown in Figs. 2–5. These calculations all represent the density of states at the

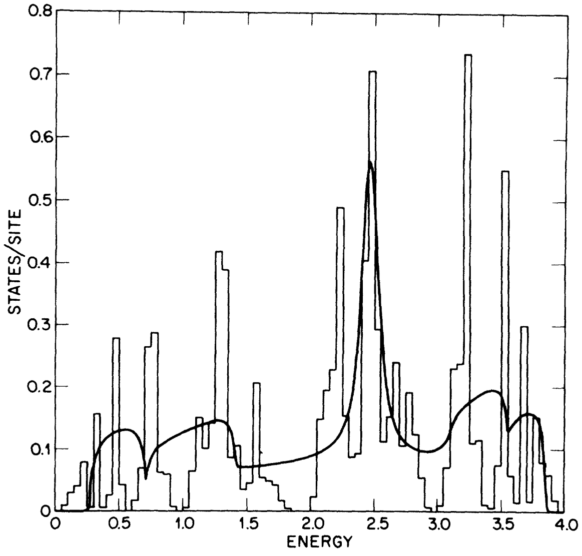

FIG. 2. Three-site CCPA or SCBS density of states compared with the exact density of states (histogram). $C_A = C_B = 0.5$, $W_0 = 1.0$, $E_A = -E_B = 2.0$.

center of the cluster. δ is chosen to be 2.0 so the bands are just split, all calculations are for $C_A = C_B = 0.5$ except for Fig. 5 which shows the impurity band of a 75–25% alloy. Figures 2, 3, 4, and 5 are for three, five, seven, and five sites, respectively. Figures 2–4 may be compared with Fig. 1(c) which shows the CPA result for the same parameters.

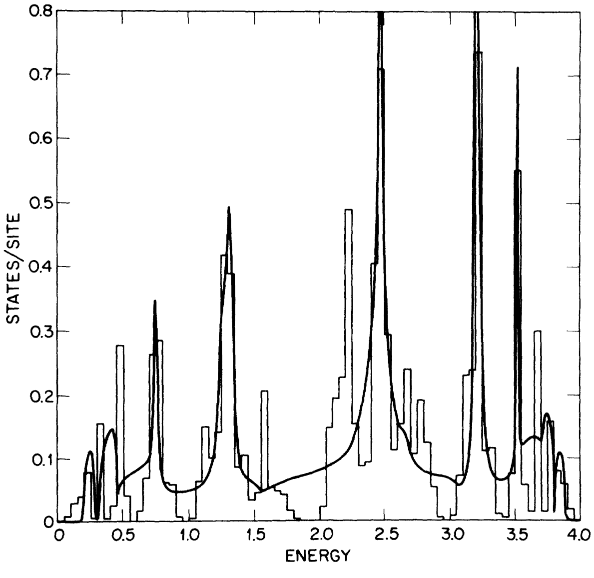

FIG. 3. Five-site CCPA or SCBS density of states compared with the exact density of states (histogram). Parameters are the same as for Fig. 2.

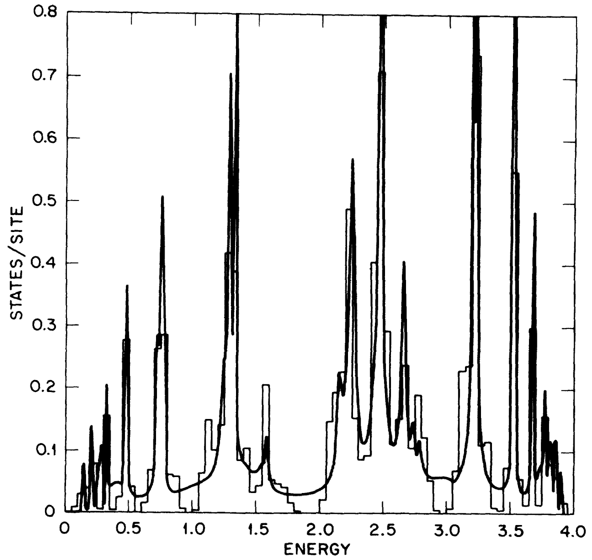

FIG. 4. Seven-site CCPA or SCBS density of states compared with the exact density of states (histogram). Parameters are the same as for Figs. 2 and 3.

III. SELF-CONSISTENT CENTRAL-SITE APPROXIMATION

In this section we define the self-consistent central-site approximation and discuss the reason for its failure in the strong scattering regime. This technique has been proposed previously by ourselves and several other authors.[13–16]

We originally proposed the approximation as a

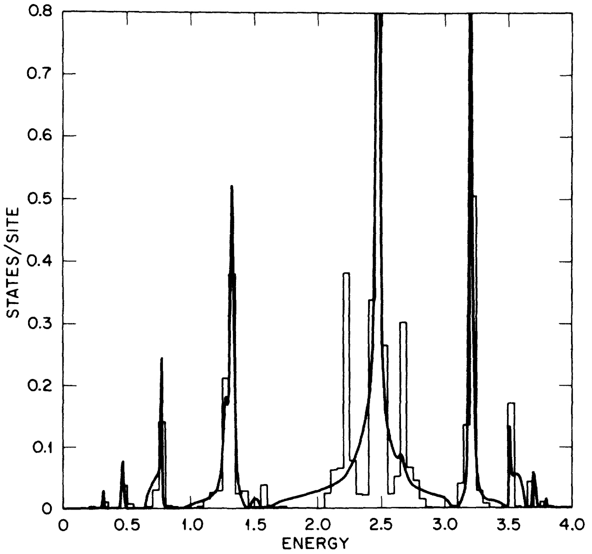

FIG. 5. Five-site CCPA or SCBS density of states compared with the exact density of states (histogram). Parameters are the same as for Figs. 2–4, except that $C_A = 0.25$ and $C_B = 0.75$. Only the impurity band is shown.

means of avoiding the complexity of the $n\times n$ coherent potential matrix Σ (2.15) of the CCPA. Clearly, it would be much nicer to work with a scalar coherent potential, i.e., $\Sigma=\sigma I_n$ (I_n is the $n\times n$ unit matrix) as in the usual CPA. Use of a scalar for Σ, however, gives one only a single parameter in $\bar{H}$ to adjust making it impossible (apparently) to satisfy Eq. (2.18) which requires that all n^2 elements of $(\bar{t}_\alpha)$ average vanish.

In the equivalent equation (2.19), one would not try to obtain equality between all n^2 elements of $\langle\{\alpha|\tilde{G}|\alpha\}\rangle_{\text{av}}$ and $\{\alpha|\bar{G}|\alpha\}$. One would, however, do what appeared to be the most reasonable thing one could do within the limitations of the scalar coherent potential *Anzatz*, namely, choose σ so that the density of states per site at the center of the cluster is consistent with the external medium, i.e.,

$$\langle n|\tilde{G}|n\rangle=\langle n|\bar{G}|n\rangle\,. \qquad (3.1)$$

Here $|n\rangle$ is the orbital on the site at the center of the cluster.

The SCCS approximation is admittedly an *ad hoc* prescription. Our main justification for proposing it was that in many cases it yielded a density of states which appeared to agree rather well with the CCPA and the exact results as is evident in Fig. 6.

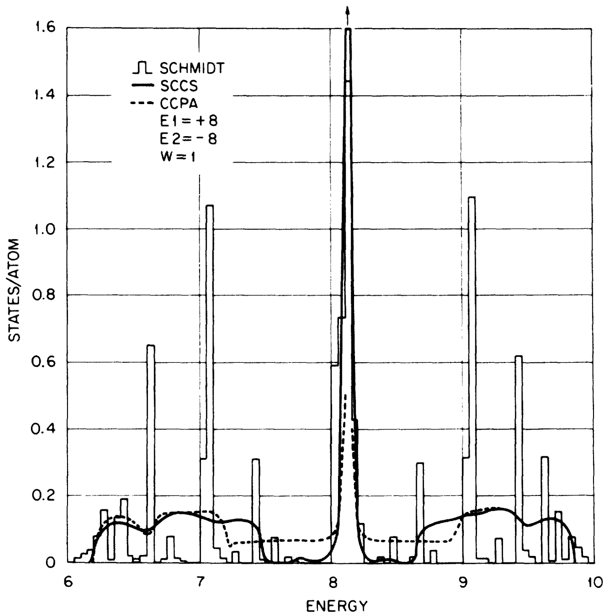

FIG. 6. Three-site SCCS approximation density of states (solid line) compared with the three-site CCPA density of states (dashed line) and the exact results (histogram). The parameters are $\delta=8.0$, $C_A=C_B=0.5$. Only one of the two symmetric bands is shown. There is a branch point in the SCCS Green's function just above the real E axis at real $E\simeq 8.1$.

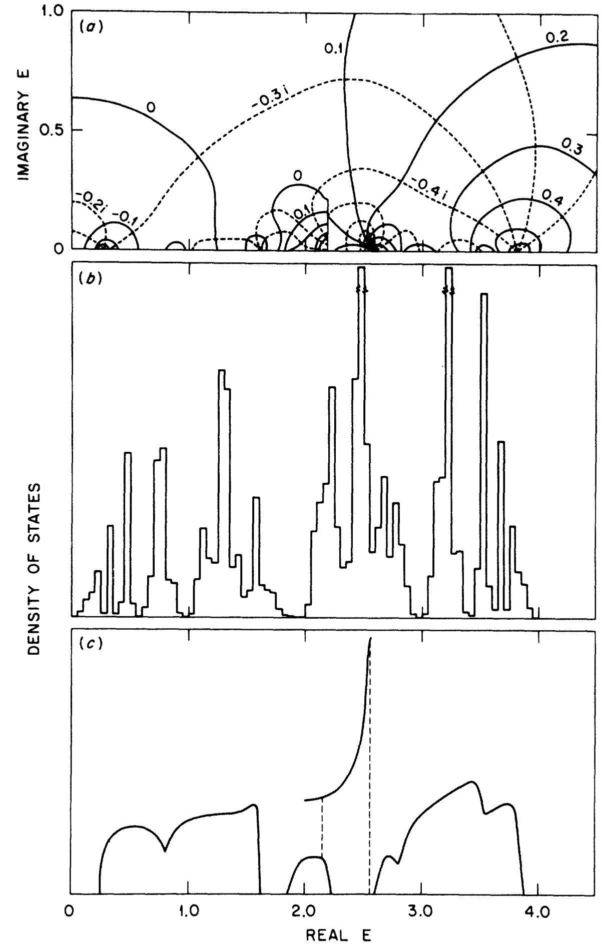

FIG. 7. (a) Contours of real and imaginary parts of the Green's function $\bar{G}_{00}$ in the SCCS approximation. The solution has been chosen so that $\bar{G}(E)\simeq E^{-1}$ for large E. (b) Exact density of states. (c) Density of states for the SCCS approximation. The dashed line at Re$E\simeq 2.1$ indicates where the branch cut has been drawn. The dashed line at Re$E\simeq 2.3$ is due to an uncertainty in the density of states associated with a singularity on the ReE axis. The Green's function is continuous at Re$E\simeq 2.3$ for ImE slightly greater than zero. Parameters are the same as Figs. 2–4.

Unfortunately, the SCCS has a serious flaw which is apparent in Fig. 7. The Green's function $\bar{G}(z)$ is not an analytic function of the energy parameter z in the strong scattering regime. As δ is increased branch points appear in $\bar{G}(z)$ off of the real z axis.[17] A Green's function with off-axis branch points violates causality. In addition, the sum rule for the integrated density of states is not satisfied.

This effect is easily missed in numerical calculations for two reasons: (a) It does not exist in the weak-scattering limit. Thus, if $\delta=(E_A-E_B)/(\text{half-band-width})$ then the effect does not show up for $\delta=0.5$ (Fig. 5 of Ref. 16 and Fig. 4 of Ref. 14) for the one-dimensional 50–50% alloy. We do not know the lowest value of δ for which the nonanalyticity occurs, but for the 50–50% alloy it is quite apparent at $\delta = 1.0$. For comparison, the actual bands do not split until $\delta = 2.0$. (b) In the extreme split-band limit, the branch points occur for values of real z which correspond to peaks in the density of states. Since $G(z)$ is changing rapidly as a function of real z in this region it is quite easy to overlook the fact that ones numerical algorithim has "switched branches."

The origin of this nonanalytic behavior of $G(z)$ is easily understood. Let us consider a three-site cluster in the extreme split-band limit. We label the sites of the cluster from left to right 1, 2, 3. The equation we desire to solve in the SCCS approximation is

$$\sum_{\{E_i\}} P(E_1, E_2, E_3)\tilde{G}_{22}(z, \sigma, E_1, E_2, E_3) = \overline{G}_{00}(z - \sigma). \tag{3.2}$$

$P(E_1, E_2, E_3)$ is the probability of any particular configuration of the energies E_i ($i = 1, 2, 3$). Now one configuration will consist of an A atom surrounded by two B atoms. It can be shown that the contribution to the sum on the left-hand side of Eq. (3.2) due to this configuration is

$$\begin{aligned} P(E_B, E_A, E_B)\tilde{G}_{22}(z, \sigma, E_B, E_A, E_B) &= P(E_B, E_A, E_B)\{z - E_A - 2W_0^2 \\ &\quad \times [z - E_B - A(z-\sigma)]^{-1}\}^{-1}, \end{aligned} \tag{3.3}$$

where $A(z - \sigma)$ satisfies

$$A = W_0^2/(z - \sigma - A). \tag{3.4}$$

In the extreme split-band limit, $E_A - E_B \gg W_0$, and for $z \sim E_A$, Eq. (3.3) becomes

$$\begin{aligned} P(E_B, E_A, E_B)\tilde{G}_{22}(z, \sigma, E_B, E_A, E_B) \\ \simeq P(E_B, E_A, E_B)(z - E_A + i\epsilon)^{-1}. \end{aligned} \tag{3.5}$$

The term represented by Eq. (3.5) will be the dominant contribution to the left-hand side of Eq. (3.2) near the peak at $z \sim E_B$ while the right-hand side has the simple form

$$\overline{G}_{00}(z - \sigma) = [(z - \sigma)^2 - 4W_0^2]^{-1/2}. \tag{3.6}$$

The function $\overline{G}_{00}(z - \sigma)$ is illustrated in Fig. 8. Note that its analytic properties in the upper-half $z - \sigma$ plane are determined by $\mathrm{Im}G$ on the real axis, i.e., by the density of states curve. As $\mathrm{Im}(z - \sigma)$ increases the real and imaginary parts of $\overline{G}(z - \sigma)$ become smoother and less sharply peaked.

To see the origin of the nonanalytic behavior of the Green's function let us set Eq. (3.5) equal to (3.6):

$$P(E_B, E_A, E_B)/(z - E_A + i\epsilon) = [(z - \sigma)^2 - 4W_0^2]^{-1/2}, \tag{3.7}$$

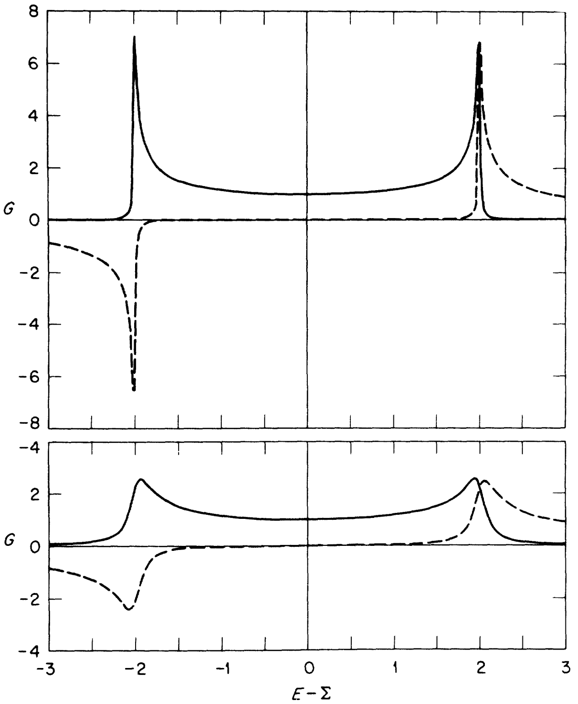

FIG. 8. $\overline{G}_{00}(z - \sigma)$ for the one-dimensional nearest-neighbor tight-binding lattice. The abscissa $E - \Sigma$ is $\mathrm{Re}(z - \sigma)$. The ordinate is $-\mathrm{Im}\overline{G}_{00}$ (solid line) and $\mathrm{Re}\overline{G}_{00}$ (dashed line). For the upper graph, $\mathrm{Im}(z - \sigma) = 0.01$ and for the lower graph, $\mathrm{Im}(z - \sigma) = 0.1$.

and imagine that we adjust σ until both real and imaginary parts of Eq. (3.7) are satisfied. Since ϵ is a small positive quantity the left-hand side of Eq. (3.7) will become quite large for $z \sim E_A$. Let us vary z from $z = E_A + \Delta$ to $z = E_A - \Delta$. The imaginary part of the left-hand side of Eq. (3.7) will follow a Lorentzian curve with a peak at $z = E_A$. The real part will follow a curve that is essentially the derivative of a Lorentzian. Now for each value of E we imagine adjusting σ on the right-hand side of Eq. (3.7) in order to satisfy the equality. Clearly, $\mathrm{Im}\sigma$ must become very small as $z \to E_A$ in order to give the required high density of states. In addition $\mathrm{Re}\tilde{G}(z)$ must change sign as z passes through E_A. Thus, the solution must "jump" from the right-hand peak of Fig. 8 (upper part) to the left-hand peak as z passes through E_A.

This same result may be obtained more directly by solving Eq. (3.7) for σ,

$$\sigma = z \pm 2W_0[1 + (z - E_A + i\epsilon)^2/4W_0^2P^2]^{1/2} \tag{3.8}$$

for $z = E_A + \Delta$ and $P(E_B, E_A, E_B) = P$, Eq. (3.8) becomes

$$\sigma = E_A + \Delta \pm 2W_0\left(1 + \frac{\Delta^2 - \epsilon^2 + 2i\epsilon\Delta}{4W_0^2P^2}\right)^{1/2}$$

$$\simeq E_A + \Delta \pm 2W_0\left(1 + \frac{\Delta^2 - \epsilon^2 + 2i\epsilon\Delta}{8W_0^2P^2}\right) . \qquad (3.9)$$

The root in Eq. (3.9) must be chosen so that $\operatorname{Im}\sigma < 0$, otherwise the density of states will be negative. Thus,

$$\begin{aligned} \sigma &= E_A - 2W_0, \quad \Delta = 0^+ \\ \sigma &= E_A + 2W_0, \quad \Delta = 0^- . \end{aligned} \qquad (3.10)$$

For smaller values of δ the effect becomes more complicated but numerical calculations show that a branch point exists off the real axis for δ as low as 1.0 for the 50–50% alloy.

In three dimensions the situation is slightly different because of the different analytic form of the Green's function, however, the same basic arguments apply. Let us consider a simple cubic tight-binding Hamiltonian with nearest-neighbor interactions only. The SCCS equation for a cluster consisting of a central site 0 and its nearest-neighbor sites, numbered 1 through 6, is

$$\sum_{\{E_i\}} P(E_0, E_1 \cdots E_6)\tilde{G}_{00}(z, \epsilon, E_0 \cdots E_6) = \overline{G}_{00}(z-\sigma) . \qquad (3.11)$$

The form of $\overline{G}_{00}(z-\sigma)$ is indicated in Fig. 9. Note the approximately flat top to the density of states curve $-\operatorname{Im}G(E+i0)$. One thing is clear immediately. The SCCS approximation applied to this model [or any model for which $\operatorname{Im}G(E+i0)$ is finite for all E] can never give a density of states greater than the maximum density of states of the perfect lattice.

We have applied the SCCS approximation to the simple cubic tight-binding Hamiltonian. To simplify the calculations we made the additional approximation suggested by Brouers *et al.*[15] of expressing the quantity analogous to A [Eq. (3.4)] in terms of $\overline{G}_{00}(z-\sigma)$. This approximation is exact in one dimension.

For $\delta = 2.0$ (bands just split) and $c = 0.5$ we could find no solutions to Eq. (3.11) for certain energy ranges. Extrapolation showed that the solution disappeared whenever $\pi\rho(E)$ exceeded $\max[-\operatorname{Im}\overline{G}\times(E+i0)]$. The general considerations mentioned above lead us to believe that this difficulty is inherent in the SCCS approximation and does not arise because of the additional approximation.

It may be possible in some cases to get around this difficulty by solving Eq. (3.11) sufficiently far off the real axis and extrapolating to $\operatorname{Im}z = 0$ to find the density of states. We have not tried this technique since it seems that its success or failure might depend on the analytic form of $\overline{G}(z)$. Indeed one would expect that for a more realistic Hamiltonian with several maxima one would have the problem of nonanalytic solutions as well as nonexistent solutions.

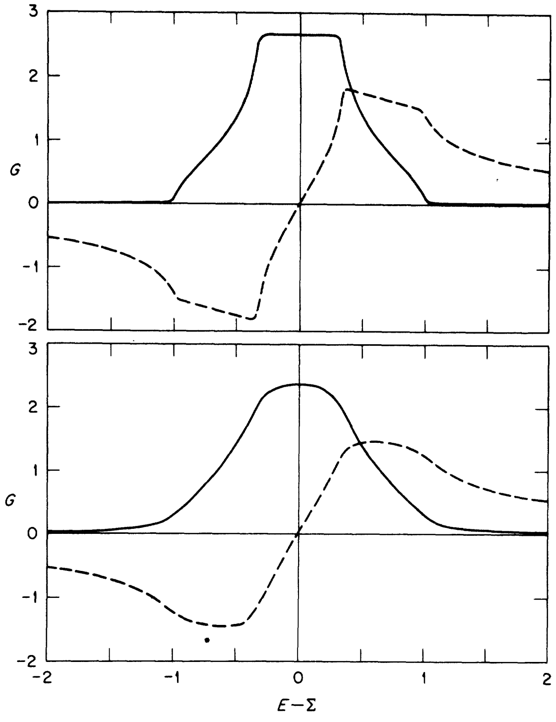

FIG. 9. $\overline{G}_{00}(z-\sigma)$ for the simple cubic nearest-neighbor tight-binding lattice. The abscissa $E-\Sigma$ is $\operatorname{Re}(z-\sigma)$. The ordinate is $-\operatorname{Im}\overline{G}_{00}$ (solid line) and $\operatorname{Re}\overline{G}_{00}$ (dashed line). For the upper graph, $\operatorname{Im}(z-\sigma) = 0.01$ and for the lower graph, $\operatorname{Im}(z-\sigma) = 0.1$.

IV. SELF-CONSISTENT BOUNDARY-SITE APPROXIMATION

It is clear that a basic difficulty in the physics of the SCCS approximation lies in the fact that the density of states per site at site n ($\sim \operatorname{Im}[G_{nn}]$) at the center of the cluster is almost independent of the external medium if the mean free path is much less than the distance from the center of the cluster to its boundary. As a consequence, determining the medium by making the density of states at the center of the cluster consistent with the external medium is not always possible.

A site at the boundary of a cluster, however, is in intimate contact with the medium and therefore the density of states per site for a boundary site will depend quite strongly on the external medium. Thus if we require consistency between a diagonal element of the Green's function for a boundary site ($\tilde{G}_{nn}$ where n is a boundary site) and a diagonal element of the Green's function for the uniform external medium we should avoid the most obvious difficulty with the SCCS approximation.

We call this new approximation the self-consistent boundary-site approximation or SCBS. Like the SCCS, the SCBS approximation is an *ad hoc* theory and must be compared with exact model calculations before it can be accepted with confidence. When we applied the SCBS approximation to the one-dimensional nearest-neighbor tight-binding alloy we found that the SCBS density of states was for this model identical to that of the cellular CPA (CCPA) discussed in Sec. II. This is quite a surprising result because the self-energy in the CCPA is an $n \times n$ matrix (n being the number of sites in the cluster), whereas the SCBS approximation employs a constant scalar coherent potential.

The reason that an approximation using a constant scalar coherent potential can yield the same density of states as the CCPA which employs a much more complicated coherent potential lies in the fact that the density of states is calculated within the cluster. As far as the Green's function within the cluster is concerned the external medium enters only as a boundary condition. For the one-dimensional model which we are considering this boundary condition involves a single parameter.

We can derive an expression which shows how the external medium enters the cluster Green's function for a tight-binding system in one, two or three dimensions. We require only that the interactions between sites fall off sufficiently fast that we can to a good approximation take it to be zero between sites separated by a few lattice parameters. Let us divide the lattice into groups of sites. Group 1 will consist of a single site which we take to be the center of our cluster. Group 2 we take to be all sites that interact with group one. Group 3 will be all sites that interact with group two not already included in group two or group one, etc. Let us define $\underline{h}_1$, $\underline{h}_2$, $\underline{h}_3$ to be block matrices which represent interactions among the sites of group 1, 2, and 3, respectively. Let $\underline{\omega}_{12}$ represent interactions between group 1 and group 2, $\underline{\omega}_{23}$ between group 2 and group 3, etc. Using these definitions we can write our Hamiltonian in block tridiagonal form:

$$\underline{H} = \begin{bmatrix} \underline{h}_1 & \underline{\omega}_{12} & & & \\ \underline{\omega}_{21} & \underline{h}_2 & \underline{\omega}_{23} & & \\ & \underline{\omega}_{32} & \underline{h}_3 & \underline{\omega}_{34} & \\ & & \underline{\omega}_{43} & \underline{h}_4 & \\ & & & & \ddots \end{bmatrix} . \tag{4.1}$$

Let us suppose that we are interested in the Green's function for this Hamiltonian, but only within the cluster that consists of the sites in groups 1, 2, and 3. Now there is a matrix identity for inverting block matrices. If

$$\underline{M} = \begin{pmatrix} \underline{A} & \underline{B} \\ \underline{C} & \underline{D} \end{pmatrix}, \tag{4.2}$$

then

$$\underline{M}^{-1} = \begin{pmatrix} (\underline{M}/\underline{D})^{-1} & -\underline{A}^{-1}\underline{B}(\underline{M}/\underline{A})^{-1} \\ -\underline{D}^{-1}\underline{C}(\underline{M}/\underline{D})^{-1} & (\underline{M}/\underline{A})^{-1} \end{pmatrix}, \tag{4.3}$$

where $(\underline{M}/\underline{D}) = \underline{A} - \underline{B}\,\underline{D}^{-1}\underline{C}$ is known as the Schur complement of $\underline{D}$ in $\underline{M}$. Equation (4.3) may be verified by matrix multiplication.

Applying Eq. (4.3) to (4.1) gives, for the cluster Green's function, $\underline{G}^c$:

$$\underline{G}^c = \begin{bmatrix} z - \underline{h}_1 & -\underline{\omega}_{21} & \\ -\underline{\omega}_{21} & z - \underline{h}_2 & -\underline{\omega}_{23} \\ & -\underline{\omega}_{32} & z - \underline{h}_3' \end{bmatrix}^{-1} , \tag{4.4}$$

$$\underline{h}_3' = \underline{h}_3 - \underline{\omega}_{34}\,\underline{G}_4^e\,\underline{\omega}_{43} . \tag{4.5}$$

$\underline{G}_4^e$ is the Green's function for propagation between sites of group 4 in the region external to the cluster, the electron not being allowed to visit any site within the cluster. Our point here is that the effect of the external medium enters the cluster Green's function only through modification of the interactions between sites on the boundary of the cluster. One can change the external medium at will, so long as the matrix $\underline{\omega}_{34}\underline{G}_4^e\underline{\omega}_{43}$ is unaffected, without affecting the cluster Green's function.

We shall now write out in detail the SCBS equations for the one-dimensional nearest-neighbor tight-binding model and then show that for this model they are equivalent to the CCPA. For simplicity, we shall write the equations for a three-site cluster. Extension to more sites is trivial.

We consider a cluster of three sites with site energies E_1, E_2, and E_3 immersed in a medium described by a site energy σ,

$$\tilde{H} = \begin{bmatrix} \ddots & & & & & & & \\ & \sigma & W_0 & & & & & \\ & W_0 & \sigma & W_0 & & & & \\ & & W_0 & E_1 & W_0 & & & \\ & & & W_0 & E_2 & W_0 & & \\ & & & & W_0 & E_3 & W_0 & \\ & & & & & W_0 & \sigma & W_0 \\ & & & & & & W_0 & \sigma \\ & & & & & & & \ddots \end{bmatrix} . \tag{4.6}$$

Let $\tilde{G} = z - \tilde{H}$.

Also let $\bar{H}$ be equal to $\tilde{H}$ except that E_1, E_2, and E_3 are all replaced by σ, and define $\bar{G} = z - \bar{H}$.

In the SCBS approximation the coherent potential σ is determined by requiring that the average diagonal element of the Green's function evaluated at a boundary site $\langle \tilde{G}_{11}\rangle_{\text{av}}$ be equal to a diagonal element of the Green's function for the uniform medium $\bar{G}_{nn}$.

For the SCBS we can obtain the following results for the Green's function within the cluster by applying (4.3) recursively:

$$\tilde{G}^c = \begin{pmatrix} z-E_1-A & -W_0 & \\ -W_0 & z-E_2 & -W_0 \\ & -W_0 & z-E_3-A \end{pmatrix}^{-1} . \qquad (4.7)$$

The boundary parameter A is related to the coherent potential σ through

$$A = A(\sigma) = W_0^2/[z-\sigma-A(\sigma)] . \qquad (4.8)$$

Equations (4.7) and (4.8) are derived with more detail in the Appendix. From Eq. (4.7) the 1, 1 element of $\tilde{G}^c$ is given by

$$\tilde{G}^c_{11} = \{z-E_1-A-W_0^2[z-E_2-W_0^2(z-E_3-A)^{-1}]^{-1}\}^{-1} . \qquad (4.9)$$

A diagonal element of $\bar{G}$ is given by

$$\bar{G} = (z-\sigma-2A)^{-1} = (W_0^2/A-A)^{-1} . \qquad (4.10)$$

Thus, the SCBS approximation for σ becomes

$$\sum_{\{E_1E_2E_3\}} P(E_1, E_2, E_3)\{z-E_1-A-W_0^2 \times[z-E_2-W_0^2(z-E_3-A)^{-1}]^{-1}\}^{-1} = (W_0^2/A-A)^{-1} . \qquad (4.11)$$

Note that σ only enters through the boundary parameter A. In fact we need never calculate σ to obtain the density of states. Once A is determined using Eq. (4.11), one can use the central site of the cluster to determine the density of states

$$\pi\rho(E) = -\operatorname{Im}\langle \tilde{G}_{22}(E+i0)\rangle_{\text{av}} , \qquad (4.12)$$

$$\tilde{G}_{22}(z, E_1, E_2, E_3, A) = \left(z-E_2-\frac{W_0^2}{z-E_1-A}-\frac{W_0^2}{z-E_3-A}\right)^{-1} . \qquad (4.13)$$

We shall now show that Eq. (4.10) is equivalent to the CCPA. For the CCPA, Eq. (4.6) becomes

$$\tilde{H} = \begin{bmatrix} \ddots & & & & \\ & \Sigma & & & \\ & & \Sigma & & \\ & & & \mathcal{E}_0 & \\ & & & & \Sigma \\ & & & & & \ddots \end{bmatrix} + W , \qquad (4.14)$$

where

$$W = \begin{bmatrix} \ddots & & & & \\ & 0 & W_0 & & \\ & W_0 & 0 & W_0 & \\ & & W_0 & 0 & W_0 \\ & & & W_0 & 0 \\ & & & & & \ddots \end{bmatrix} \qquad (4.15)$$

and

$$\Sigma = \begin{pmatrix} \sigma_1 & \sigma_2 & \sigma_3 \\ \sigma_2 & \sigma_4 & \sigma_2 \\ \sigma_3 & \sigma_2 & \sigma_1 \end{pmatrix} . \qquad (4.16)$$

Here we have used symmetry to reduce the number of different elements of Σ from 9 to 4:

$$\mathcal{E}_0 = \begin{pmatrix} E_1 & 0 & 0 \\ 0 & E_2 & 0 \\ 0 & 0 & E_3 \end{pmatrix} . \qquad (4.17)$$

Again we only need the Green's function within the central cluster. Application of Eq. (4.3) yields (see Appendix)

$$\tilde{G}^c = \begin{pmatrix} z-E_1-A & -W_0 & \\ -W_0 & z-E_2 & -W_0 \\ & -W_0 & z-E_3-A \end{pmatrix}^{-1} . \qquad (4.18)$$

Equation (4.18) is equivalent to (4.7) except that the boundary parameter A is now given by

$$A = W_0^2(X^{-1})_{11} , \qquad (4.19)$$

$$X = \begin{pmatrix} z-\sigma_1 & -\sigma_2-W_0 & -\sigma_3 \\ -\sigma_2-W_0 & z-\sigma_4 & -\sigma_2-W_0 \\ -\sigma_3 & -\sigma_2-W_0 & z-\sigma_1-A \end{pmatrix} . \qquad (4.20)$$

Application of Eq. (4.3) to (4.19) and (4.20) yields

$$A = W_0^2[z-\sigma_1-UY(A)U^T]^{-1} , \qquad (4.21)$$

where U and $Y(A)$ are given by

$$U = (-\sigma_2-W_0, \ -\sigma_3) \qquad (4.22)$$

and

$$Y(A) = \begin{pmatrix} z-\sigma_4 & -\sigma_2-W_0 \\ -\sigma_2-W_0 & z-\sigma_1-A \end{pmatrix}^{-1} . \qquad (4.23)$$

U^T is the transpose of U.

The Green's function $\bar{G}$ where $\mathcal{E}_0$ in $\tilde{G}$ is replaced by Σ is

$$\overline{G}^c=\begin{bmatrix} z-\sigma_1-A & -\sigma_2-W_0 & -\sigma_3 \\ -\sigma_2-W_0 & z-\sigma_4 & -\sigma_2-W_0 \\ -\sigma_3 & -\sigma_2-W_0 & z-\sigma_1-A \end{bmatrix}^{-1}. \quad (4.24)$$

The boundary parameter A is again given by Eq. (4.21).

Thus, the CCPA is determined by setting $\overline{G}^c$ [Eq. (4.24)] equal to the configurational average of $\tilde{G}^c$ [Eq. (4.18)]. This appears to be a set of four equations in four unknowns σ_1, σ_2, σ_3, σ_4. Note however that $\overline{G}^c$ is determined once A is known. We can obtain a single equation for A that does not involve σ_1, σ_2, σ_3, and σ_4.

The 1, 1 element of $\overline{G}^c$ [Eq. (4.24)] is given by

$$\overline{G}^c_{11}=[z-\sigma_1-A-UY(A)U^T]^{-1} \quad (4.25)$$

or equivalently, using Eq. (4.21),

$$(\overline{G}^c)_{11}=(W_0^2/A-A)^{-1}. \quad (4.26)$$

Thus the equation which determines the boundary parameter A in the CCPA is obtained by equating (4.26) to $\langle\tilde{G}_{11}\rangle_{\text{av}}$ calculated from (4.18):

$$\sum_{\{E_1E_2E_3\}} P(E_1,\, E_2,\, E_3)\{z-E_1-A-W_0^2 \times[z-E_2-W_0^2(z-E-A)^{-1}]^{-1}\}^{-1}=(W_0^2/A-A)^{-1} \quad (4.27)$$

Equation (4.27) is clearly identical to (4.11) so that the SCBS is equivalent to the CCPA for this model. To extend the proof to any number of sites one need merely note that the right-hand side is independent of the number of sites in the cluster and that $\langle\tilde{G}^c_{11}\rangle_{\text{av}}$ has the same form for the SCBS approximation (4.7) as for the CCPA [Eq. (4.18)] regardless of the number of sites.

V. DISCUSSION AND CONCLUSIONS

A great deal of theoretical and empirical work indicates that the CPA is a reliable self-consistent single-site approximation for the density of states of a disordered alloy. We emphasize the extensive empirical model calculations as well as the exact theoretical investigations of limiting cases because as far as we know there is no general proof that the CPA Green's function has the requisite analytical properties.[20] The CPA has "worked" in all cases for which it has been tried to date. However, we might well remember that all calculations with the exceptions of the CCPA calculations reported here and by Tsukada have involved zero range potentials.

Assuming that there exists a general theorem stating that the CPA Green's function has the required analytic properties it is clear that this theorem must hold for the CCPA as well since the CCPA can be considered to be a CPA for a special extended potential. This is important because of recent work which indicates that self-consistency arbitrarily applied often leads to a nonphysical Green's function especially in the strong scattering regime.[17] The importance of the CCPA is also emphasized by the work of Leath who showed that theories which yield "cluster diagonal" coherent potentials such as the CCPA and the SCBS can interpolate between the virtual crystal and split-band limits.[21]

Given then that the CCPA is a reliable approximation which encompasses the short mean free path as well as the long mean-free-path regime there remains the question of whether or not it will be practical for application to three-dimensional physical systems. We are doubtful of the efficiency of straightforward application of the CCPA to actual physical systems without further simplification or approximation and for this reason we proposed the SCCS approximation which appears to fail in the strong scattering regime.

An investigation of the reasons for the failure of the SCCS approximation led us to the conclusion that these difficulties could be avoided by making a site on the boundary (rather than one at the center) consistent with the external medium. As a test of this SCBS approximation we applied it to a one dimensional model Hamiltonian. For this model we found that the SCBS and CCPA are identical.

The equivalence of the SCBS and CCPA is probably only true for one-dimensional systems. In two and three dimensions one usually finds that cells which reproduce the lattice when periodically continued do not have all boundary sites equivalent. For example, the smallest cell for the simple cubic lattice which has a central site and which reproduces the lattice when periodically continued has boundary sites with three different symmetries.

We feel, nevertheless, that the SCBS approximation will be useful in two and three dimensions. For most simple lattices one could imagine treating a cluster consisting of a central atom and its nearest neighbors with this approximation. In this case all of the boundary sites would be equivalent. We realize, of course, the need for further testing of this approximation.

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APPENDIX

Consider the block tridiagonal matrix $\underline{M}$ defined by

$$\underline{M}=\begin{bmatrix} \underline{B}_1 & \underline{C}_1 & 0 & 0 \\ \underline{D}_1 & \underline{B}_2 & \underline{C}_2 & 0 \\ 0 & \underline{D}_2 & \underline{B}_3 & \underline{C}_3 \\ 0 & 0 & \underline{D}_3 & \underline{B}_4 \end{bmatrix}, \tag{A1}$$

where $\underline{B}_i$ is an $n_i \times n_i$ matrix, $\underline{C}_i$ is $n_i \times n_{i+1}$, and $\underline{D}_i$ is $n_{i+1} \times n_i$. Suppose that we are interested in the upper left-hand block of the inverse of $\underline{M}$, i.e., the block corresponding to $\underline{B}_1$. Let us call this block of $\underline{M}^{-1}$, $\underline{G}_{11}$. We can derive the following formula for $\underline{G}_{11}$:

$$\begin{aligned} \underline{G}_{11}&=(\underline{B}_1-\underline{C}_1\underline{A}_1\underline{D}_1)^{-1}, \\ \underline{A}_1&=(\underline{B}_2-\underline{C}_2\underline{A}_2\underline{D}_2)^{-1}, \\ \underline{A}_2&=(\underline{B}_3-\underline{C}_3\underline{A}_3\underline{D}_3)^{-1}, \\ \underline{A}_3&=\underline{B}_4^{-1}. \end{aligned} \tag{A2}$$

Equations (A2) assume the existence of $\underline{G}_{11}$, $\underline{A}_1$, $\underline{A}_2$, and $\underline{A}_3$, but this assumption will be true for the applications in which we are interested.

The proof of (A2) is accomplished by using Eq. (4.3). For example, if we partition (A1) so that $\underline{D}$ in (4.3) corresponds to $\underline{B}_4$ in (A1) we have

$$\underline{G}_{11}=\left(\begin{bmatrix} \underline{B}_1 & \underline{C}_1 & \\ \underline{D}_1 & \underline{B}_2 & \underline{C}_2 \\ & \underline{D}_2 & \underline{A}_2 \end{bmatrix}^{-1}\right)_{11} \tag{A3}$$

and

$$\underline{A}_2=(\underline{B}_3-\underline{C}_3\underline{B}_4^{-1}\underline{D}_3)^{-1}. \tag{A4}$$

Applying (4.3) to (A3) we have

$$\underline{G}_{11}=\left(\begin{bmatrix} \underline{B}_1 & \underline{C}_1 \\ \underline{D}_1 & \underline{A}_1 \end{bmatrix}^{-1}\right)_{11} \tag{A5}$$

and

$$\underline{A}_1=(\underline{B}_2-\underline{C}_2\underline{A}_1\underline{D}_2)^{-1}. \tag{A6}$$

Finally, if we apply (4.3) to (A5) we have

$$\underline{G}_{11}=(\underline{B}_1-\underline{C}_1\underline{A}_1\underline{D}_1)^{-1}. \tag{A7}$$

This matrix continued-fraction formalism is especially useful for treating periodic block tridiagonal matrices. Let $\underline{P}$ be such a matrix

$$\underline{P}=\begin{bmatrix} \ddots & & & & \\ & \underline{B} & \underline{C} & & \\ & \underline{D} & \underline{B} & \underline{C} & \\ & & \underline{D} & \underline{B} & \\ & & & & \ddots \end{bmatrix} \tag{A8}$$

One can obtain a diagonal block of the inverse of $\underline{P}$ without resorting to momentum space integrals. Let $\underline{G}$ be a diagonal block of the inverse of $\underline{P}$. Then

$$\underline{G}=[\underline{B}-\underline{C}\,\underline{A}_1\underline{D}-\underline{D}\,\underline{A}_2\underline{C}]^{-1}, \tag{A9}$$

$$\underline{A}_1=(\underline{B}-\underline{C}\,\underline{A}_2\underline{D})^{-1}, \tag{A10}$$

$$\underline{A}_2=(\underline{B}-\underline{D}\,\underline{A}_2\underline{C})^{-1}. \tag{A11}$$

Thus $\underline{G}$ is determined if the matrix equations (A10) and (A11) can be solved for $\underline{A}_1$ and $\underline{A}_2$, respectively. Note that these equations are quadratic in $\underline{A}_1$ and $\underline{A}_2$ so that there will be two possible solutions for $\underline{A}_1$ and $\underline{A}_2$. The solution which one chooses depends upon the desired boundary condition at infinity.

A few simple examples will show how the procedure works. Consider the problem of obtaining a diagonal element of the Green's function for a periodic one-dimensional nearest-neighbor tight-binding Hamiltonian. The Green's function is given by

$$(z\underline{I}-\underline{H})^{-1}\begin{bmatrix} \ddots & & & \\ & z-\sigma & -w_0 & \\ & -w_0 & z-\sigma & -w_0 \\ & & -w_0 & z-\sigma \\ & & & & \ddots \end{bmatrix}^{-1}, \tag{A17}$$

where z, σ, and w_0 are scalars. Application of (A9)–(A11) yields an expression for a diagonal element of (A17)

$$G_{nn}=(z-\sigma-w_0^2A_1-w_0^2A_2)^{-1}. \tag{A18}$$

where A_1 and A_2 are determined by

$$A_1=A_2=(z-\sigma-w_0^2A_1)^{-1}. \tag{A19}$$

Solving (A19) for A_1 yields

$$A_1=\tfrac{1}{2}\{(z-\sigma)\pm[(z-\sigma)^2-4w_0^2]^{1/2}\}w_0^{-2}. \tag{A20}$$

We choose the minus sign in (A20) because it gives $\mathrm{Im}(G_{nn})<0$ and also because it can be shown that this choice of sign corresponds to outgoing waves at infinity for $\mathrm{Im}(z) > 0$. Using (A20) in (A18) yields

$$G_{nn} = [(z-\sigma)^2 - 4w_0^2]^{-1/2} . \qquad \text{(A21)}$$

This result agrees with the usual expression obtained from a momentum space integration.

The technique described above is especially useful when one wants the Green's function for a Hamiltonian consisting of an impurity cluster in an otherwise periodic medium. Consider for example the Hamiltonian (4.6). The Green's function within the cluster can be written

$$\underline{\tilde{G}} = \begin{pmatrix} z - E_1 - w_0^2 A & -w_0 & 0 \\ -w_0 & z - E_2 & -w_0 \\ 0 & -w_0 & z - E_3 - w_0^2 A \end{pmatrix}^{-1} . \qquad \text{(A21)}$$

where A is given by (A19) or (A20). The important point to note is that A is determined entirely by the medium exterior to the cluster so that it is not affected when the matrix elements of the Hamiltonian within the cluster are changed. It can be seen that Eq. (A21) is equivalent to (4.7).

As a third example consider the problem of obtaining $\overline{G}$ in the three-site one-dimensional CCPA. The Hamiltonian is given by (4.14). Let us write

$$\underline{\Sigma} = \begin{pmatrix} \sigma_1 & \sigma_2 & \sigma_3 \\ \sigma_2 & \sigma_4 & \sigma_2 \\ \sigma_3 & \sigma_2 & \sigma_1 \end{pmatrix} . \qquad \text{(A22)}$$

We can then write $zI - \overline{H}$ in the form of (A8) with

$$\underline{B} = \begin{pmatrix} z - \sigma_1 & -(\sigma_2 + w_0) & -\sigma_3 \\ -(\sigma_2 + w_0) & z - \sigma_4 & -(\sigma_2 + w_0) \\ -\sigma_3 & -(\sigma_2 + w_0) & z - \sigma_1 \end{pmatrix} , \qquad \text{(A23)}$$

$$\underline{C} = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ w_0 & 0 & 0 \end{pmatrix} , \qquad \text{(A24)}$$

and

$$\underline{D} = \underline{C}^T . \qquad \text{(A25)}$$

Equation (A9) then yields

$$\underline{G} = \begin{pmatrix} z - \sigma_1 - A & -(\sigma_2 + w_0) & -\sigma_3 \\ -(\sigma_2 + w_0) & z - \sigma_4 & -(\sigma_2 + w_0) \\ -\sigma_3 & -(\sigma_2 + w_0) & -\sigma_1 - A \end{pmatrix}^{-1} , \qquad \text{(A26)}$$

where A is obtained from the (1, 1) element of $\underline{A}_1$ or the (3, 3) element of $\underline{A}_2$. Note that $\underline{C}\,\underline{A}_1\underline{C}^T$ yields w_0^2 times the (1, 1) element of $\underline{A}_1$ and $\underline{C}^T\underline{A}_2\underline{C}$ yields w_0^2 times the (3, 3) element of $\underline{A}_2$. Thus,

$$A = w_0^2 \left(\begin{bmatrix} z - \sigma_1 & -(\sigma_2 + w_0) & \\ -(\sigma_2 + w_0) & z - \sigma_4 & -(\sigma_2 + w_0) \\ -\sigma_3 & -(\sigma_2 + w_0) & z - \sigma_1 - A \end{bmatrix}^{-1} \right)_{11} . \qquad \text{(A27)}$$

This establishes Eqs. (4.19) and (4.24).

Finally, let us obtain the cluster Green's function $\underline{\tilde{G}}$ [Eq. (4.18)] needed for the cellular CPA. This is obtained trivially because our Hamiltonian (4.14) does not differ from (2.14) except within the central cell. For this reason the boundary parameter A which represents the effect of the region exterior to the cell is unchanged. Thus,

$$\underline{\tilde{G}} = \begin{pmatrix} z - E_1 - A & -w_0 & 0 \\ -w_0 & z - E_2 - A & -w_0 \\ 0 & -w_0 & z - E_3 - A \end{pmatrix}^{-1} ,$$

where A is again given by (A27).

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