Self-consistent boundary site approximation in the cluster theories of disordered alloys*

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A simple method is proposed for applying the self-consistent boundary site approximation (SCBSA) in cluster theories of electronic states in disordered alloys. This method is applicable to lattices of any dimensionality. The electronic densities of states are calculated for binary alloys having the simple cubic and the diamond lattice structures. These results are compared with the results obtained from the method of moments, the disordered field formalism, the coherent-potential approximation, and a few other methods. In addition to this, the averaged Green's function has been calculated in the complex energy plane to study its analytic structure. It is found that though the SCBSA is computationally simple and yields densities of states which agree quite well with the available exact results, in three dimensions, the SCBSA shows some unphysical features such as the negative partial densities of states and branch points off the real axis for the averaged Green's function in the strong-scattering regime.

I. INTRODUCTION

During the last few years several extensions of the coherent-potential approximation (CPA) have been proposed in order to incorporate the cluster effects in the study of electronic states in disordered alloys.[1] A theoretical advance in this direction was made by Tsukada,[2] who proposed the molecular CPA (MCPA). However, from a practical viewpoint, the complete implementation of such a theory to real systems is extremely difficult. Approximate theories like the self-consistent central-site approximation[3-6] (SCCSA) and the self-consistent boundary-site approximation[7,8] (SCBSA) have been suggested, which simplify the calculations a great deal. The SCCSA[7,9-11] yields the fine structure in the density-of-states curves as observed in exact machine calculations, and its results agree fairly well with the MCPA results,[7] but it suffers from the difficulties of nonanalyticity in the strong-scattering regime,[8,12] where the clustering effects become quite important. Butler,[7] however, showed that the SCBSA was equivalent to the MCPA[13] for a linear chain. This equivalence of the SCBSA and the MCPA does not hold for real three-dimensional lattices. Nevertheless, with this unexpected success of the SCBSA, for a linear chain, it was naturally very tempting to test the usefulness of the SCBSA for three-dimensional lattices. The authors[8] suggested a simple generalization of the SCBSA approach which is applicable to lattices of any dimensionality. Using a simple tight-binding model description, it was found that the nonanalyticities observed in the SCCSA for a diamond lattice were not there in the

SCBSA for a 50-50 binary alloy $A_{1-x}B_x$, with $\delta = (\epsilon_B - \epsilon_A)/\omega = 1.0$. Here ϵ_A and ϵ_B are the atomic energy levels of the pure A and the pure B constituents and ω is the half bandwidth which is assumed to be the same for both the constituents. Further it was observed that the SCBSA yielded a density of states which was not much different from the CPA and failed to reproduce the fine structure in the density of states. It is important to mention that we calculated the densities of states at the boundary of the cluster. As the number of nearest neighbors increases (e.g., the cubic lattices), the computational effort needed increases a lot because the configurational averages have to be performed over a large number of configurations. Here we propose another simpler method in which the number of distinct configurations is greatly reduced by making an assumption that for a fixed number of different kinds of atoms on the shell of nearest neighbors, the different configurations of the atoms on the shell are not distinguished. This has been applied to calculate the electronic densities of states for binary alloys having the simple cubic and the diamond lattice structures. These results have been compared with the other available results obtained from various cluster theories, namely the method of moments,[11] the disorder field formalism,[15] the SCCSA,[5,8,16] and the cluster CPA of Kumar *et al.*[17] It has been found that the SCBSA reproduces well the fine structure if the densities of states are calculated at the center of the cluster, rather than at the boundary of the cluster. This has also been emphasized earlier by Butler.[7] But, in the strong-scattering regime, it yields some unphysical features such as

negative partial densities of states. To study the analyticity of the Green's function in this approximation we extended our calculations for complex energies. It has been found that the SCBSA yields average Green's functions which have singularities off the real axis. Therefore this approximation would not be acceptable in the strong-scattering regime for three-dimensional lattices. The region of analyticity of the SCBSA is much greater[8,18] than that of the SCCSA. This indicates that the SCBSA is superior to the SCCSA.

In Sec. II we present the general formulation of the SCBSA. In Sec. III results of the averaged densities of states and the partial densities of states for binary alloys having the diamond lattice and the simple cubic lattice structures have been presented and discussed.

II. FORMULATION

We consider a binary alloy $A_{1-x}B_x$ described within a single-band tight-binding approximation. The one-electron Hamiltonian is

$$\underline{H} = \sum_i |i\rangle\langle i| \epsilon_i + \sum_{ij; i\neq j} h_{ij} |i\rangle\langle j| = \underline{D} + \underline{W}. \tag{1}$$

Only the diagonal terms ϵ_i's are assumed to be random and can have values ϵ_A or ϵ_B with the probability $1-x$ or x, respectively. The transfer integrals h_{ij} are assumed to be nonzero only between nearest neighbors.

The alloy Green's function is defined as

$$\underline{G}(z) = (z\underline{I} - \underline{H})^{-1}, \tag{2}$$

where $z = E + i\eta$ is the complex energy having an infinitesimal positive imaginary part η and $\underline{I}$ is the unit matrix.

In the MCPA formalism the whole system is divided into clusters containing several sites. The coherent potential matrix Σ which describes the effective medium, is then an $n \times n$ matrix,[14] where n is the number of sites in the cluster. Within the SCBSA one chooses it to be a scalar coherent potential as in the usual CPA, i.e., $\Sigma = \sigma I_n$, where I_n is the $n \times n$ unit matrix. The effective-medium Green's function is then

$$\overline{\underline{G}}(z) = [(z - \sigma)\underline{I} - \underline{W}]^{-1}. \tag{3}$$

Here we consider clusters consisting of a central site and its Z nearest neighbors. Then analogous to the single-site CPA, one such cluster c is thought to be immersed in the effective medium. The Green's function $\underline{G}^c$ for such a system can be written

$$\underline{G}^c = \left(\overline{\underline{G}}^{-1} - \sum_{i\in c} |i\rangle(\epsilon_i - \sigma)\langle i|\right)^{-1}. \tag{4}$$

This can be expressed in terms of a Green's function G^s of a system in which the central site is also occupied by a fictitious atom with site energy σ. Then,

$$\underline{G}^c = \underline{G}^s + \underline{G}^s \underline{V}^0 \underline{G}^c, \tag{5}$$

where $\underline{V}^0 = |0\rangle(\epsilon_0 - \sigma)\langle 0|$, and 0 denotes the central site.

Now the Green's function G^s can easily be expressed in terms of the effective-medium Green's function $\overline{G}$:

$$\underline{G}^s = \overline{\underline{G}} + \overline{\underline{G}} \underline{T}^s \overline{\underline{G}}, \tag{6}$$

where

$$\underline{T}^s = \underline{V}^s(\underline{I} + \overline{\underline{G}} \underline{T}^s), \tag{7}$$

and

$$\underline{V}^s = \sum_{i\in s} |i\rangle(\epsilon_i - \sigma)\langle i|. \tag{8}$$

s denotes the shell of nearest neighbors.

In order to determine the effective medium within the SCBSA, we choose the following condition:

$$\sum_{p_c} \left(\frac{1}{Z} \sum_{i\in s} G^c_{ii}\right) p_c = \overline{G}(0), \tag{9}$$

where p_c is the weighted probability of a cluster configuration and $\overline{G}(0)$ is the diagonal matrix element of $\overline{G}$.

The matrix elements of G^c are obtained from Eq. (5):

$$\frac{1}{Z}\sum_{i\in s} G^c_{ii} = \frac{1}{Z}\sum_{i\in s} G^s_{ii} + \frac{V^0_{00}}{1 - V^0_{00}G^s_{00}} \frac{1}{Z}\sum_{i\in s} G^s_{0i}G^s_{i0}. \tag{10}$$

Equation (6) is then solved to obtain

$$G^s_{00} = \overline{G}(0) + \overline{G}^2(R)\sum_{ij\in s} T^s_{ij} = \overline{G}(0) + Z\overline{G}^2(R)T, \tag{11}$$

where

$$T = \frac{1}{Z}\sum_{ij\in s} T^s_{ij},$$

$\overline{G}(R)$ is the matrix element of $\overline{G}$ between two nearest-neighbor sites, and R denotes the nearest-neighbor separation. For a single-band model the matrix elements of $\overline{G}$ depend only on the separation between the two sites. Also,

$$\frac{1}{Z}\sum_{i\in s} G^s_{ii} = \overline{G}(0) + \frac{1}{Z}[\overline{G}(0) - \overline{\Gamma}]^2 \sum_{i\in s} T^s_{ii}$$
$$+ [2\overline{\Gamma}\,\overline{G}(0) + (Z-2)\overline{\Gamma}^2]T \tag{12}$$

and

$$\frac{1}{Z}\sum_{i\in s} G^s_{0i}G^s_{i0} = \overline{G}^2(R)(1 + Z\overline{\Gamma}T)^2\left(1 + \frac{2}{Z}[\overline{G}(0) - \overline{\Gamma}]\sum_{i\in s} t_{ii}\right.$$
$$\left. + \frac{1}{Z}[\overline{G}(0) - \overline{\Gamma}]^2 \sum_{i\in s} t^2_{ii}\right), \tag{13}$$

where

$$t_{ii} = V_{ii}^s / \{1 - V_{ii}^s [\overline{G}(0) - \overline{\Gamma}]\} .$$ (14)

Here the matrix elements of the effective-medium Green's function between two different sites of the shell s are approximated by $\overline{\Gamma}$, which is defined as

$$\overline{\Gamma} = \frac{1}{Z-1} \sum_{j \neq i; \, j \in s} \overline{G}_{ij} .$$ (15)

This approximation was initially suggested by Brouers et al.[5,9] to simplify the calculations in their study of the SCCSA. It is exact in the case of a linear chain.

Expressions for T and T_{ii}^s are obtained from Eq. (7):

$$T = \frac{1}{Z}(1 + Z\overline{\Gamma}T) \sum_{i \in s} t_{ii}$$ (16)

and

$$\frac{1}{Z} \sum_{i \in s} T_{ii}^s = \frac{1}{Z} \sum_{i \in s} t_{ii} + \frac{\overline{\Gamma}}{Z}(1 + Z\overline{\Gamma}T) \sum_{i \in s} t_{ii}^2 .$$ (17)

The quantities $\overline{G}(R)$ and $\overline{\Gamma}$ can easily be expressed[9,10] in terms of $\overline{G}(0)$ to obtain

$$\overline{G}(R) = [(z - \sigma)\overline{G}(0) - 1]/\omega$$ (18)

and

$$\overline{\Gamma} = [Z(z - \sigma)\overline{G}(R)/\omega - \overline{G}(0)]/(Z-1) .$$ (19)

Once the effective medium is determined by solving the condition (9), the partial and the total averaged densities of states are then determined in the two following ways: (i) at the boundary of the cluster using the following expressions for the partial and total averaged densities of states:

$$\rho^c(E) = -\frac{1}{\pi Z} \text{Im} \sum_{i \in s} G_{ii}^c$$ (20)

and

$$\rho(E) = -1/\pi \, \text{Im}\overline{G}(0) ,$$ (21)

respectively; and (ii) at the center of the cluster using the relations

$$\rho^c(E) = -1/\pi \, \text{Im}G_{00}^c$$ (22)

and

$$\rho(E) = \sum_{p_c} p_c \rho^c(E) .$$ (23)

The expression for G_{00}^c can be obtained from (5)

$$G_{00}^c = G_{00}^s / (1 - G_{00}^s V_{00}^0) ,$$ (24)

where G_{00}^s is given by Eq. (11).

III. RESULTS AND DISCUSSION

We have calculated the densities of states for binary alloys having the simple cubic and the dia-

mond lattice structures. The input densities of states for the pure constituents were calculated using the continued fraction coefficients.[19] The densities of states calculated at the boundary site of the cluster using the condition (21) are represented as SCBSA(B), whereas the densities of states calculated at the center of the cluster using the condition (23) are represented as SCBSA(C).

A. Simple cubic lattice

Our results for binary alloys having the simple cubic lattice structure are shown in Figs. 1–5. The half bandwidth of the pure constituents is taken to be unity. In Fig. 1, we have shown the minority band of an alloy with $\delta = 1.25$, and $x = 0.05$. The CPA result, and the results obtained from two other cluster theories, the SCCSA[16] and the Bethe-Peierls approximation[5] (BPA) of Brouers et al., and the method of moments[11] have also been shown for comparison. It can be easily noticed from the figure that the various peaks in the SCBSA(B) and the SCBSA(C) are centered at about the same energies as in the SCCSA, the BPA, and the method of moments. However, we also notice a difference in the results obtained from the SCBSA(B), and the SCBSA(C). In the case of the SCBSA(B) various peaks are less prominent as compared to the results obtained from other methods. Particularly the central peak in the SCBSA(B) which looks very similar to the one in the CPA, is not well defined. The results of the SCBSA(C) agree fairly well with the SCCSA, the BPA, and the method of moments, except that the peaks in the SCBSA(C) are more intense. The method of moments gives a band which is wider than the one obtained from any other method mentioned here. This is because of the smaller size of the cluster considered in the SCBSA, or the SCCSA, as compared to the method of moments where a cluster of 7175 atoms has been used. Lifshitz[20] has argued that the tailing becomes more prominent as we increase the cluster size very much. The results of the moment method given here are more or less the same as the exact results obtained by Alben et al.[21] Therefore the SCBSA(C) results are in good agreement with the exact results.

Figure 2 corresponds to an alloy with $\delta = 1.0$, and $x = 0.5$. The SCBSA(B) results are more or less the same as the CPA results (not shown in the figure). The SCBSA(C) result shows peaks at $E \simeq \pm 0.635$ which agrees well with the one obtained from the method of moments. This corresponds to configurations where a $B(A)$ atom is surrounded by $6A$ or $5A$ ($6B$ or $5B$) atoms as can be seen from Fig. 3 where we have plotted the partial densities of states in the SCBSA(C). However, the
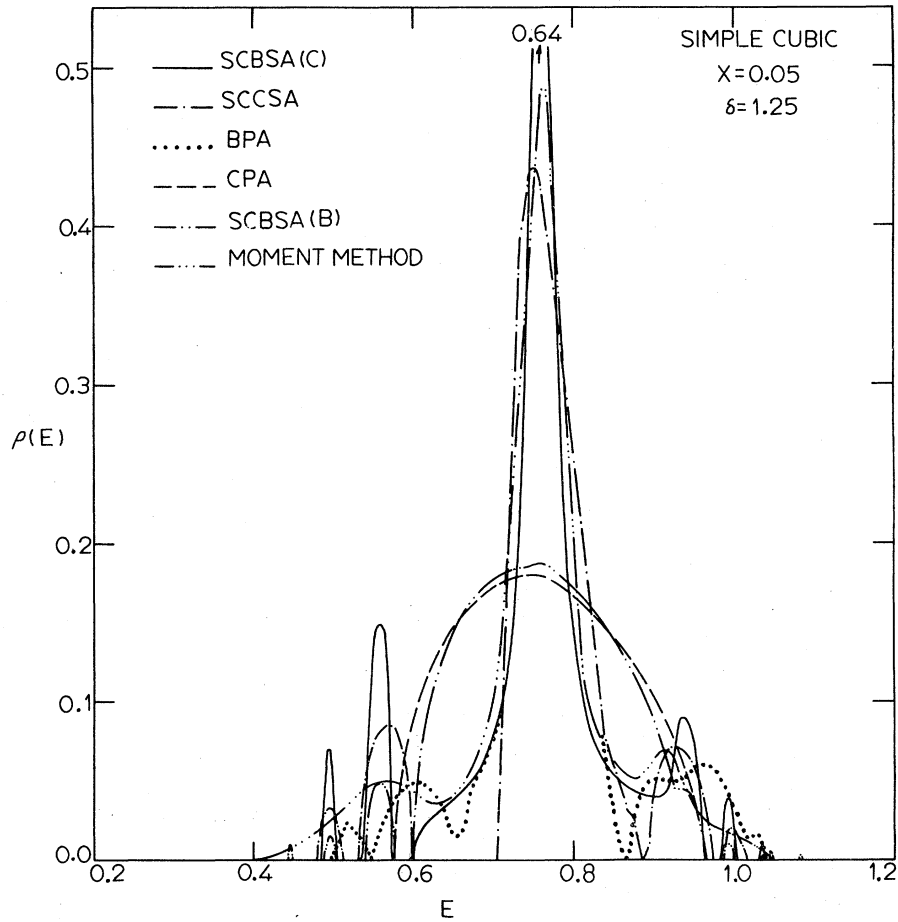
FIG. 1. Minority band of
the density-of-states
curves for a binary alloy
having the simple cubic
(sc) lattice structure. The
half bandwidth ω is taken
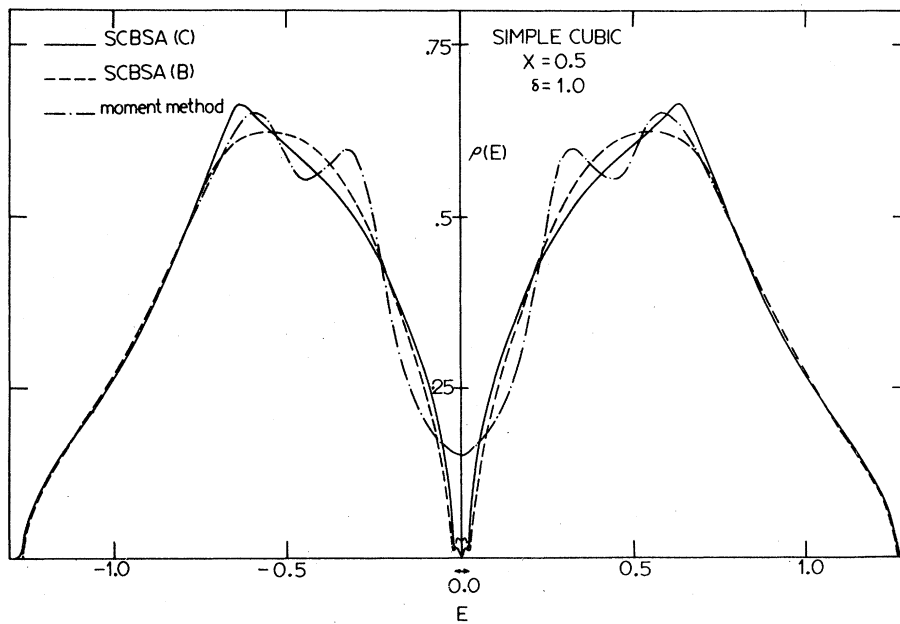to be unity, $\delta = 1.25$, and
$x = 0.05$.

FIG. 2. Density-of-
states curves for a binary
alloy having sc lattice
structure. $\delta = 1.0$, and
$x = 0.5$. The arrow shows
the region where nonphy-
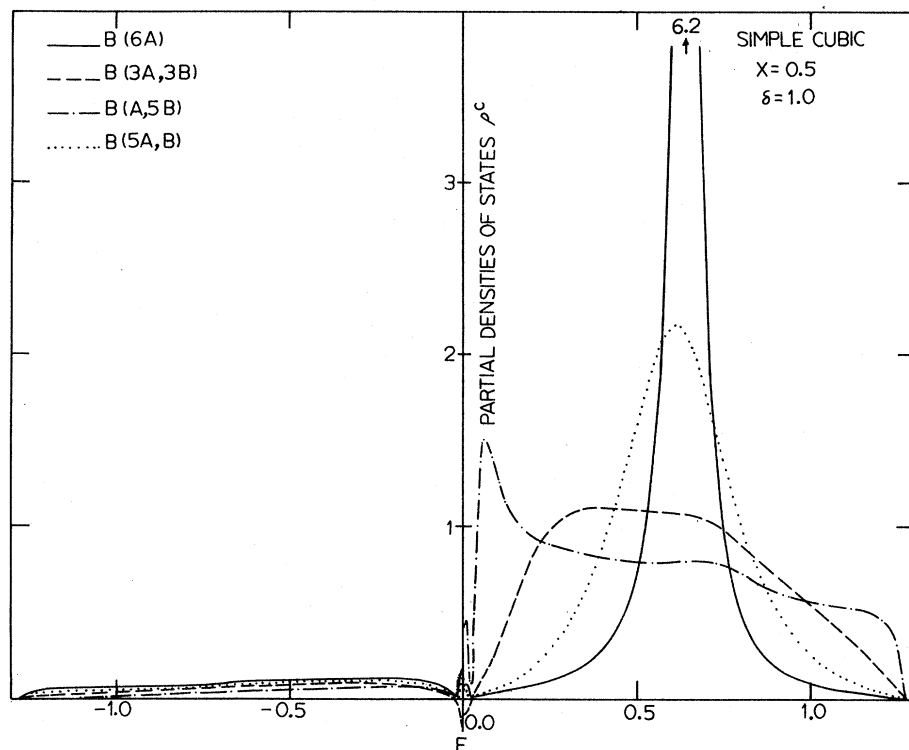sical results are obtained
in the SCBSA.

FIG. 3. Representative plots of the partial densities of states. The parameters are the same as in Fig. 2. The curves are discontinuous at $E = 0.0$. The solid, dashed, dash-dot and dotted lines, respectively, correspond to cluster configurations where an impurity atom B is surrounded by $6\,A$, $3\,A$ and $3\,B$, $1\,A$ and $5\,B$, and $5\,A$ and $1\,B$.

SCBSA(C) misses peaks at $E \simeq \pm 0.325$ and shows some unphysical results in the energy interval $E \simeq -0.02$ to $E \simeq +0.02$. In this region some of the partial densities of states become negative which is obvious from Fig. 3. It is further noticed from Fig. 3 that the partial densities of states do not match at $E = 0.0$, i.e., there are discontinuities in the partial densities-of-states curves. This is a sign of nonanalyticity. This aspect will be discussed in detail when we consider results for an alloy having $\delta = 2.2$, and $x = 0.1$. The overall agreement with the moment method is reasonably good except near $E = 0$.

In Fig. 4 we have shown the minority band of an alloy with $\delta = 2.2$, and $x = 0.1$. This corresponds to a split band case. It is obvious from the figure that the SCBSA(B) result is not much different from the CPA result. However, the SCBSA(C) reproduces the fine structure as observed in the result of the moment method. The central peak in the SCBSA(C) is more intense compared to the result of the method of moments, whereas the other peaks are subdued. The partial densities of states are found to become negative in the energy region below $E = 0.91$. At certain energies even the total averaged density of states is found to be negative. The results in this energy region are not reliable at all. To investigate the analyticity of the SCBSA,
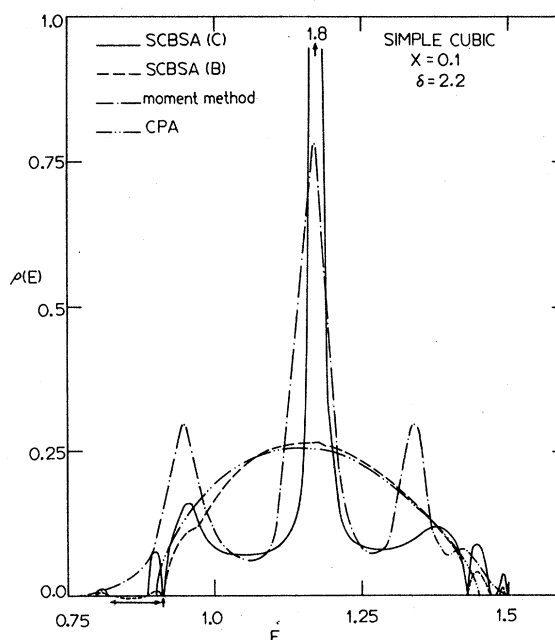

FIG. 4. Minority band of the density-of-states curves for the simple cubic binary alloy with $\delta = 2.2$, and $x = 0.1$. The vertical arrow shows the region where the branch points occur off the real axis. The horizontal arrow shows the region where some of the partial densities of states are negative.
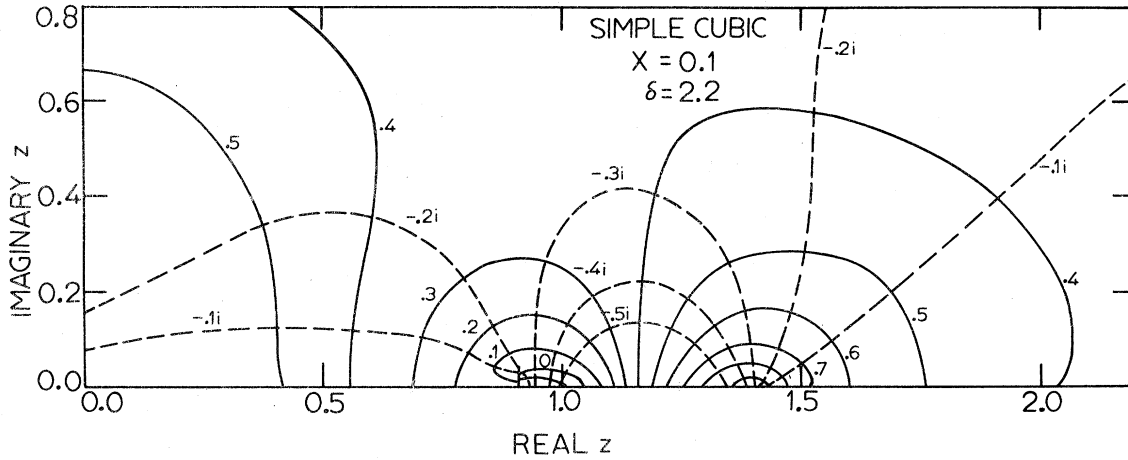
FIG. 5. Contours of equal real and imaginary parts of the averaged Green's function $\overline{G}(0)$ in the SCBSA. The various parameters are the same as in Fig. 4. The solution has been chosen in such a manner that $\overline{G}(z) \approx 1/z$ as $z \to \infty\,(\mathrm{Im}\,z > 0)$. A branch cut has been drawn at $\mathrm{Re}\,z \approx 0.91$.

we extended these calculations to the complex energy plane. In Fig. 5, we have plotted contours of equal, real, and imaginary parts of the averaged Green's function. The correct solution was chosen by starting at a very large value of the energy where we know the asymptotic behavior of the averaged Green's function $(G \approx 1/z)$. This root was then followed towards the energy region of interest. It is noticed that branch points off the real axis occur for $\mathrm{Re}\,z \approx 0.91$ where a branch cut has been drawn parallel to imaginary z axis. The density of states is different if we cross $E = 0.91$ from right to left, and from left to right. From this calculation it is apparent that the SCBSA is nonanalytic in the strong scattering regime and

for concentrated alloys. It is our conjecture that one will face the problem of nonanalyticity of the averaged Green's function in a region where the partial densities of states become negative. These difficulties have already been discussed in detail by Nickel and Butler[12] and Butler.[7]

B. Diamond lattice

Our results for binary alloys having the diamond lattice structure are shown in Figs. 6–9. The half bandwidth of the pure constituents has been taken to be 4. In Fig. 6 we have shown the results for $\delta = 1.0$, and $x = 0.5$. The curves are symmetric about $E = 0$. As in the case of the simple cubic
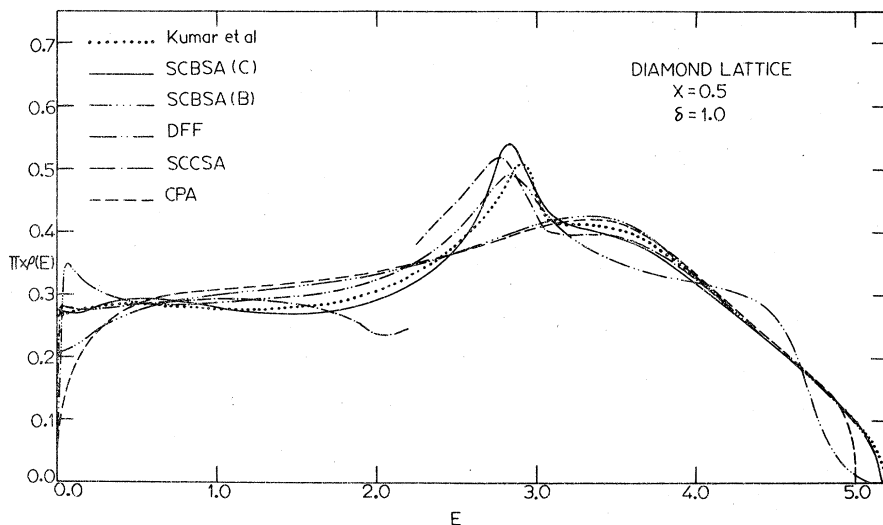

FIG. 6. Density-of-states curves for a binary alloy having the diamond lattice structure. $\delta = 1.0$, $x = 0.5$, and $\omega = 4.0$. The curves are symmetric about $E = 0$. The SCCSA result shows a discontinuity at $E \approx 2.25$. The result of SCBSA(C) and those of Kumar *et al.* are very much similar.
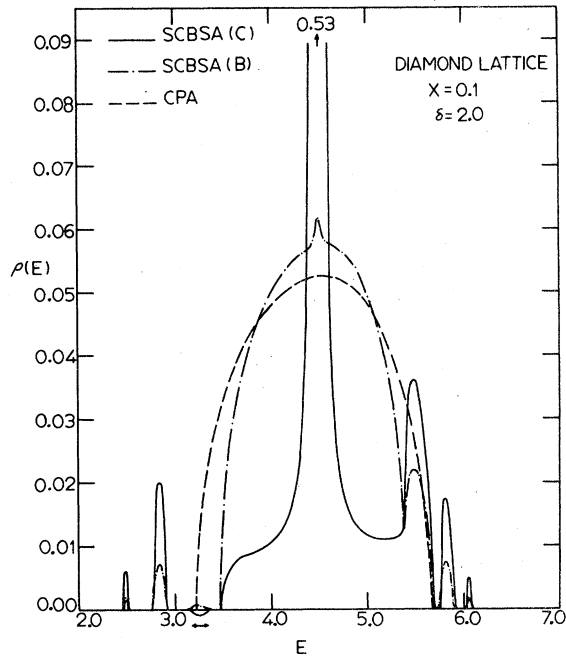
FIG. 7. Minority band of the density-of-states curves for a binary alloy having the diamond lattice structure $\delta = 2.0$, $x = 0.1$, and $\omega = 4.0$. The horizontal arrow shows the region where some of the partial densities of dates are negative.

lattice, the SCBSA(B) results are not much different from the CPA results, except that in the case of the SCBSA(B) the band is wider and there is no band gap. On the other hand the SCBSA(C) shows a peaky structure. This matches well with the results obtained from the disorder field formalism[15] (DFF), and the cluster CPA of Kumar et al.[17] The only marked distinction between the SCBSA(C) result and the DFF is that in the DFF the band splits, whereas in the SCBSA(C) it does not. In fact the DFF results obtained by Mookerjee are not reliable at the band edges and at the center of the band because of some mistakes in the calculation of the environment.[22] The DFF is equivalent[23] to using a full cluster self-energy as in the MCPA. Therefore we see that the SCBSA(C) is a good approximation for the diamond lattice. In contrast to the simple cubic lattice, here there is no difficulties of nonanalyticity or negative partial densities of states with $\delta = 1.0$, and $x = 0.5$. The SCCSA is nonanalytic for this case. We expect that even for the diamond lattice, the band will not split for $\delta = 1.0$, and $x = 0.5$, if an exact calculation is done similar to the one done by Alben et al.[21] for the simple cubic lattice.

In Fig. 7 we have shown the minority band of relatively dilute binary alloy with $\delta = 2.0$, and x

= 0.1. This corresponds to the split band region. The SCBSA(B), as well as the SCBSA(C) show fine structure in the densities of states. However, the peaks are more intense in the case of SCBSA(C). There are no results available for this particular case from other methods. As in the case of the simple cubic alloys, here we also face the problem of negative partial densities of states. In the case of the SCBSA(B) the partial densities of states are shown in Fig. 8. In a small region of energy between $E \approx 3.461$, and $E \approx 3.473$, some of the partial densities of states become negative (this feature is shown in an insert at the lower part of the figure), whereas the total averaged density of states is positive. In the case of the SCBSA(C) the partial densities are positive in this region. But near $E \approx 3.2$, in both the SCBSA(B) and the SCBSA(C),
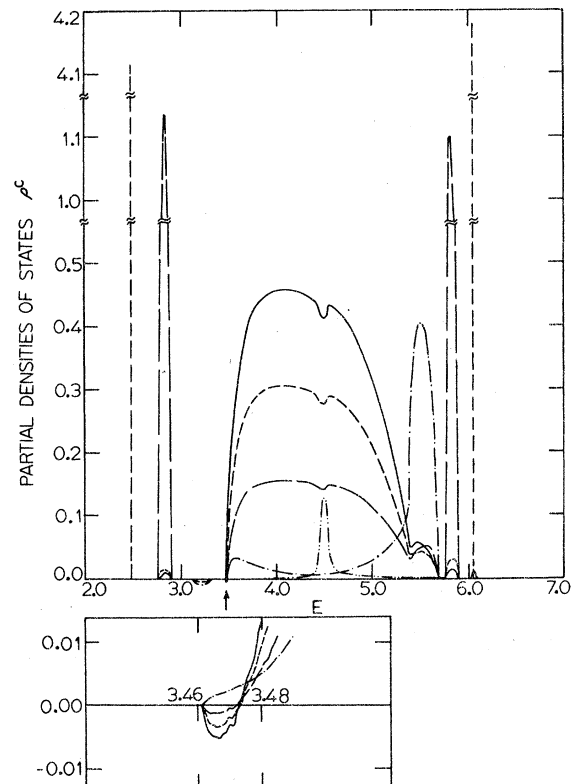

FIG. 8. Plots of the partial densities of states in the minority band in the SCBSA(B). The parameters are the same as in Fig. 7. The solid, dashed, long-dash, dash-dot, and dash–double-dot lines, respectively, correspond to cluster configurations in which an impurity atom B is surrounded by 4 B, 3 B, and 1 A, 2 B and 2 A, 1 B, and 3 A and 4 A. See the missing peaks near $E \approx 3.2$. The arrow indicates the region where some of the partial densities of states become negative. This has been shown on an enlarged scale in the lower part of the figure. Also in the region near $E \approx 3.2$ some of the partial densities of states are negative.
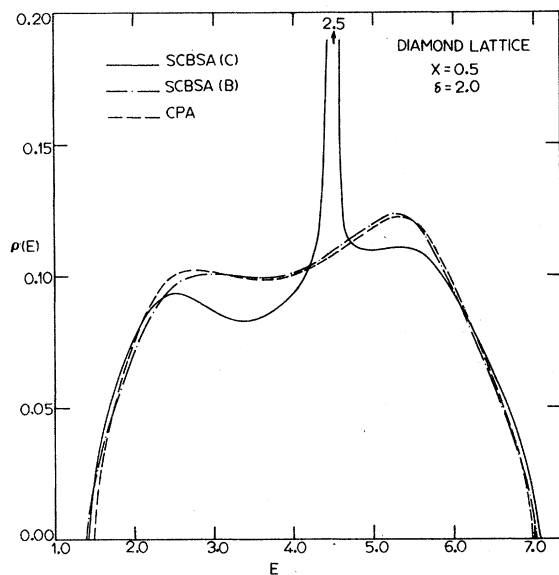
FIG. 9. Densities-of-states curves for binary alloys with $\delta = 2.0$, and $x = 0.5$, and having the diamond lattice structure. The curves are symmetric about $E = 0$.

some of the partial densities of states are negative. In the SCBSA(C) even the total averaged density of states is negative. This shows that the applicability of the SCBSA for the diamond lattice in the strong-scattering regime is limited and questionable.

In Fig. 9 results have been presented for an alloy with $\delta = 2.0$, and $x = 0.5$. The SCBSA(B) is more or less similar to the CPA result, but the SCBSA(C) shows a peaky structure. Here we do not face any problem of nonanalyticity or the negative partial densities of states.

C. Conclusion

From these results we conclude that the SCBSA(C) is reasonably good approximation for the calculation of the electronic structure of disordered alloys. But it should be applied with care, because in the strong-scattering regime it leads to negative partial densities of states and averaged Green's functions which have singular points off the real axis. Our calculations show that the region of analyticity of the SCBSA is much greater[18] than

the SCCSA, and that it depends on the underlying lattice structure of the alloy. This is apparent from our calculations on the simple cubic and the diamond lattice structures. The SCBSA(C) is found to be successful for diamond lattice over a larger range of parameters in contrast to the simple cubic lattice.

The negative partial densities of states observed in both the simple cubic and the diamond lattices, are unphysical. We feel that this defect is inherent in the boundary-site condition and it does not stem from the additional approximation that we introduced through Eq. (15). Equation (15) approximates the matrix elements of $\overline{G}$ between two different sites of the shell by their averaged value $\overline{\Gamma}$ (this is also equivalent to neglecting detailed configurations of the shell for a fixed number of different kinds of atoms) and is exact on a diamond lattice. We have not searched for the lowest value of δ and x at which the nonanalytic behavior of the averaged Green's function (or the negative partial densities of states) starts showing up, but for the simple cubic alloys with $\delta = 1.0$, and $x = 0.5$, and for alloys having the diamond lattice structure with $\delta = 2.0$, and $x = 0.1$, these unphysical features are there as seen in Figs. 3 and 8, respectively. Therefore, whereas the SCBSA is equivalent to the MCPA in the case of a linear chain, it is found not to be so for three-dimensional lattices. We feel that the problem of nonanalyticity will be unavoidable in any cluster theory where the coherent-potential matrix is approximated by a scalar coherent potential. Perhaps one should use smaller clusters with proper symmetries, and then treat these exactly.

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