Self-consistent cluster coherent-potential approximation for the tight-binding linearized-muffin-tin-orbitals approach to random binary alloys

Abhijit Datta, Prabhat Kumar Thakur, and Abhijit Mookerjee
S.N. Bose National Centre for Basic Sciences, DB 17, Sector 1, Salt Lake, Calcutta 700064, India
(Received 4 January 1993)

We have used the augmented-space formalism (ASF) to discuss the configuration averaging of random observables that one encounters in random systems, viz. the one-electron Green function or other related properties. The Hamiltonian of the constituents is obtained within the first-principles tight-binding linearized-muffin-tin-orbitals scheme. A self-consistent approach for the cluster coherent-potential function has been developed for substitutional binary alloys. Configuration averaging for the single-site coherent-potential approximation (CPA) and its cluster generalization (CCPA) is discussed using the ASF.

I. INTRODUCTION

The linearized-muffin-tin-orbitals method (LMTO) has been successfully used for the study of electronic band structure and other related properties for pure metals and semiconductors, and their disordered alloys,[1-7] as well as for solid surfaces and interfaces.[4,8] It has been shown by Andersen and others[2-9] that the original infinite-ranged MTO basis sets can be transformed into new basis sets with different degrees of screening in real space. An especially simple and accurate description of solids can be obtained within the so-called orthogonal LMTO representation in the atomic-sphere approximation (ASA) (the γ representation) and the most localized LMTO (the β representation). In either of the two representations, one may construct a tight-binding (TB) Hamiltonian having basic parameters and canonical structure constants describing, respectively, the scattering properties of the lattice-site atoms and the geometry of the lattice.[2]

Recently, Kudrnovsky and others have discussed in detail the application of the LMTO formalism to the evaluation of the electronic structure for disordered binary alloys[5-9] and pseudobinary alloys[7] within the coherent-potential approximation (CPA) first introduced by Soven and Taylor.[10] The resulting single-site CPA (SCPA) within the LMTO has many similarities with the traditional TB-SCPA theory. The parameters in the TB-LMTO Hamiltonians for the solids (both ordered and disordered) contain much more detailed physical features regarding the bands of the constituents than the empirical TB Hamiltonian, so that one can rely much more on these first-principles approaches than the parameter-fitting exercises. In the TB-LMTO picture the detailed band information of the pure constituents can be expressed in terms of the relevant potential parameters for the band positions, bandwidths, and band shapes.

The importance of the generalization of the single-site CPA has been realized for some time in various contexts such as incorporating short-range correlations, cluster effects, and off-diagonal disorders.[11-17] These works concentrate mainly on traditional tight-binding models.[12-15,17] Augmented-space formalism (ASF), first introduced and originally developed within a tight-binding framework by Mookerjee, provides a self-consistent cluster coherent-potential approximation (CCPA) in which one can go beyond the CPA in a systematic way.[12-15] In this method, the effective medium is determined by the self-consistency condition that the average scattering from all possible configurations of the real cluster embedded in the effective medium is zero. Unlike the molecular CPA,[18] the ASF CCPA gives a translationally invariant effective medium.[14,15] The ideas of ASF are rather general and can be combined with the conventional first-principles methods, such as the Korringa-Kohn-Rostoker (KKR), LMTO, etc., methods. In this spirit a self-consistent cluster theory within the KKR theory has previously been developed.[16]

In this paper we present a self-consistent cluster theory which combines augmented-space formalism and conventional TB-LMTO methods to determine the effective medium corresponding to the potential function which can be expressed in terms of the bare potential parameters of the LMTO approach. Our motivation is to determine self-consistently the coherent-potential function of the disordered alloys within a cluster generalized approach.

II. THE TB-LMTO FORMALISM

The conventional MTO and the screened version of the same have been discussed in detail elsewhere in the literature.[2] We quote here only those results which are of direct relevance to the central issue of this paper, namely, configuration averaging of the Green function in the *most localized* or β representation. In this representation the Hamiltonian is given by

$$H^{\beta}=h^{\beta}(I+o^{\beta}h^{\beta})+(I+h^{\beta}o^{\beta})E_{\nu}(o^{\beta}h^{\beta}+I)\ , \tag{1}$$

and the overlap is given by

$$O^{\beta}=(I+h^{\beta}o^{\beta})(o^{\beta}h^{\beta}+I)\ , \tag{2}$$

where

$$h^{\beta}=(C^{\beta}_{RL}-E_{\nu RL})\delta_{RR'}\delta_{LL'}+(\Delta^{\beta}_{RL})^{1/2}S^{\beta}_{RL,R'L'}(\Delta^{\beta}_{R'L'})^{1/2} .$$

The parameters C^{β}_{RL} and Δ^{β}_{RL} introduced above are the potential parameters directly related to the potential function P^{β}_{RL}, which is in turn expressed in terms of the phase shifts.

In practice, $S^{\beta}_{RL,R'L'}$, the structure matrix element, vanishes beyond second-nearest neighbor for close-packed lattices. The feasibility of the representation is that the quantities $X_{RL}=X^{i}_{L}\delta_{LL'}$, $P_{RL}=P^{i}_{L}\delta_{LL'}$, and $\mu_{RL}=\mu^{i}_{L}\delta_{LL'}$, which enter into the calculation of Green functions and which are described below, are also diagonal matrices. The Green function in the β representation has the following form:

$$G^{\beta}_{RL,R'L'}=X^{\beta}_{L}(z)\delta_{RR'}\delta_{LL'}+\mu^{\beta}_{L}(z)g^{\beta}_{RL,R'L'}\mu^{\beta}_{L'}(z) , \quad (3)$$

where

$$\begin{aligned} &g^{\beta}_{RL,R'L'}=\{[P^{\beta}(z)-S^{\beta}]^{-1}\}_{RL,R'L'} ,\\ &X^{\beta}_{L}(z)=(\gamma_L-\beta_L)\mu^{\beta}_{L}(z)/\Delta^{1/2}_{L} ,\\ &\mu^{\beta}_{L}(z)=[\dot{P}^{\beta}_{L}(z)]^{1/2}=\frac{\Delta_L}{[\Delta_L+(\gamma_L-\beta_L)(z-c_L)]} ,\\ &P^{\beta}_{L}(z)=\frac{z-c_L}{[\Delta_L+(\gamma_L-\beta_L)(z-c_L)]} . \end{aligned} \quad (4)$$

Note that this is a very useful representation for performing averaging of the Green functions of random alloys. In this representation $P^{\beta}_{L}(z)$, $X^{\beta}_{L}(z)$, and $\mu^{\beta}_{L}(z)$ are all site diagonal and the structure factor matrix is nonrandom.

In a binary random alloy, A_xB_{1-x}, characterized by the random site-diagonal potential parameters, viz., band-center position C_L, bandwidth Δ_L, and band-shape parameter γ_L, regularly takes two values with probability x for type A and $(1-x)$ for type B.

III. CONFIGURATION AVERAGING WITHIN THE AUGMENTED-SPACE FORMALISM AND THE GENERALIZATION OF THE COHERENT POTENTIAL APPROXIMATION

In a binary alloy, A_xB_{1-x}, characterized by the random site-diagonal potential parameters, viz., band-center position C_L, bandwidth Δ_L, and band-shape parameter γ_L, regularly takes two values with probability x and $1-x$ for A and B types. The quantities $P^{\beta,i}_{L}(z)$, $X^{\beta,i}_{RL}(z)$, and $\mu^{\beta,i}_{RL}(z)$ also take on two values with probabilities x and $1-x$, where $i=A$ or B, respectively. The structure matrix element $S^{\beta}_{RL,R'L'}$ is not random. As a consequence, the configuration averaging of the Green function is configuration averaging of an auxiliary Green function g which involves the site-diagonal random potential function $P^{\beta,i}_{L}(z)$ only. It has been shown by Kudrnovsky *et al.* that the CPA matrix $P^{\beta}(z)$ for cubic random alloys may be determined by a set of coupled CPA equations:

$$P_L(z)=\langle P^{\beta}_{L}(z)\rangle+[P^{\beta}_{A,L}(z)-P^{\beta}_{L}(z)]\phi^{\beta}_{L}(z)\times[P^{\beta}_{B,L}(z)-P^{\beta}_{L}(z)] , \quad (5)$$

where

$$\phi^{\beta}_{L}(z)=\frac{1}{N}\sum_{k}\{[P^{\beta}(z)-S^{\beta}(k)]^{-1}\}_{LL}\cdots , \quad (6)$$

with $P^{\beta}(z)=[\delta_{LL'}P_L(z)]$ and $S^{\beta}(k)=[S^{\beta}_{LL'}(k)]$, where $S^{\beta}_{LL'}(k)$ is the Bloch transform of $S^{\beta}_{RL,R'L'}$.

There exists considerable literature on the use of the ASF for configuration averaging of any random function which contains random physical parameters of the system.[11–16] It has been discussed in the literature how one can incorporate cluster effects, off-diagonal disorder, and short-ranged order within this formalism. Here we shall give an outline of the procedure for obtaining self-consistent cluster CPA generalizations.

For a binary-alloy problem the random occupation variable for each site n_i on the lattice enters the Hamiltonian. The binary probability distribution $p(n_i)$ is expressed as

$$\begin{aligned} p(n_i)&=x\delta(n_i-1)+y\delta(n_i)\\ &=-1/\pi\,\mathrm{Im}\langle f^{(i)}_{0}|(n_iI-M^{i})^{-1}|f^{(i)}_{0}\rangle , \end{aligned} \quad (7)$$

where $n_i=1$ or 0 according to whether site i is occupied by an A or a B type of atom, respectively. The operator $M^{(i)}$ is the analog of the tight-binding Hamiltonian H and can be expressed as

$$\begin{aligned} M^{(i)}=&x|f^{i}_{0}\rangle\langle f^{i}_{0}|+y|f^{i}_{1}\rangle\langle f^{i}_{1}|\\ &+(xy)^{1/2}(|f^{i}_{0}\rangle\langle f^{i}_{1}|+|f^{i}_{1}\rangle\langle f^{i}_{0}|) . \end{aligned} \quad (8)$$

Note that for a binary alloy the basis states are $|f^{i}_{0}\rangle$ and $|f^{i}_{1}\rangle$. The total configuration space Φ for n sites of a binary random alloy is the direct product space $\prod\otimes\phi_i$ and is spanned by states like

$$|f^{1}_{0}\otimes\cdots f^{1}_{1}\otimes\cdots f^{2}_{2}\cdots\rangle .$$

Any member of the basis may be completely determined by the sequence $\{i_1,i_2,\ldots,i_C\}=\sigma$, which is called the cardinality sequence, where C is the cardinality. The augmented-space theorem gives us

$$\langle A\rangle_{\mathrm{au}}=\langle\varnothing|\tilde{A}(\{M^{(i)}\})|\varnothing\rangle . \quad (9)$$

$\varnothing$ is the null sequence. The operator function $\tilde{A}(\{M^{(i)}\})$ is the same function of $M^{(i)}$ as that of $A(\{n_i\})$.

It has been discussed by Kudrnovsky *et al.*[5–9] that the configuration averaging of the actual resolvent can be carried out through the calculation of an auxiliary resolvent, as is evinced in Eqs. (12) and (13). Note that the first of Eqs. (13) can be written as a Hamiltonian-like operator representation in the following way:

$$g^{\beta}_{iL,jL}=[A^{\beta}]^{-1}$$

where

$$A^{\beta}=\sum_{iL}P^{\beta,i}_{iL}|iL\rangle\langle iL|-\sum_{iL,jL'}S^{\beta}_{iL,jL'}|iL\rangle\langle jL'| , \quad (10)$$

or in matrix form,

$$[A^{\beta}]_{iL,jL'}=\{P_{iL}^{\beta,i}\delta_{LL'}-S_{iL,iL'}^{\beta}\delta_{LL'} -S_{iL,iL'}^{\beta}(1-\delta_{LL'})\}\delta_{ij}-S_{iL,jL'}^{\beta} . \quad (11)$$

Note that the term within the parentheses is purely site diagonal; the third term there, however, has a contribution from $L=L'$ terms as well. The last term is off-diagonal both in site and angular momentum indices. The structure function is independent of disorder and depends *only* on the lattice, but

$$P_{iL}'^{\beta}=P_{iL}^{\beta}-S_{iL,iL}^{\beta}=P'^{\beta}_{A,L}(1-n_i)+P'^{\beta}_{B,L}n_i .$$

From Eq. (3) we may configuration-average both sides to obtain

$$\langle G_{iL,iL}^{\beta}\rangle=\langle X_{iL}^{\beta}\rangle+\langle \mu_{iL}^{\beta}(z)g_{iL,iL}^{\beta}(z)\mu_{iL}^{\beta}(z)\rangle . \quad (12)$$

Henceforth we shall assume that we are always working in the β representation and drop this index. Here, $\mu_{iL}=\mu_{B,L}+\delta\mu n_i$ and $\delta\mu=\mu_A-\mu_B$. We may rearrange Eq. (12) with these values substituted to

$$\begin{aligned}G_{iL,iL}&=X_{iL}+[\mu_{B,L}(z)+\delta\mu n_i]g_{iL,iL}(z)[\mu_{B,L}+\delta\mu n_i]\\&=X_{iL}(z)+\mu_{B,L}(z)g_{iL,iL}(z)\mu_{B,L}(z)+\cdots+\mu_{B,L}(z)g_{iL,iL}(z)\delta\mu_L n_i\\&\quad+\delta\mu_L n_i g_{iL,iL}(z)\mu_{B,L}(z)+\cdots\delta\mu_L n_i g_{iL,iL}(z)\delta\mu_L n_i . \quad (13)\end{aligned}$$

The augmented-space theorem gives the configuration average as

$$\begin{aligned}\langle G_{iL,iL}\rangle&=\langle X_{iL}(z)\rangle+\mu_{B,L}^2(z)\langle\varnothing|\tilde{g}_{iL,iL}|\varnothing\rangle+\cdots+\mu_{B,L}(z)\langle\varnothing|\tilde{g}_{iL,iL}\otimes\tilde{M}^{(i)}|\varnothing\rangle\delta\mu_L\\&\quad+\delta\mu_L\langle\varnothing|\tilde{M}^{(i)}\otimes\tilde{g}_{iL,iL}|\varnothing\rangle\mu_{B,L}\cdots+\delta\mu_L\langle\varnothing|\tilde{M}^{(i)}\otimes\tilde{g}_{iL,iL}\otimes\tilde{M}^{(i)}|\varnothing\rangle\delta\mu_L . \quad (14)\end{aligned}$$

We have to evaluate the following quantities

(i) $\langle i\varnothing|\tilde{g}(\{\tilde{M}^{(i)}\})|i\varnothing\rangle$,

(ii) $\langle i\varnothing|\tilde{g}(\{\tilde{M}^{(i)}\})\otimes\tilde{M}^{(i)}|i\varnothing\rangle=x\langle i\varnothing|\tilde{g}(\{\tilde{M}^{(i)}\})|i\varnothing\rangle+(xy)^{1/2}\langle i,\{i\}|\tilde{g}(\{\tilde{M}^{(i)}\})|i\varnothing\rangle$,

(iii) $\langle i\varnothing|\tilde{M}^{(i)}\otimes\tilde{g}(\{\tilde{M}^{(i)}\})|i\varnothing\rangle=x\langle i\varnothing|\tilde{g}(\{\tilde{M}^{(i)}\})|i\varnothing\rangle+(xy)^{1/2}\langle i,\{i\}|\tilde{g}(\{\tilde{M}^{(i)}\})|i\varnothing\rangle$,

(iv) $\langle i\varnothing|\tilde{M}^{(i)}\otimes\tilde{g}(\{M^{(i)}\})\otimes M^{(j)}|i\varnothing\rangle=x^2\langle i\varnothing|\tilde{g}(\{\tilde{M}^{(i)}\})|i\varnothing\rangle+\cdots+x(xy)^{1/2}[\langle i\varnothing|\tilde{g}(\{\tilde{M}^{(i)}\})|i,\{i\}\rangle+\langle i,\{i\}|\tilde{g}(\{\tilde{M}^{(i)}\})|i\varnothing\rangle]+xy\langle i,\{i\}|\tilde{g}(\{\tilde{M}^{(i)}\})|i,\{j\}\rangle$,

where $\tilde{g}(\{\tilde{M}^{(i)}\})$ is the same functional of $\tilde{M}_i$ as $g(n_i)$ is of n_i.

In order to obtain a $\mathcal{C}$-cluster CPA, we partition the augmented-space Ψ in two subspaces: Ψ_1, spanned by the cluster $\mathcal{C}$ and its configurations, and $\Psi_2=\Psi/\Psi_1$. This involves partition of $A(\{M^{(i)}\})$ as follows:

$$\tilde{A}=\begin{bmatrix}A_1 & A'\\ A'^{T} & A_2\end{bmatrix} ,$$

where A_1 is in subspace Ψ_1 and A_2 is in subspace Ψ_2. By applying the partition theorem, the inverse of A in subspace Ψ_1 can be written as

$$[A^{-1}]_1=[A_1-A'A_2^{-1}A'^{T}]^{-1}=\tilde{A}^{-1} ,$$

$$\begin{aligned}A_1&=\sum_{i\in\mathcal{C}}P'_{i,\sigma}|i\rangle\langle i|\otimes\sum_{\alpha\in\mathcal{C}}|\sigma\rangle\langle\sigma|\\&\quad+\delta P'\sqrt{xy}\sum_{i\in\mathcal{C}}|i\rangle\langle i|\otimes\sum_{\substack{\sigma,\sigma'\in\mathcal{C}\\ \sigma\neq\sigma'}}|\sigma\rangle\langle\sigma'|\\&\quad-\sum_{\substack{i,j\in\mathcal{C}\\ i\neq j}}S_{ij}|i\rangle\langle j|\otimes\sum_{\sigma\in\mathcal{C}}|\sigma\rangle\langle\sigma| ,\end{aligned}$$

where $P'_{i,\sigma}=\langle P'\rangle_{\mathrm{av}}$ if the configuration at site i is $\uparrow$, and xP_B+yP_A if it is $\downarrow$. The approximation now involves ignoring any configuration fluctuations outside the space Ψ_1 and replacing the operator A is that subspace by an effective operator:

$$\begin{aligned}A_2&\cong\left[P'_{\mathrm{eff}}\sum_{k\in\mathcal{C}'}|k\rangle\langle k|-\sum_{\substack{k,m\in\mathcal{C}'\\ k\neq m}}[S_{km}+s_{km}]|k\rangle\langle m|\right]\\&\quad\otimes|\varnothing\rangle\langle\varnothing| ,\\A'&=-\sum_i\sum_k[S_{ik}+s_{ik}]|i\rangle\langle k|\otimes\sum_{\sigma\in\mathcal{C}}|\sigma\rangle\langle\varnothing| ,\\A_{21}&=A_{12}^{\dagger} .\end{aligned}$$

s_{kl} are site off-diagonal corrections in P'; the diagonal corrections are already contained in P'_{eff}. We shall define the sum $S_{ik}+s_{ik}$ as S_{eff}^{ik}. The elements of $[A^{-1}]$ can be found if we can evaluate the triple product $(A'A_2^{-1}A'^{T})$. Since A_2 is the matrix element in the effective medium with cluster $\mathcal{C}$ removed from the medium, we may write $A_2^{-1}=g_{\mathrm{eff}}^{(\mathcal{C})}$. The superscript $\mathcal{C}$ inside the parentheses indicates the fact that g is calculated from the lattice from

which cluster $\mathcal{C}$ has been removed.

From the above equations,

$$A' A_2^{-1} A'^T = \sum_{i,j\in\mathcal{C}} \sum_{k,l\in\mathcal{C}'} S_{\rm eff}^{ik} g_{kl}^{(\mathcal{C})} S_{\rm eff}^{lj} |i\rangle\langle j| \otimes \sum_{\sigma\in\mathcal{C}} |\sigma\rangle\langle\sigma|$$
$$= \sum_{i,j\in\mathcal{C}} \xi_{\mathcal{C}}^{ij} |i\rangle\langle j| \otimes \sum_{\sigma\in\mathcal{C}} |\sigma\rangle\langle\sigma| ,$$

where $\xi_{\mathcal{C}}^{ij} = \sum\sum_{k,l} S'_{ik} g_{kl}^{(\mathcal{C})} S'_{lj}$ for $i,j\in\mathcal{C}$ and $K,l\in\mathcal{C}'$.

The matrix $A' A_2^{-1} A'^T$ is diagonal in the configuration space Φ. The off-diagonal parts in A thus come from A_1 only:

$$\tilde{A} = \left[\sum_{i\in\mathcal{C}} (P' - \xi_{\mathcal{C}}^{ii}) |i\rangle\langle i| - \sum_{\substack{i,j\in\mathcal{C} \\ i\neq j}} (S_{\rm eff}^{ij} + \xi_{\mathcal{C}}^{ij}) |i\rangle\langle j| \right] \otimes \sum_{\sigma\in\mathcal{C}} |\sigma\rangle\langle\sigma| + \delta P \sum |i\rangle\langle i| \otimes \tilde{M}^{(i)} .$$

Now let us further partition $\tilde{A}$ in subspace 1 spanned by $|i,\varnothing\rangle$, $i\in\mathcal{C}$, and is of rank m, where m is the size of the cluster. Subspace 2 is the complement of subspace 1 and has rank $m\times(2^m-1)$. The inverse of $\tilde{A}$ in subspace 1 is given by

$$[\tilde{A}^{-1}]_1 = (\tilde{A}_1 - \tilde{A}_{12} \tilde{A}_2^{-1} \tilde{A}_{21})^{-1} = a^{-1} .$$

Since the ranks of the matrices involved on the right-hand side are small, in general we can easily invert the above:

$$a = \sum_{i\in\mathcal{C}} (\langle P'\rangle - \xi_{\mathcal{C}}^{ii}) |i\rangle\langle i| - \sum_{\substack{i,j\in\mathcal{C} \\ i\neq j}} (S_{\rm eff}^{ij} + \xi_{\mathcal{C}}^{ij}) |i\rangle\langle j| .$$

For the translationally invariant effective medium,

$$A_{\rm eff} = P'_{\rm eff} \sum_{i\in\mathcal{C}} |i\rangle\langle i| - \sum_{\substack{i,j\in\mathcal{C} \\ i\neq j}} (S_{\rm eff}^{ij}) |i\rangle\langle j| .$$

Since subspace 1 is spanned by configuration $|\varnothing\rangle$ alone, the augmented-space theorem tells us that $\langle g\rangle = a^{-1}$, but by the definition of the effective medium, it is also $A_{\rm eff}^{-1}$. This leads to the self-consistency equations

$$P'_{\rm eff} = \langle P'\rangle - \langle i| \tilde{A}_{12} \tilde{A}_2^{-1} \tilde{A}_{21} |i\rangle , \qquad (15)$$
$$S_{\rm eff}^{ij} = S_{ij} + \langle i| \tilde{A}_{12} \tilde{A}_2^{-1} \tilde{A}_{21} |j\rangle \quad \text{for } i\neq j .$$

The other three elements (ii)–(iv) are obtained from $[\tilde{A}^{-1}]_{12}$, $[\tilde{A}^{-1}]_{21}$, and $[\tilde{A}^{-1}]_2$. The partition theorem gives

$$[\tilde{A}^{-1}]_{12} = -[\tilde{A}_1 - \tilde{A}_{12} \tilde{A}_2^{-1} \tilde{A}_{21}]^{-1} A_{12} A_2^{-1} ,$$
$$[\tilde{A}^{-1}]_{22} = \tilde{A}_2^{-1} - [\tilde{A}^{-1}]_{21} \tilde{A}_{12} \tilde{A}_2^{-1} . \qquad (16)$$

Once we have obtained the effective $P'_{\rm eff}$ and $S_{\rm eff}^{ij}$ using the self-consistent equations (22), we immediately obtain expressions for the three other averages involved in (ii)–(iv):

$$\langle g_{ii} n_i\rangle = \langle g_{ii}\rangle [x + \Delta P' \delta P'^{-1}] - \sum \langle g_{ij}\rangle \Delta S_{ji} \delta P'^{-1} ,$$
$$\langle n_i g_{ii}\rangle = [x + \delta P'^{-1} \Delta P'] \langle g_{ii}\rangle - \sum \delta P'^{-1} \Delta S_{ij} \langle g_{ji}\rangle ,$$
$$\langle n_i g_{ii} n_i\rangle = [x + \delta P'^{-1} \Delta P'] \langle g_{ii}\rangle [x + \delta P'^{-1} \Delta P'] + \sum_j \delta P'^{-1} \Delta S_{ij} \langle g_{ji}\rangle \Delta P' \delta P'^{-1} + \sum_j \delta P'^{-1} \Delta P' \langle g_{ij}\rangle \Delta S_{ji} \delta P^{-1} + \sum_k \sum_j \delta P'^{-1} \Delta S_{ik} \langle g_{kj}\rangle \Delta S_{ki} \delta P'^{-1} , \qquad (17)$$

where $\Delta P' = P'_{\rm eff} - \langle P'\rangle$ and $\Delta S_{ij} = S_{\rm eff}^{ij} - S_{ij}$.

Substitution into the Eq. (19) gives the result

$$\langle G_{ii}\rangle = \langle X_i\rangle + \mu^{\rm eff}(z)^\dagger \langle g_{ii}(z)\rangle \mu^{\rm eff}(z) - \sqrt{xy}\,[\mu'(z)^\dagger h(z) \delta P'^{-1} \delta\mu + \delta\mu^\dagger (\delta P'^\dagger)^{-1} h'(z) \mu'(z)] - xy \delta\mu^\dagger (\delta P'^\dagger)^{-1} K(z) \delta P'^{-1} \delta\mu ,$$

where

$$\mu^{\rm eff}(z) = \langle \mu(z)\rangle + \sqrt{xy}\,\Delta P \delta P'^{-1} \delta\mu, \quad \delta\mu = \mu_A - \mu_B$$
$$\mu'(z) = \mu_B + \sqrt{xy}\,\Delta P \delta P'^{-1} \delta\mu ,$$
$$h(z) = \int_{\rm BZ} \frac{d^3\mathbf{k}}{8\pi^3} \langle g(\mathbf{k})\rangle \Delta S(\mathbf{k}) , \qquad (18)$$
$$h'(z) = \int_{\rm BZ} \frac{d^3\mathbf{k}}{8\pi^3} \Delta S^\dagger(\mathbf{k}) \langle g(\mathbf{k})\rangle ,$$
$$K(z) = \int_{\rm BZ} \frac{d^3\mathbf{k}}{8\pi^3} \Delta S^\dagger(\mathbf{k}) \langle g(\mathbf{k})\rangle \Delta S(\mathbf{k}) .$$

IV. CONCLUSION

We have proposed here a generalization of the coherent-potential method for the TB LMTO to take into account the effect of clusters. It has been felt through experience while dealing with strongly disordered alloys with either diagonal disorder or off-diagonal disorder that statistical correlation between the sites within a cluster may be a physically relevant issue in order to study its electronic density of states, electrical conductivity, etc. In this regard we should mention that alloys like $Cu_{1-x}Pd_x$, $Au_{1-x}Pd_x$, and several other transition-metal alloys may be systems of relevant studies. The single-site CPA theory, from the very beginning, is far from complete, although the recent versions of it incorporate both kinds (diagonal and off-diagonal) of disorder. So a multisite or cluster CPA problem was always a formidable problem. We think that with this formulation in the near future one can do realistic calculations for electronic structures of several other alloys as well.

ACKNOWLEDGMENTS

We acknowledge the S. N. Bose National Centre for Basic Sciences, Calcutta, for making its research facilities available to us. Dr. Prabhat K. Thakur would like to thank C.S.I.R., India, for financial support under the Scientist Pool scheme.

[1]O. K. Andersen, O. Jepsen, and M. Sôb, in *Electronic Band Structure and its Applications,* edited by M. Yussouff (Springer-Verlag, Berlin, 1987); O. K. Andersen, O. Jepsen, and D. Glötzel, in *Highlights in Condensed Matter Theory,* edited by F. Bassani, F. Fumi, and M. P. Tosi (North-Holland, New York, 1985).

[2]O. K. Andersen, Z. Pawalowska, and O. Jepsen, Phys. Rev. B **34**, 5253 (1986); O. K. Andersen and O. Jepsen, Physica (Utrecht) B **91**, 317 (1977).

[3]W. R. L. Lambrecht and O. K. Andersen, Surf. Sci. **178**, 256 (1986).

[4]H. L. Skriver and N. M. Rosengaard, Phys. Rev. B **43**, 9538 (1991).

[5]J. Kudrnovsky, V. Drchal, and J. Masêk, Phys. Rev. B **35**, 2487 (1987).

[6]R. W. L. Lambrecht and O. K. Andersen, Phys. Rev. B **34**, 2439 (1986).

[7]J. Kudrnovsky, V. Drchal, M. Sôb, N. E. Christensen, and O. K. Andersen, Phys. Rev. B **40**, 10 029 (1989).

[8]G. P. Das, Pramana **38**, 545 (1992); also see Ref. 4.

[9]J. Kudrnovsky and V. Drchal, Phys. Rev. B **41**, 7515 (1990).

[10]P. Soven, Phys. Rev. **156**, 809 (1967); D. W. Taylor, *ibid.* **156**, 1017 (1967).

[11]A. Mookerjee, J. Phys. C **6**, L205 (1973).

[12]L. J. Gray and T. Kaplan, Phys. Rev. B **24**, 1872 (1981).

[13]A. Mookerjee, V. K. Srivastava, and V. Chowdhury, J. Phys. C **16**, 4555 (1983).

[14]A. Mookerjee and Prabhat K. Thakur, Phys. Rev. B **38**, 3798 (1988).

[15]V. Kumar, A. Mookerjee, and V. K. Srivastava, J. Phys. C **15**, 1939 (1982); Prabhat K. Thakur, A. Mookerjee, and V. A. Singh, J. Phys. F **17**, 1523 (1987).

[16]S. S. A. Razee, S. S. Pajput, R. Prasad, and A. Mookerjee, Phys. Rev. B **42**, 9391 (1990).

[17]R. Mills and P. Ratanavararaksha, Phys. Rev. B **18**, 5291 (1978); R. Mills, L. J. Gray, and T. Kaplan, *ibid.* **27**, 3252 (1983).

[18]M. Tsukuda, J. Phys. Soc. Jpn. **26**, 684 (1969); **32**, 1475 (1972).