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Coherent-Potential Approximation for Alloys with Random Off-Diagonal Elements*

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The single-site coherent-potential approximation for substitutional disordered alloys is extended to include the effects of random off-diagonal elements and of the formation of clusters. Our results are in good agreement with the exact numerical computations performed on a one-dimensional system over most of the energy region.

I. INTRODUCTION

Recently, the one-electron theory of disordered binary alloys has been studied most intensively. Because of the lack of crystal symmetry in disordered alloys, their properties evaluated by statistical averages over all configurations are difficult to calculate. Therefore various approximations have emerged. The virtual crystal[1] and the t-matrix[2] approximations are the conventional approaches. More recently the coherent-potential approximation (CPA)[3–5] has been shown to be the most powerful method to treat the disordered alloys. It is a self-consistent method which serves as an interpolating scheme for the entire range of concentrations and scattering strengths in disordered alloys.

The CPA is developed within the framework of multiple scattering theory introduced by Lax.[6] Soven[3] and Taylor[4] first used the CPA to calculate the electronic density of states (EDS) and the phonon spectrum in disordered substitutional binary alloys. They introduced the concept of a coherent potential which, when placed on every site of the alloy lattice, will simulate the EDS or the phonon spectrum of the actual alloy, respectively. To determine the coherent potential, one generally requires that a single scatterer imbedded in this effective medium should produce no further scattering on the average. A detailed discussion of the CPA can be found in Velický *et al.*[5] This theory, based on a single-site approximation (SCPA), suffers from three major drawbacks: (i) its failure to produce a tail in the edge of the density of states, (ii) its restriction to alloys with composition independent off-diagonal elements, and (iii) its neglect of the effects due to the formation of clusters. The first point has been discussed by Eggarter *et al.* using a percolation theory[7] and by Schwartz using an extended CPA,[8] which includes the effects due to pairs at all distances, but excludes effects of random off-diagonal elements. The second point has been treated by Soven in the CPA for a system of muffin tin potentials,[9] in which the pure constituents have different bandwidths, and by Blackman *et al.* using the CPA in a locator expansion[10] in which the effects of clustering have not been considered. The third point has been discussed by Freed *et al.* in a cluster theory,[11] in which there is an infinite hierarchy of equations of motions [in which the n-atom Green's functions are coupled to the $(n+1)$-atom Green's function] and which provides an improvement over the SCPA and becomes more and more accurate by inclusion of larger and larger clusters. One problem is to know the optimum size of clusters convenient for machine computation and for reproducing the features of the true spectra at the same time. The SCPA corresponds to truncation in the equation of motion of a 1-atom Green's function. Berk[12] has considered the last two points in the weak-coupling limit. Montgomery *et al.*[13] have treated amorphous

Heisenberg ferromagnets using a similar perturbation approach. On the other hand, a truncation of the hierarchy to a rather low n can be justified providing the mean free path of the electron is short, as in the case of a highly disordered system.[14] The authors have proposed a two-site CPA (TCPA)[15] in which the last two points have been taken into account on the same footing.

Tanaka *et al.*[16] have proposed a similar theory as ours. Their one-dimensional results seem in disagreement with our predictions and Dean's exact solutions.[17] They treat the total Hamiltonian as a collection of uncorrelated pair potentials. Their assumption implies that, for example, in the one-dimensional case a single site may be occupied by $\frac{1}{2}A$ and $\frac{1}{2}B$ atoms simultaneously, which is unrealistic. Furthermore, one can easily show that both their diagonal and off-diagonal coherent potentials do not agree with the perturbation theory in the weak scattering limit [Eq. (27)].

In Sec. II, a modified CPA including the effects of off-diagonal randomness (TCPA) is derived. Some deficiencies of our theory (mainly due to the truncation process) are discussed in Sec. III by comparison with the perturbation theory. In this section, we have extended Montgomery's theory to substitutional alloys and derived it in detail. In Sec. IV, we discuss the TCPA and compare its numerical results with Dean's exact spectra for a finite one-dimensional alloy model (N atoms).

II. MODIFIED COHERENT-POTENTIAL APPROXIMATION

We consider a disordered binary alloy $A_{1-x}B_x$, where x is the concentration of B atom. Let us consider a tight-binding model Hamiltonian

$$H=\sum_n \epsilon_n|n\rangle\langle n| + \sum_{nm} h_{nm}|n\rangle\langle m| \ , \tag{1}$$

where the diagonal element ϵ_n is the atomic level associated with a Wannier wave function $|n\rangle$ at site n, and the off-diagonal element h_{nm} represents the hopping integral between sites n and m. Here we consider that both ϵ_n and h_{nm} are composition dependent. The energy level ϵ_n is equal to ϵ_A or ϵ_B, if the n site is occupied by an atom of type A or B, and the hopping integral h_{nm} is equal to h_{AA}, h_{BB}, or h_{AB} $(=h_{BA})$, if the n and m sites are occupied by two A atoms, two B atoms, or one A and one B atom, respectively.

The essence of the coherent-potential approximation is as follows: The alloy is considered as consisting of a random array of scatterers (type A or B) placed in an effective medium. This effective medium is described by the coherent Hamiltonian, which is to be determined self-consistently. In the single-site approximation, the criterion for the choice of the coherent potential is that a scatterer in this effective medium will produce on the average no further scattering. The single-site approximation is well justified, provided that all scatterers are point scatterers or, in other words, all elements have the same bandwidth. A direct comparison between the SCPA and Dean's exact numerical calculation shows that while there is reasonable agreement over most of the energy region, there is serious disagreement in the impurity band region.[4] The exact solution shows a great deal of structure in the impurity band which may be attributed to isolated clusters of impurity atoms. When one considers the cluster effect, the simplest and lowest-order contributions come from pairs of defects. In our case we have to consider not only the scattering due to the diagonal elements but also the scattering from the off-diagonal elements as well. To include the effect of the off-diagonal scattering, the dominant contributions come from pairs of nearest-neighbor defects. Therefore one must modify the criterion used to determine the coherent potential, and require that a pair of scatterers imbedded in the effective medium produces no further scattering on the average.

We introduce a Hamiltonian H_{eff} to describe the effective medium, the matrix elements of which are generally complex and energy dependent[3]; H_{eff} retains the full symmetry of the crystal. The Fourier coefficients of H_{eff} can be written in terms of a coherent self-energy $\Sigma'(\vec{k}, E)$

$$\langle\vec{k}|H_{\text{eff}}(E)|\vec{k}'\rangle = \delta_{\vec{k}\vec{k}'}\,[s(\vec{k})+\Sigma'(\vec{k}, E)] \ , \tag{2}$$

where $s(\vec{k})$ is the $\vec{k}$-dependent band energy. The associated Green's function can be expressed as

$$\begin{aligned} G(\vec{k}, E) &= \langle\vec{k}|\,[E-H_{\text{eff}}(E)]^{-1}\,|\vec{k}\rangle \\ &= [E-\Sigma(\vec{k}, E)]^{-1} \ , \end{aligned} \tag{3}$$

where

$$\Sigma(\vec{k}, E) = s(\vec{k}) + \Sigma'(\vec{k}, E) \ . \tag{4}$$

Here we assume that $\Sigma(\vec{k}, E)$ has the same functional form as the tight-binding expression for $s(\vec{k})$. In the one-dimensional case, it would read

$$\Sigma(\vec{k}, E) = \Sigma_0(E) + \Sigma_1(E)\cos ka \ . \tag{5}$$

The first term Σ_0 is the usual coherent potential (diagonal element) and Σ_1 is by definition the coherent hopping integral (off-diagonal element). The scatterers within this effective medium have the "scattering strengths" $(\epsilon_A-\Sigma_0)$ or $(\epsilon_B-\Sigma_0)$ for the diagonal part, depending on whether the site is occupied by an atom of type A or type B, and $(h_{AA}-\Sigma_1)$, $(h_{BB}-\Sigma_1)$, or $(h_{AB}-\Sigma_1)$ for the off-diagonal part, depending on whether the pair of sites are occupied by two atoms of type A, type B, or one atom of type A and one of type B.

In the spirit of the SCPA, we consider a single pair of scatterers (nearest neighbors) placed in the

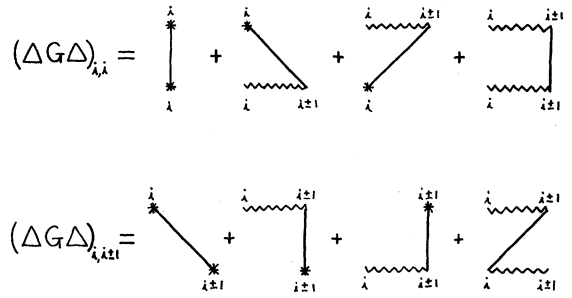

FIG. 1. Diagrammatic equations.

effective medium, and we determine the coherent potentials Σ_0 and Σ_1 by requiring no further scattering from this single pair of scatterers. The scattering potentials of this pair include the contributions from the diagonal elements of each atom and the off-diagonal elements connecting the pair of atoms. By this criterion, we neglect the scattering from atoms next to this pair, or in other words, we truncate the three-atom cluster effect.

Let us consider a pair of scatterers of type α and type β at sites 1 and 2, respectively. Their scattering potentials are given by

$$V^{\alpha\beta} = V_{11}^{\alpha\beta} |1\rangle\langle 1| + V_{22}^{\alpha\beta} |2\rangle\langle 2| + V_{12}^{\alpha\beta} |1\rangle \times \langle 2| + V_{21}^{\alpha\beta} |2\rangle\langle 1| \ , \quad (6)$$

where

$$V_{11}^{\alpha\beta} = \epsilon_\alpha - \Sigma_0, \quad V_{22}^{\alpha\beta} = \epsilon_\beta - \Sigma_0, \quad V_{12}^{\alpha\beta} = V_{21}^{\alpha\beta} = h_{\alpha\beta} - \Sigma_1 \ . \quad (7)$$

The t matrix for this pair of sites can be obtained by solving

$$\underline{T} = \underline{V} + \underline{V}\,\underline{G}\,\underline{T} \ , \quad (8)$$

where $\underline{G}$ is the coherent Green's function (corresponding to the coherent potential), and we obtain

$$T_{11}^{\alpha\beta} = [V_{11}^{\alpha\beta}(1 - V_{22}^{\alpha\beta} G_{22} - V_{21}^{\alpha\beta} G_{12}) + V_{21}^{\alpha\beta}(V_{11}^{\alpha\beta} G_{12} + V_{12}^{\alpha\beta} G_{22})]/D$$

and

$$T_{21}^{\alpha\beta} = [V_{21}^{\alpha\beta}(1 - V_{11}^{\alpha\beta} G_{11} - V_{12}^{\alpha\beta} G_{21}) + V_{11}^{\alpha\beta}(V_{21}^{\alpha\beta} G_{11} + V_{22}^{\alpha\beta} G_{21})]/D \ , \quad (9)$$

where

$$D = (1 - V_{11}^{\alpha\beta} G_{11} - V_{12}^{\alpha\beta} G_{21})(1 - V_{21}^{\alpha\beta} G_{12} - V_{22}^{\alpha\beta} G_{22}) - (V_{11}^{\alpha\beta} G_{12} + V_{12}^{\alpha\beta} G_{22})(V_{21}^{\alpha\beta} G_{11} + V_{22}^{\alpha\beta} G_{21}) \ . \quad (10)$$

Here $G_{11}\,(= G_{22})$ and $G_{12}\,(= G_{21})$ are the matrix elements of $\underline{G}$ corresponding to sites 1 and 2. In the two-site CPA, the criterion to determine Σ_0 and Σ_1 becomes

$$\langle T_{ij} \rangle \equiv \sum_{\alpha\beta} P(\alpha, \beta)\, T_{ij}^{\alpha\beta} = 0 \ , \quad (11)$$

where $ij = 11$ and 21, $\alpha\beta = AA$, BB, AB, and BA. The quantity $P(\alpha, \beta)$ represents the probability of finding an α atom at site 1 and a β atom at site 2. For a completely random disordered alloy, we have $P(A, A) = (1 - x)^2$, $P(B, B) = x^2$, and $P(A, B) = x(1 - x)$. The effect of the short-range order can be taken into account in a straightforward manner but will not be discussed in this paper. Thus the density of states can be determined from

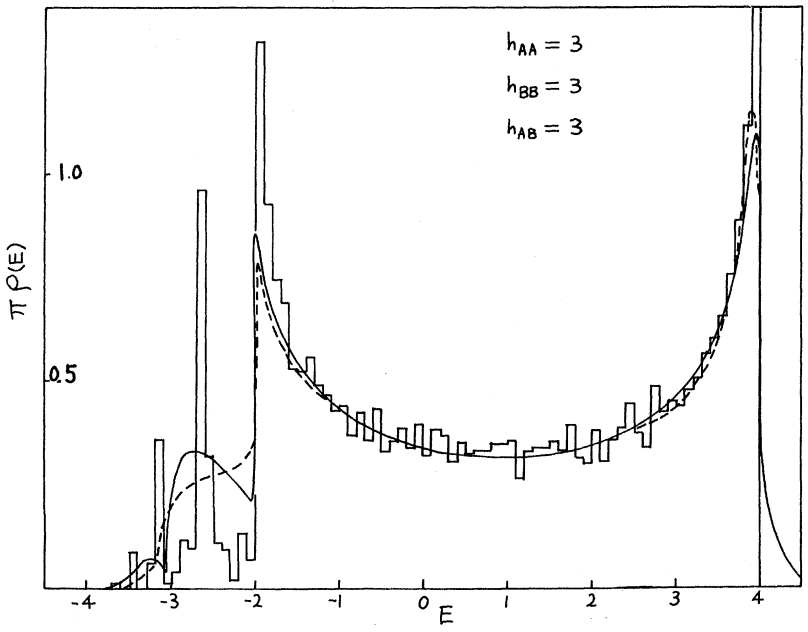

FIG. 2. Electronic density of states $\pi\rho(E)$ calculated via (1) Dean's method (histogram), (2) the SCPA (dashed line), and (3) the TCPA (solid line). $h_{AA} = h_{AB} = h_{BB} = 3$, $\epsilon_A = -\epsilon_B = 1$, $x = 0.1$, and $N = 5000$.

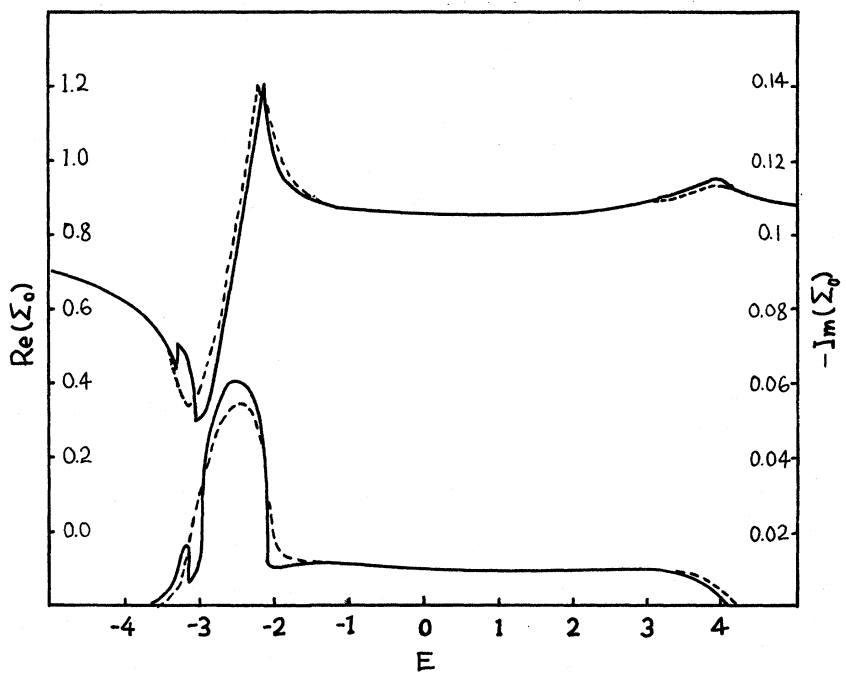

FIG. 3. Real part (upper curves) and imaginary part (lower curves) of the coherent potential Σ_0 in the SCPA (dashed line) and the TCPA (solid line). $h_{AA}=h_{AB}=h_{BB}=3$, $\epsilon_A=-\epsilon_B=1$, and $x=0.1$.

$$\rho(E)=-(\pi)^{-1}\mathrm{Im}G_{11}(E+i\eta)\ , \tag{12}$$

where η is a positive infinitesimally small number. (For the sake of convergence in computation, we take η to be 0.05.)

III. PERTURBATION THEORY: WEAK SCATTERING LIMIT

In this section, we will extend the perturbation theory introduced by Montgomery *et al.*[13] for the amorphous magnets to the disordered alloys. For convenience, we write the alloy Hamiltonian as

$$\underline{H}=\underline{\overline{H}}+\underline{\Delta}\ , \tag{13}$$

where $\underline{\overline{H}}$ is the Hamiltonian in the virtual crystal approximation, i.e., replacing ϵ_i by

$$\overline{\epsilon}=(1-x)\epsilon_A+x\epsilon_B\ , \tag{14a}$$

and h_{ij} by

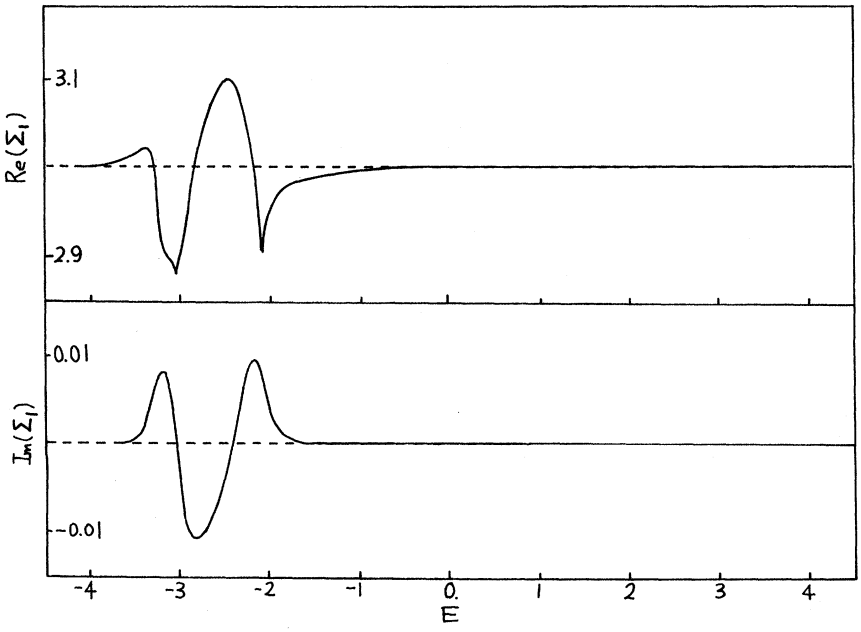

FIG. 4. Real part (upper curves) and imaginary part (lower curves) of the coherent hopping Σ_1 in the SCPA (dashed line) and the TCPA (solid line). $h_{AA}=h_{AB}=h_{BB}=3$, $\epsilon_A=-\epsilon_B=1$, and $x=0.1$.

$$\bar{h} = (1-x)^2 h_{AA} + 2x(1-x)h_{AB} + x^2 h_{BB} \ , \tag{14b}$$

and $\underline{\Delta}$ is the deviation from the mean Hamiltonian $\underline{\bar{H}}$. The exact Green's function can be expanded in power series of $\underline{\Delta}$ as

$$\underline{G} = \underline{\bar{G}} + \underline{\bar{G}}\,\underline{\Delta}\,\underline{\bar{G}} + \underline{\bar{G}}\,\underline{\Delta}\,\underline{\bar{G}}\,\underline{\Delta}\,\underline{\bar{G}} + \cdots \ . \tag{15}$$

The alloy properties are assumed to depend only on the composition average of the Green's function,

$$\langle \underline{G} \rangle = \underline{\bar{G}} + \underline{\bar{G}} \langle \underline{\Delta}\,\underline{\bar{G}}\,\underline{\Delta} \rangle \underline{\bar{G}} + \cdots \ , \tag{16}$$

where the linear term in $\underline{\Delta}$ vanishes as a consequence of averaging. In the perturbation theory, we will neglect all higher-order terms and replace them by a geometric series in $\langle \underline{\Delta}\,\underline{\bar{G}}\,\underline{\Delta} \rangle$. Here we will make a further approximation by neglecting the correlations involving three sites. Under these conditions, the Fourier transformation of $\langle \underline{G} \rangle$ becomes

$$\langle \bar{G}(\vec{k}) \rangle = \frac{\bar{G}(\vec{k})}{1 - \bar{\Sigma}'(\vec{k})\bar{G}(\vec{k})} \ , \tag{17}$$

where

$$\bar{G}(\vec{k}) = [E - \bar{H}(\vec{k})]^{-1} \tag{18}$$

and

$$\bar{\Sigma}'(\vec{k}) = \bar{\Sigma}_0' + \bar{\Sigma}_1' \cos ka \ , \tag{19}$$

for a one-dimensional model, and

$$\bar{\Sigma}_0' = \langle \underline{\Delta}\,\underline{\bar{G}}\,\underline{\Delta} \rangle_{ii} \ , \tag{20}$$

which is the diagonal element, and

$$\bar{\Sigma}_1' = \langle \underline{\Delta}\,\underline{\bar{G}}\,\underline{\Delta} \rangle_{ii+1} \ , \tag{21}$$

which is the off-diagonal element. By substituting (18) into (17), we obtain

$$\langle \bar{G}(\vec{k}) \rangle = [E - \bar{H}(\vec{k}) - \bar{\Sigma}'(\vec{k})]^{-1} \ . \tag{22}$$

Therefore we can define a self-energy

$$\bar{\Sigma}(\vec{k}) = \bar{H}(\vec{k}) + \bar{\Sigma}'(\vec{k}) = \bar{\Sigma}_0 + \bar{\Sigma}_1 \cos ka \tag{23}$$

and

$$\bar{\Sigma}_0 = \bar{\epsilon} + \bar{\Sigma}_0' \ , \tag{24}$$

$$\bar{\Sigma}_1 = \bar{h} + \bar{\Sigma}_1' \ . \tag{25}$$

In the following, we will use a diagrammatic method to discuss $\bar{\Sigma}$. The notation * is used to represent the diagonal scattering potential Δ_{ii}, the wavy line to represent the off-diagonal scattering potential $\Delta_{ii\pm1}$, and the solid line to represent a propagator (or a Green's function). The time order is from top to bottom. The initial position of the electron is at the i site and the final position can be at either the i site or the $i \pm 1$ site corresponding to the diagonal or the off-diagonal part, respectively. The diagrammatic equations are shown in Fig. 1 and can be summed up as follows:

$$\bar{\Sigma}_0' = \langle (\delta v)^2 \rangle G_0 + 4 \langle \delta v \, \delta h \rangle G_1 + 2 \langle (\delta h)^2 \rangle G_0 \tag{26}$$

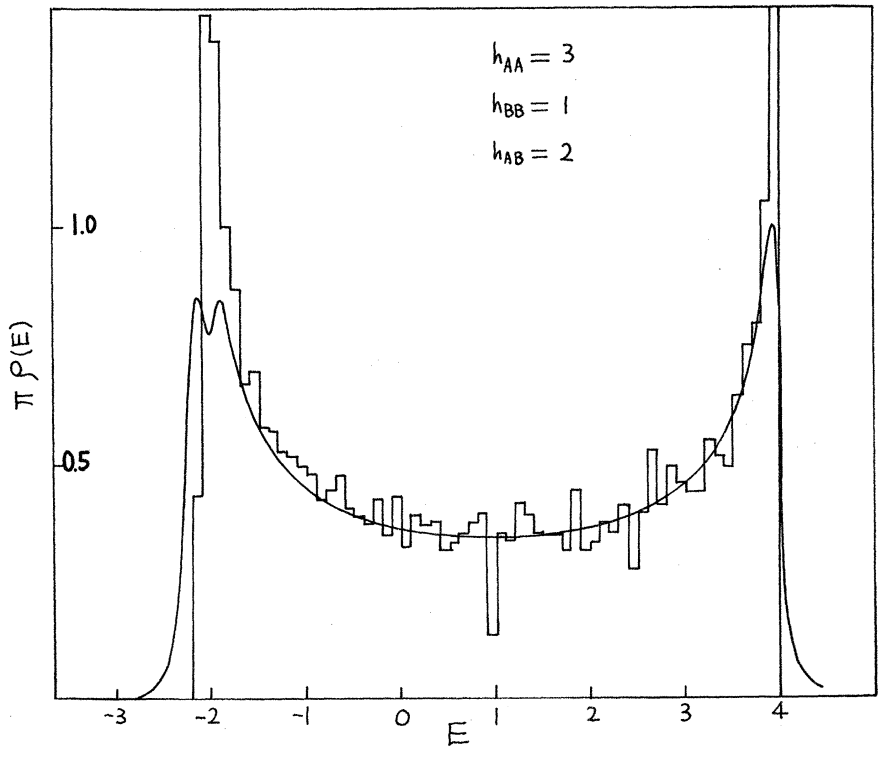

FIG. 5. Electronic density of states $\pi\rho(E)$ calculated via (1) Dean's method and (2) the TCPA. $h_{AA}=3$, $h_{AB}=2$, $h_{BB}=1$, $\epsilon_A = -\epsilon_B = 1$, $x=0.1$, and $N=5000$.

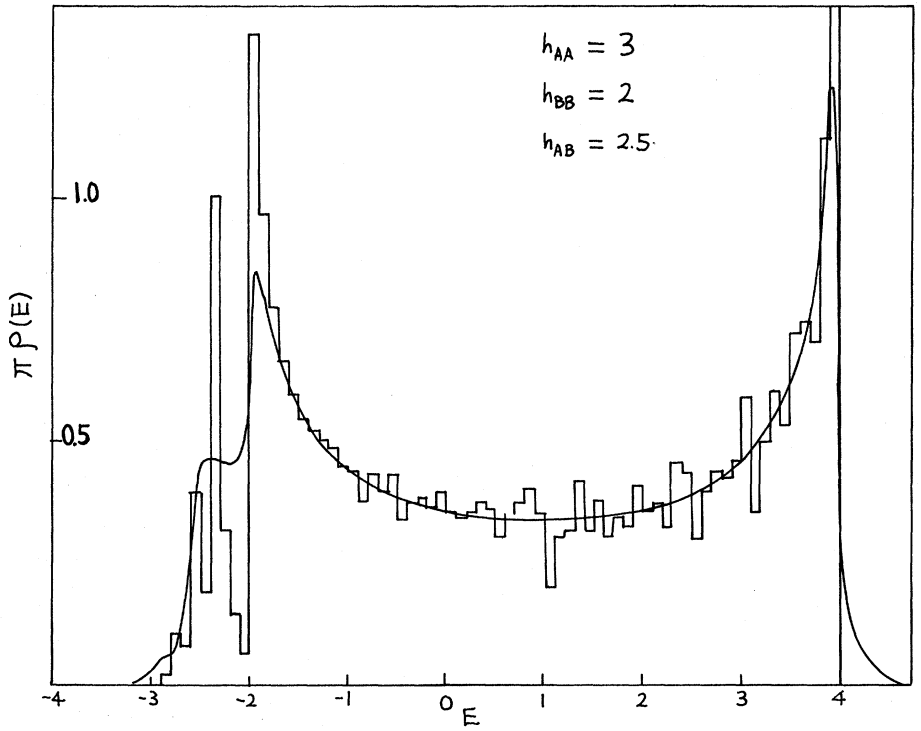

FIG. 6. Electronic density of states calculated via (1) Dean's method and (2) the TCPA. $h_{AA}=3$, $h_{AB}=2.5$, $h_{BB}=2$, $\epsilon_A=-\epsilon_B=1$, $x=0.1$, and $N=5000$.

and

$$\bar{\Sigma}_1' = \langle \delta v\, \delta v \rangle G_1 + 2\langle \delta v\, \delta h \rangle G_0 + \langle (\delta h)^2 \rangle G_1 \ , \qquad (27)$$

where $\langle\ \rangle$ represents the composition average. G_0 and G_1 denote, respectively, the matrix elements (ii) and $(i, i\pm 1)$ of the Green's function and

$$\langle (\delta v)^2 \rangle = \langle (\epsilon_i - \bar{\epsilon})^2 \rangle \ ,$$
$$\langle (\delta h)^2 \rangle = \langle (h_{ij} - \bar{h})^2 \rangle \ ,$$
$$\langle \delta v\, \delta v \rangle = \langle (\epsilon_i - \bar{\epsilon})(\epsilon_j - \bar{\epsilon}) \rangle = 0 \ , \qquad (28)$$

and

$$\langle \delta v\, \delta h \rangle = \langle (\epsilon_i - \bar{\epsilon})(h_{ij} - \bar{h}) \rangle \ .$$

Since we have neglected correlations involving three sites,

$$\langle \delta h\, \delta h \rangle = \langle (h_{ij} - \bar{h})(h_{jk} - \bar{h}) \rangle = \langle \delta h \rangle \langle \delta h \rangle = 0 \ . \qquad (29)$$

In the weak-coupling limit, the coherent potential Σ_0 and the coherent hopping Σ_1 can be expanded in terms of the scattering potentials by using Eqs. (9)–(11). To second order in the scattering potentials, they read

$$\Sigma_0 = \bar{\epsilon} + \langle (\delta v)^2 \rangle G_0 + \langle (\delta h)^2 \rangle G_0 + 2\langle \delta v\, \delta h \rangle G_1$$

and

$$\Sigma_1 = \bar{h} + \langle \delta v\, \delta v \rangle G_1\, 2\langle \delta v\, \delta h \rangle G_0 + \langle (\delta h)^2 \rangle G_1 \ . \qquad (30)$$

Since in the single-site approximation, the correlation between two sites has been also neglected and only alloys with composition-independent hopping integrals are considered, we have

$$\langle \delta v\, \delta h \rangle = 0 \ , \quad \langle (\delta h)^2 \rangle = 0 \qquad (31)$$

because

$$\delta h = 0 \ .$$

Then

$$\Sigma_0 = \bar{\epsilon} + \langle (\delta v)^2 \rangle G_0 \ , \quad \Sigma_1 = \bar{h} \ . \qquad (32)$$

By comparison with equations (27) and (30), we find that Σ_1 agrees with $\bar{\Sigma}_1$, but Σ_0 is underestimated and slightly different from $\bar{\Sigma}_0$. This can be attributed to the way we truncate the t-matrix equations in which only one nearest neighbor of site i has been considered. This difficulty is expected in any kind of self-consistent calculation in which truncation is required. Since Σ_0 describes the location of the center of the energy band and Σ_1 describes the bandwidth, the TCPA may provide a reasonable prediction of the density of states over most of the energy region. However, the location of the impurity cluster band deviates somewhat from the exact results.

In order to prove the effectiveness of such truncation and the validity of our assumption concerning the "minimum" cluster, a comparison with exact numerical computations will be presented for a one-dimensional model in Sec. IV.

IV. ONE-DIMENSIONAL ALLOY MODEL

In this section, we consider a one-dimensional

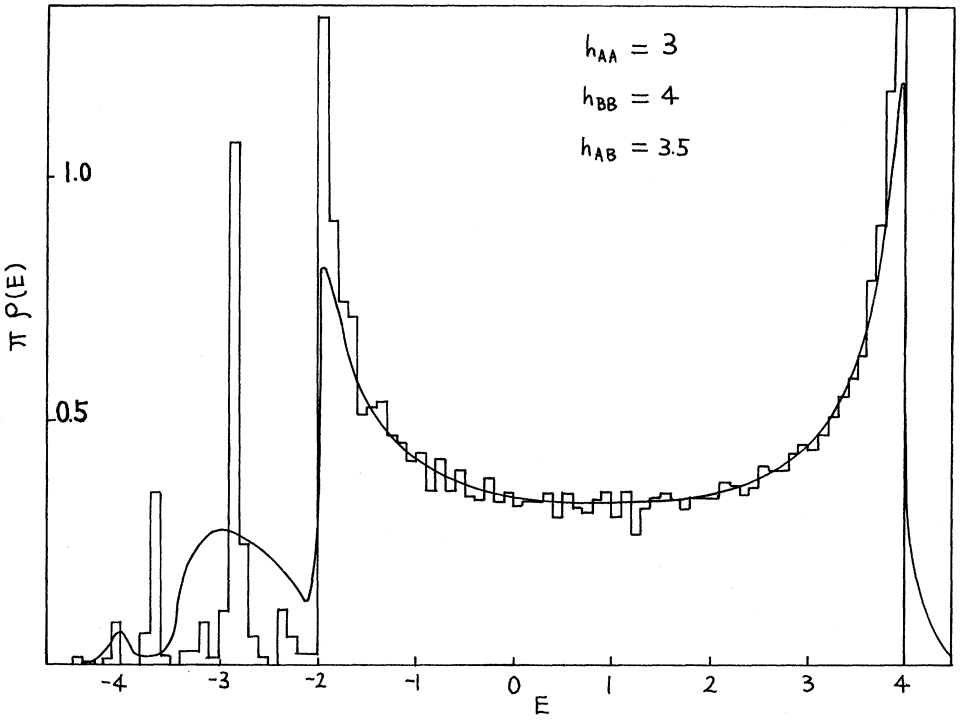

FIG. 7. Electronic density of states calculated via (1) Dean's method and (2) the TCPA. $h_{AA}=3$, $h_{AB}=3.5$, $h_{BB}=4$, $\epsilon_A=-\epsilon_B=1$, $x=0.1$, and $N=5000$.

alloy model with Hamiltonian given by (1). The corresponding coherent Green's function between sites l and l' is

$$G_{ll'}(E)=N^{-1}\sum_k \frac{e^{ik(l-l')}}{E-\Sigma_0-\Sigma_1\cos ka}\,, \tag{33}$$

where N is the total number of sites, and the summation is over the first Brillouin zone. The Green's functions G_{11} and G_{12} entering (9) are readily found to be

$$G_0\equiv G_{11}=[(E-\Sigma_0)^2-\Sigma_1^2]^{-1/2}\,,$$

$$G_1\equiv G_{12}=\Sigma_1^{-1}\,[(E-\Sigma_0)G_0-1]\,. \tag{34}$$

It remains to solve (11) to obtain Σ_0 and Σ_1 self-consistently.

It is convenient to express ϵ_A and ϵ_B in dimensionless units such that

$$\epsilon_A=1 \quad \text{and} \quad \epsilon_B=-1\,. \tag{35}$$

For convenience we will use the same energy units for the hopping integrals.

Since there is a serious disagreement between the SCPA and the exact numerical calculation in the impurity band region, we will put emphasis on this region in order to indicate whether any modification or improvement on the SCPA results from our TCPA. We consider first a dilute alloy of $x=0.1$, with composition-independent hopping integrals, for example, $h_{AA}=h_{AB}=h_{BB}=3$. The EDS calculated via the exact numerical method[17] (histogram), the SCPA (dash line), and our TCPA (solid line) are shown in Fig. 2. One sees that there is an excellent agreement in the host energy band, throughout the interval between $E=-2$ and -4. The interval between -4 and -2 is called the impurity band because the presence of these states is due to impurity effects. In the impurity band region, the histogram shows two dominant peaks, one at $E=-2.65$ and the other $E=-3.15$. The TCPA curve also shows two peaks which roughly coincide with those in the histogram, both in positions and strengths. The peak at $E=-2.65$ can be identified as the local resonant mode associated to AB pairs, while the other peak, much weaker, is due to the rarer impurity pair BB. However, one cannot identify these two peaks in the SCPA. The tails, appearing at the band edges, are due to the finite value of η. It is noticeable that although $h_{AA}=h_{AB}=h_{BB}$ for this case, the fact that Σ_1 in (5) is energy (composition) dependent modifies the general "impurity band spectrum." No such structure has been found in the perturbation theory treatment.[12] Only a shift in band edges (due to the Saxon-Hutner theorem) and some vague line-shape modification were observed. Hence at low concentration and equal bandwidths, our formalism offers already a promising improvement over the SCPA. The corresponding coherent potentials Σ_0 and Σ_1 are plotted in Figs. 3 and 4, respectively.

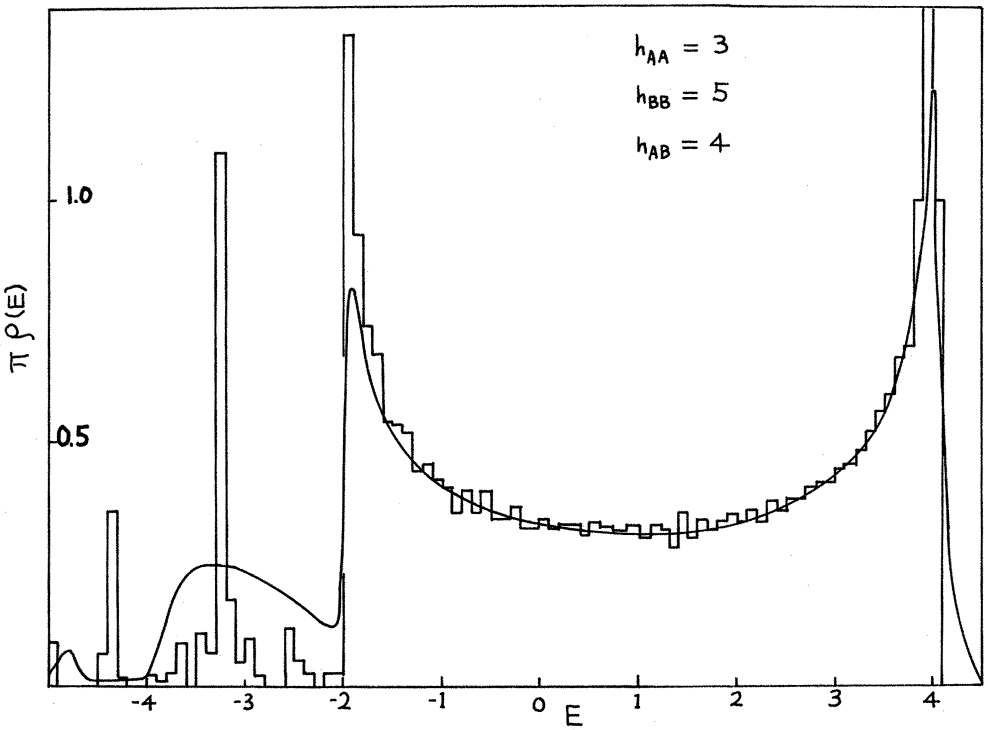

FIG. 8. Electronic density of states calculated via (1) Dean's method and (2) the TCPA. $h_{AA}=3$, $h_{AB}=4$, $h_{BB}=5$, $\epsilon_A = -\epsilon_B = 1$, $x=0.1$, and $N=5000$.

The deviations in the coherent potentials between the TCPA (solid line) and the SCPA (dashed line) also occur at the impurity band region, i.e., $-4.0 < E < -2.0$.

We then set the hopping integral of the crystal between host atoms at $h_{AA}=3$, while varying h_{BB}

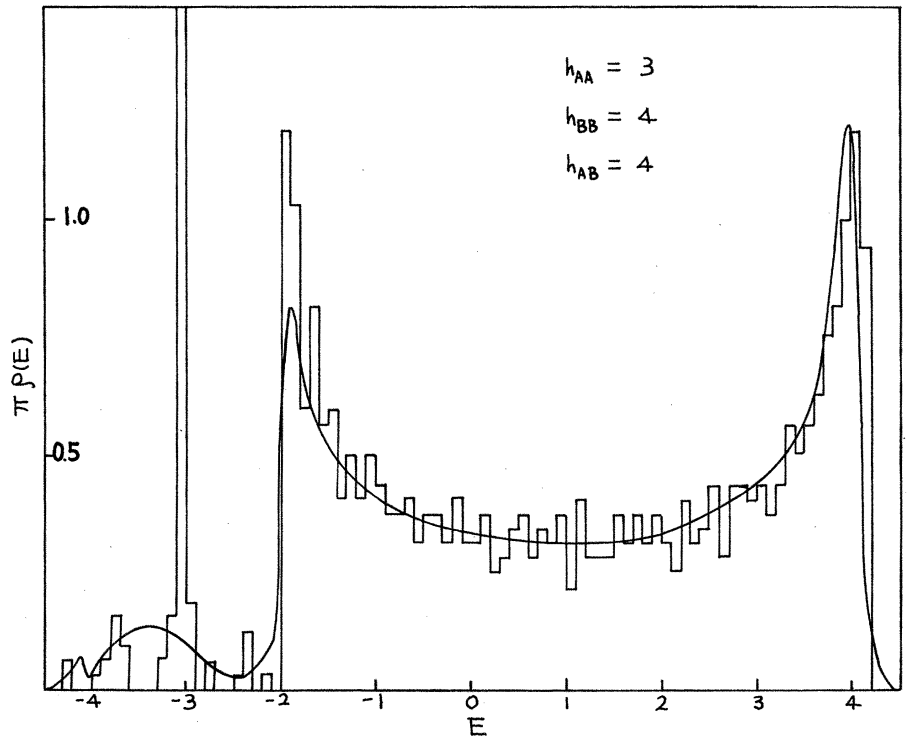

FIG. 9. Electronic density of states calculated via (1) Dean's method and (2) the TCPA. $h_{AA}=3$, $h_{AB}=h_{BB}=4$, $\epsilon_A=-\epsilon_B=1$, $x=0.1$, and $N=1000$.

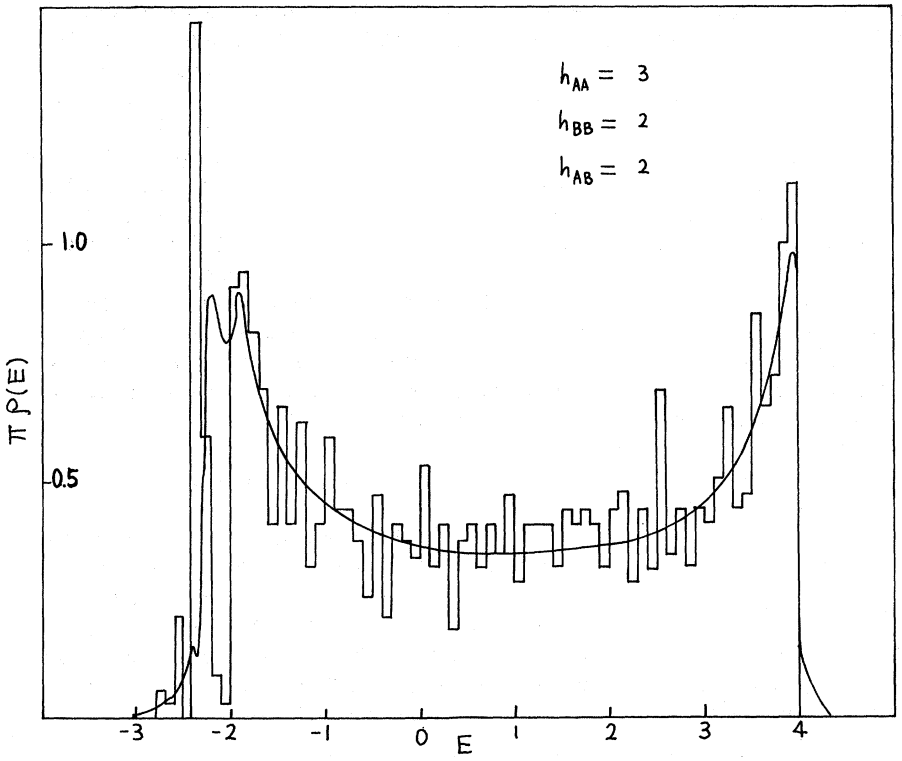

FIG. 10. Electronic density of states calculated via (1) Dean's method and (2) the TCPA. $h_{AA}=3$, $h_{AB}=h_{BB}=2$, $\epsilon_A=-\epsilon_B=1$, $x=0.1$, and $N=1000$.

from 1 to 5, and let $h_{AB}=\frac{1}{2}(h_{AA}+h_{BB})$. The EDS in the TCPA is compared with the exact solution in Figs. 5–11. For $h_{BB}<h_{AA}$, we notice that the impurity band moves closer to and partially merges with the host band. For $h_{BB}>h_{AA}$, the two peaks in the impurity band region move away from the host

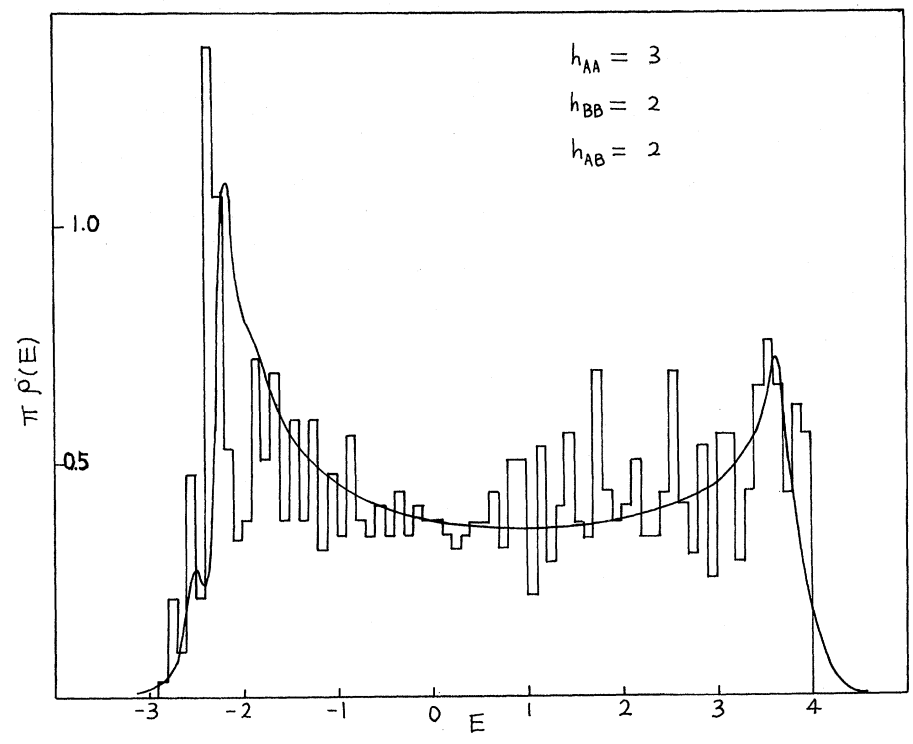

FIG. 11. Electronic density of states calculated via (1) Dean's method and (2) the TCPA. $h_{AA}=3$, $h_{AB}=h_{BB}=2$, $\epsilon_A=-\epsilon_B=1$, $x=0.2$, and $n=1000$.

band. The TCPA results are generally in good agreement with the exact solutions, especially for the larger peak corresponding to the AB pairs. The smaller peak in solid line which corresponds to the BB pairs does not coincide, however, with that in the histogram. The disagreement may be attributed to our underestimating the correction due to all nearest neighbors. This disagreement becomes less obvious when the randomness in hopping integrals becomes smaller, or when the impurity band is not well defined. In Fig. 9, we consider the case of $h_{AA}=3$, $h_{AB}=h_{BB}=4$, and $x=0.1$. One sees that the impurity states are reasonably reproduced. In Figs. 10 and 11, we consider cases of $h_{AA}=3$, $h_{AB}=h_{BB}=2$, with $x=0.1$ and 0.2, respectively. For $x=0.1$, there are three well-defined peaks in the lower-energy region. For $x=0.2$, one of the peaks in the lower-energy region has merged into the host band and the band edge in the higher-energy side becomes damped.

V. CONCLUSION

The two-site coherent-potential theory proposed in this paper is similar in some ways to the two-atom Green's-function truncation of the cluster theory.[11] Clearly this approach suffers (like all similar approximations) from some deficiencies. In particular, because only one neighbor is taken into account in the truncation process the effects of clustering and disorder on Σ_0 may be underestimated while the effects on Σ_1 are probably more accurate, thus suggesting that when the "scattering strengths" are large, the calculated location of the impurity cluster band is less reliable. On the other hand this theory has the advantage of taking into account both clustering and the off-diagonal elements and treating these two effects self-consistently and on the same footing. This method can be applied to a three-dimensional model as well. Such calculation is now in progress.[18]

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