Configuration-averaged Green's function within the Korringa-Kohn-Rostoker cluster coherent-potential approximation

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We derive an exact expression for the configuration-averaged Green's function within the Korringa-Kohn-Rostoker cluster coherent-potential approximation for a general cluster size. In an earlier publication [Phys. Rev. B **42**, 9391 (1990)], the expression for the configuration-averaged Green's function was derived using the restricted-averaging method. Using these two expressions, we have calculated the density of states for a one-dimensional muffin-tin alloy, which shows a very small difference between the results of the two methods; the gross features remain the same, except for the height of some of the peaks. However, for the dilute alloy, there is a qualitative difference between the two results in the impurity band.

I. INTRODUCTION

The Korringa-Kohn-Rostoker (KKR) Green's-function method has emerged as a powerful tool for calculating the electronic structure of disordered substitutional alloys from first principles. Within the coherent-potential approximation (CPA), this method[1-3] (KKR-CPA) has been very successful in predicting the electronic properties of a wide variety of disordered alloys. However, the KKR-CPA, being a single-site approximation, might fail when applied to systems in which correlated scattering from different atoms is important. In a recent publication,[4] we developed a self-consistent-field cluster generalization of the KKR-CPA by combining the augmented space cluster CPA (Ref. 5) and the conventional KKR Green's function formalism.[3] This formulation, which we called the KKR cluster CPA (KKR-CCPA), can be made fully charge self-consistent within the local-density-functional theory, and therefore is a first-principles parameter-free theory of the electronic structure of disordered alloys.

In Ref. 4, the configuration-averaged Green's function was calculated by the restricted-averaging method. This method is essentially a single-site approach, and therefore is an approximate one. In this paper, we show that this approximation can be avoided and the configuration-averaged Green's function can be determined exactly within the KKR-CCPA. We find that, for a general cluster size, the expression for the configuration-averaged Green's function obtained by this method is different from that obtained by the restricted-averaging method. However, for a one-atom cluster, the two expressions are identical, thus giving the correct limit.

We have calculated the averaged density of states (DOS) for a one-dimensional muffin-tin alloy using these two methods. For the numerical calculations within the KKR-CCPA, we have taken a two-atom cluster. We find that, for the dilute alloy, there is a qualitative difference between the two results in the impurity band; using the exact method we find two peaks in the impurity band in contrast to the one obtained by the method of Ref. 4. Otherwise, in general, the two approaches give almost identical results. But, nevertheless, one should use the present expression for the configuration-averaged Green's function, since it is the exact expression within the KKR-CCPA, unlike that in Ref. 4.

The outline of the paper is as follows. In Sec. II, we briefly outline the KKR-CCPA formulation. Also, we discuss some of the features of the KKR-CCPA, which were not discussed in Ref. 4. In Sec. III, we derive an expression for the configuration-averaged Green's function within the KKR-CCPA. In Sec. IV, we present our results for the one-dimensional muffin-tin alloy, and in Sec. V, we give our conclusions.

II. THE KKR CLUSTER CPA

The Green's function for an array of muffin-tin potentials is[3]

$$G(\mathbf{r},\mathbf{r}')=\sum_{L,L'} Z_L^i(\mathbf{r}_i)T_{LL'}^{ij}Z_{L'}^j(\mathbf{r}'_j) -\delta_{ij}\sum_L Z_L^i(\mathbf{r}_i)J_L^i(\mathbf{r}'_j)\ , \tag{1}$$

where $\mathbf{r}_i$ and $\mathbf{r}'_j$ lie on the ith and jth cells, respectively. The functions $Z_L^i(\mathbf{r}_i)$ and $J_L^i(\mathbf{r}_i)$ are, respectively, the regular and irregular solutions of the Schrödinger equation for a single muffin-tin potential centered on the ith site, and L ($\equiv l,m$) is a composite index. $T_{LL'}^{ij}$ are on-the-energy-shell matrix elements of scattering-path operators and are given by[4]

$$T_{LL'}^{ij}=(A^{-1})_{LL'}^{ij}\ , \tag{2}$$

where

$$A=\sum_i C^i|i\rangle\langle i|-\sum_{i,j\ (i\neq j)} B^{ij}|i\rangle\langle j|\ . \tag{3}$$

In Eq. (3) we have suppressed the angular momentum indices L. C^i is the inverse t matrix for a single muffin-tin potential on the ith site and B^{ij} are the real-space version of the KKR structure constants. We now express A in terms of random variables n_i, which take the value 1

when the ith site is occupied by an A atom, and 0 when occupied by a B atom. Thus we have[4]

$$A(\{n_i\})=C^B\sum_i|i\rangle\langle i|+\delta C\sum_i|i\rangle\langle i|n_i - \sum_{i,j\ (i\neq j)}B^{ij}|i\rangle\langle j| , \tag{4}$$

where

$$\delta C=C^A-C^B . \tag{5}$$

By the augmented space theorem,[5] the configuration-averaged path operators are given by

$$\langle T^{ij}\rangle=\langle i,F|[\tilde{A}(\{M^i\})]^{-1}|j,F\rangle , \tag{6}$$

where

$$\tilde{A}(\{M^i\})=\left[C^B\sum_i|i\rangle\langle i|-\sum_{i,j\ (i\neq j)}B^{ij}|i\rangle\langle j|\right]\otimes\sum_{F_\sigma\in\mathcal{C}}|F_\sigma\rangle\langle F_\sigma|+\delta C\sum_i|i\rangle\langle i|\otimes M^i . \tag{7}$$

In Eq. (7), M^i is an operator in the configuration space, and in matrix notation it is a 2×2 matrix in the basis $|f_0^i\rangle$ and $|f_1^i\rangle$, respectively called the ground state and excited state in the configuration space of the ith site. $\mathcal{C}$ is the set of all possible vectors $\{|F_\sigma\rangle\}$ in the configuration space of the lattice. The vectors $|F_\sigma\rangle$ are given by[6]

$$|F_\sigma\rangle=\prod_i|f_n^i\rangle \quad \text{with } n=\begin{cases}0 & \text{for } i\notin\sigma\\ 1 & \text{for } i\in\sigma\end{cases} . \tag{8}$$

The state $|F\rangle$ appearing in Eq. (6) is the ground state in the full configuration space, and corresponds to the case $\sigma=\varnothing$ (the null set) in Eq. (8).

Now, we invoke the KKR-CCPA. We partition the augmented space Ψ into subspaces Ψ_1 and Ψ_2, such that subspace Ψ_1 is spanned by $\{|i;F_\sigma\rangle, i\in\mathbb{C}, F_\sigma\in\mathcal{C}\}$ where $\mathbb{C}$ is the chosen cluster. Subspace Ψ_2 is the complement of Ψ_1 in Ψ. The space Ψ_2 is now replaced by an effective medium. If we partition $\tilde{A}(\{M^i\})$ in this scheme, then the inverse of $\tilde{A}(\{M^i\})$ in subspace Ψ_1 is given by[4]

$$(\tilde{A}^{-1})_1=(A_1-A_{12}A_2^{-1}A_{21})^{-1}=\hat{A}^{-1} , \tag{9}$$

where the matrices A_1, A_{12}, A_{21}, and A_2 are given by Eqs. (2.21), (2.22), and (2.23) in Ref. 4. By simple algebraic manipulation, one easily gets[4]

$$\hat{A}=\left[\sum_{i\in\mathbb{C}}(C^B-\xi_{\mathbb{C}}^{ii})|i\rangle\langle i|-\sum_{\substack{i,j\in\mathbb{C}\\(i\neq j)}}(B^{ij}+\xi_{\mathbb{C}}^{ij})|i\rangle\langle j|\right]\otimes\sum_{F_\sigma\in\mathcal{C}}|F_\sigma\rangle\langle F_\sigma|+\delta C\sum_{i\in\mathbb{C}}|i\rangle\langle i|\otimes M^i , \tag{10}$$

where

$$\xi_{\mathbb{C}}^{ij}=\sum_{k,l\in\mathbb{C}'}B_{\text{eff}}^{ik}T_{\text{eff}}^{(\mathbb{C})kl}B_{\text{eff}}^{lj} \quad \text{for } i,j\in\mathbb{C} . \tag{11}$$

In Eq. (11), $T_{\text{eff}}^{(\mathbb{C})kl}$ are the path operators of the effective medium calculated with the cluster removed from the lattice. We will show later that these can be completely eliminated from the computational procedure.

In the second step of the KKR-CCPA,[4] Ψ_1 is partitioned into subspaces ϕ_1 and ϕ_2 such that ϕ_1 is spanned by $\{|i;F\rangle, i\in\mathbb{C}\}$, and its complement ϕ_2 is spanned by $\{|i;F_\sigma\rangle\sigma\neq\varnothing, i\in\mathbb{C}\}$. Since, for a general cluster, this step was not described in detail in Ref. 4, we give the necessary details in this paper. The expressions derived here will be used in the next section. We partition $\hat{A}$ in the above scheme. The four constituent matrices of $\hat{A}$ can be obtained explicitly by using the following identity in the configuration space:[7]

$$M^i|F_\sigma\rangle=\begin{cases}x|F_\sigma\rangle+(xy)^{1/2}|F_{\sigma'}\rangle , & \sigma'=\sigma+i\\ \text{when } i\notin\sigma\\ y|F_\sigma\rangle+(xy)^{1/2}|F_{\sigma'}\rangle , & \sigma'=\sigma-i\\ \text{when } i\in\sigma ,\end{cases} \tag{12}$$

where x (y) is the concentration of A (B) atoms in the alloy. The four constituent matrices of $\hat{A}$ are thus given by[7]

$$\mathcal{A}_1=\sum_{i\in\mathbb{C}}(\bar{C}-\xi_{\mathbb{C}}^{ii})|i;F\rangle\langle i;F| - \sum_{\substack{i,j\in\mathbb{C}\\(i\neq j)}}(B^{ij}+\xi_{\mathbb{C}}^{ij})|i;F\rangle\langle j;F| , \tag{13}$$

$$\mathcal{A}_{12}=\omega\sum_{i\in\mathbb{C}}|i;F\rangle\langle i;F_i| , \tag{14}$$

$$\mathcal{A}_{21}=\omega\sum_{i\in\mathbb{C}}|i;F_i\rangle\langle i;F| , \tag{15}$$

and

$$\mathcal{A}_2=\left[\sum_{i\in\mathbb{C}}(C^B-\xi_{\mathbb{C}}^{ii})|i\rangle\langle i|-\sum_{\substack{i,j\in\mathbb{C}\\(i\neq j)}}(B^{ij}+\xi_{\mathbb{C}}^{ij})|i\rangle\langle j|\right]\otimes\sum_{\sigma\neq\phi}|F_\sigma\rangle\langle F_\sigma|+\delta C\sum_{i\in\mathbb{C}}|i\rangle\langle i|\otimes\sum_{\sigma\neq\phi}\sum_{\sigma'\neq\varnothing}|F_\sigma\rangle\langle F_\sigma|M^i|F_{\sigma'}\rangle\langle F_{\sigma'}| , \tag{16}$$

where

$$\bar{C}=xC^A+yC^B \tag{17}$$

and

$$\omega=(xy)^{1/2}\delta C . \tag{18}$$

Now, the inverse of $\hat{A}$ in subspace ϕ_1 is given by

$$(\hat{A}^{-1})_1=(\mathcal{A}_1-\mathcal{A}_{12}\mathcal{A}_2^{-1}\mathcal{A}_{21})^{-1} . \tag{19}$$

From Eqs. (14), (15), and (16) we get

$$\mathcal{A}_{12}\mathcal{A}_2^{-1}\mathcal{A}_{21}=\omega\Gamma\omega , \tag{20}$$

where

$$\Gamma=\sum_{i,j\in\mathbb{C}}|i;F\rangle\langle i;F_i|\mathcal{A}_2^{-1}|j;F_j\rangle\langle j;F| \ . \tag{21}$$

From Eqs. (6) and (19) we get

$$\langle T^{ij}\rangle=\langle i;F|\hat{A}^{-1}|j;F\rangle=\langle i;F|(\mathcal{A}_1-\omega\Gamma\omega)^{-1}|j;F\rangle \ . \tag{22}$$

For a translationally invariant effective medium, the path operators in the cluster subspace are given by[4]

$$T^{ij}_{\rm eff}=\langle i|\left[\sum_{k\in\mathbb{C}}(C_{\rm eff}-\xi^{kk}_{\mathbb{C}})|k\rangle\langle k| - \sum_{\substack{k,l\in\mathbb{C}\\(k\neq l)}}(B^{kl}_{\rm eff}+\xi^{kl}_{\mathbb{C}})|k\rangle\langle l|\right]^{-1}|j\rangle \ . \tag{23}$$

The self-consistency condition $\langle T^{ij}\rangle=T^{ij}_{\rm eff}$ implies that

$$\langle F|(\mathcal{A}_1-\omega\Gamma\omega)|F\rangle=\sum_{i\in\mathbb{C}}(C_{\rm eff}-\xi^{ii}_{\mathbb{C}})|i\rangle\langle i| - \sum_{\substack{i,j\in\mathbb{C}\\(i\neq j)}}(B^{ij}_{\rm eff}+\xi^{ij}_{\mathbb{C}})|i\rangle\langle j| \ . \tag{24}$$

By comparing the corresponding matrix elements on both sides of Eq. (24), we get the KKR-CCPA equations

$$C_{\rm eff}=\bar{C}-\omega\langle i;F_i|\mathcal{A}_2^{-1}|i;F_i\rangle\omega \ , \tag{25}$$

$$b^{ij}=\omega\langle i;F_i|\mathcal{A}_2^{-1}|j;F_j\rangle\omega \quad \text{for } i,j\ (i\neq j)\in\mathbb{C} \ . \tag{26}$$

Note that Eqs. (25) and (26) are self-consistent equations, which involve $C_{\rm eff}$, b^{ij}, and $\xi^{ij}_{\mathbb{C}}$ on the right-hand side as well. These equations can be solved iteratively; the starting values for $C_{\rm eff}$ and b^{ij} may be taken as $\bar{C}$ and 0 respectively. Note that $\xi^{ij}_{\mathbb{C}}$ can be calculated in terms of $\{T^{ij}_{\rm eff}\}$, $\{B^{ij}_{\rm eff}\}$ $(i,j\in\mathbb{C})$, and $C_{\rm eff}$ using Eq. (23).

It can be seen from Eq. (25) that, as in the KKR-CPA, the first-order correction to the KKR-CCPA inverse t matrices is of the order of $\omega^2=xy(\delta C)^2$. This implies that the KKR-CCPA, like the KKR-CPA, is exact in the limit when the concentration of either constituent vanishes, and also in the limit when the difference between the scattering strengths of the two constituents is small.

III. THE CONFIGURATION-AVERAGED GREEN'S FUNCTION

The Green's functions for site-diagonal (SD) and non-site-diagonal (NSD) cases can be written from Eq. (1) as[3]

$$G_{\rm SD}(\mathbf{r},\mathbf{r}')={\rm Tr}(T^{ii}F^i)-\sum_L Z^i_L(\mathbf{r}_i)J^i_L(\mathbf{r}'_i) \tag{27}$$

and

$$G_{\rm NSD}(\mathbf{r},\mathbf{r}')={\rm Tr}(T^{ij}F^{ji}) \ , \tag{28}$$

where Tr stands for trace over L and

$$F^i_{LL'}=Z^i_L(\mathbf{r}_i)Z^i_{L'}(\mathbf{r}'_i) \tag{29}$$

and

$$F^{ji}_{LL'}=Z^j_L(\mathbf{r}'_j)Z^i_{L'}(\mathbf{r}_i) \ . \tag{30}$$

Configuration averaging Eqs. (29) and (30), we get

$$\langle G_{\rm SD}(\mathbf{r},\mathbf{r}')\rangle={\rm Tr}\langle T^{ii}F^i\rangle-\sum_L[xZ^A_L(\mathbf{r}_i)J^A_L(\mathbf{r}'_i)+yZ^B_L(\mathbf{r}_i)J^B_L(\mathbf{r}'_i)] \tag{31}$$

and

$$\langle G_{\rm NSD}(\mathbf{r},\mathbf{r}')\rangle={\rm Tr}\langle T^{ij}F^{ji}\rangle \ . \tag{32}$$

The joint averages appearing in Eqs. (31) and (32) can be evaluated by the augmented space formalism if we express them in terms of the random variables n_i, i.e.,

$$F^i=F^B+\delta F n_i \tag{33}$$

and

$$F^{ji}=F^{BB}+F_1n_in_j+F_2n_i+F_3n_j \ , \tag{34}$$

where

$$\delta F=F^A-F^B \ , \tag{35}$$

$$F_1=F^{AA}+F^{BB}-F^{AB}-F^{BA} \ , \tag{36}$$

$$F_2=F^{AB}-F^{BB} \ , \tag{37}$$

and

$$F_3=F^{BA}-F^{BB} \ . \tag{38}$$

With the help of Eq. (33), we can write the joint average in Eq. (31) as

$$\langle T^{ii}F^i\rangle=T^{00}_{\rm eff}F^B+\langle T^{ii}n_i\rangle\delta F \ . \tag{39}$$

Applying the augmented space theorem,[5] we get

$$\langle T^{ii}n_i\rangle=\langle i;F|[\tilde{A}(\{M^i\})]^{-1}M^i|i;F\rangle \ . \tag{40}$$

With the help of Eq. (12) we get

$$\langle T^{ii}n_i\rangle=xT^{00}_{\rm eff}+(xy)^{1/2}\langle i;F|\tilde{A}^{-1}|i;F_i\rangle \ . \tag{41}$$

Substituting Eq. (41) in Eq. (39) we get

$$\langle T^{ii}F^i\rangle=T^{00}_{\rm eff}\bar{F}+(xy)^{1/2}\langle i;F|\tilde{A}^{-1}|i;F_i\rangle\delta F \ , \tag{42}$$

where

$$\bar{F}=xF^A+yF^B \ . \tag{43}$$

The only unknown term in Eq. (42) is $\langle i;F|\tilde{A}^{-1}|i;F_i\rangle$. This can be determined within the KKR-CCPA by following the same procedure that led to the KKR-CCPA. After the first partitioning of the augmented space, the element $\langle i;F|\tilde{A}^{-1}|i;F_i\rangle$ is the same as $\langle i;F|\hat{A}^{-1}|i;F_i\rangle$. After the second partitioning, this element falls in the top right-hand-side block of $\hat{A}^{-1}$, i.e. if we partition $\hat{A}^{-1}$ as

$$\hat{A}^{-1}=\begin{bmatrix}E_1 & E_{12}\\ E_{21} & E_2\end{bmatrix} \ , \tag{44}$$

then $\langle i;F|\hat{A}^{-1}|i;F_i\rangle$ will fall in the E_{12} block, which by partition theorem is given by

$$E_{12}=-(\mathcal{A}_1-\mathcal{A}_{12}\mathcal{A}_2^{-1}\mathcal{A}_{21})^{-1}\mathcal{A}_{12}\mathcal{A}_2^{-1} \ . \tag{45}$$

With the help of Eqs. (20) and (45) we can write

$$\langle i;F|\hat{A}^{-1}|i;F_i\rangle = -\langle i;F|(\mathcal{A}_1-\omega\Gamma\omega)^{-1}\mathcal{A}_{12}\mathcal{A}_2^{-1}|i;F_i\rangle$$
$$= -\sum_{j,k}\sum_{F_\sigma}\sum_{F_{\sigma'}}[\langle i;F|(\mathcal{A}_1-\omega\Gamma\omega)^{-1}|j;F_\sigma\rangle\langle j;F_\sigma|\mathcal{A}_{12}|k;F_{\sigma'}\rangle\langle k;F_{\sigma'}|\mathcal{A}_2^{-1}|i;F_i\rangle] . \quad (46)$$

From Eq. (14) we have

$$\langle j;F_\sigma|\mathcal{A}_{12}|k;F_{\sigma'}\rangle = \omega\delta_{jk}\delta_{FF_\sigma}\delta_{F_kF_{\sigma'}} \quad (47)$$

and thus Eq. (46) can be rewritten as

$$\langle i;F|\hat{A}^{-1}|i;F_i\rangle = -\sum_j[\langle i;F|(\mathcal{A}_1-\omega\Gamma\omega)^{-1}|j;F\rangle\omega \times\langle j;F_j|\mathcal{A}_2^{-1}|i;F_i\rangle] . \quad (48)$$

From Eq. (22) we know that

$$\langle i;F|(\mathcal{A}_1-\omega\Gamma\omega)^{-1}|j;F\rangle = T^{ij}_{\text{eff}} , \quad (49)$$

and from Eqs. (25) and (26) we have

$$\langle j;F_j|\mathcal{A}_2^{-1}|i;F_i\rangle = \omega^{-1}[(\bar{C}-C_{\text{eff}})\delta_{ij} + b^{ji}(1-\delta_{ij})]\omega^{-1} . \quad (50)$$

Substituting Eqs. (49) and (50) into Eq. (48) we get

$$\langle i;F|\hat{A}^{-1}|i;F_i\rangle = T^{00}_{\text{eff}}(C_{\text{eff}}-\bar{C})\omega^{-1} - \sum_{j\in\mathbb{C}} T^{ij}_{\text{eff}}b^{ji}\omega^{-1} . \quad (51)$$

Thus from Eq. (42) we finally get

$$\langle T^{ii}F^i\rangle = T^{00}_{\text{eff}}[\bar{F}+(C_{\text{eff}}-\bar{C})(\delta C)^{-1}\delta F] - \sum_{j\in\mathbb{C}} T^{ij}_{\text{eff}}b^{ji}(\delta C)^{-1}\delta F . \quad (52)$$

We note that the expression for the joint average within the KKR-CCPA given by Mookerjee [Eq. (16b) of

$$\langle T^{ij}n_j\rangle = xT^{ij}_{\text{eff}} + (xy)^{1/2}\langle i;F|\tilde{A}^{-1}|j;F_j\rangle , \quad (56)$$

and

$$\langle n_iT^{ij}n_j\rangle = x^2T^{ij}_{\text{eff}} + x(xy)^{1/2}(\langle i;F|\tilde{A}^{-1}|j;F_j\rangle + \langle i;F_i|\tilde{A}^{-1}|j;F\rangle) + xy\langle i;F_i|\tilde{A}^{-1}|j;F\rangle . \quad (57)$$

Putting Eqs. (55), (56), and (57) in Eq. (54), we get

$$\langle T^{ij}F^{ji}\rangle = T^{ij}\bar{\bar{F}} + (xy)^{1/2}[\langle i;F|\tilde{A}^{-1}|j;F_j\rangle(xF_1+F_3) + \langle i;F_i|\tilde{A}^{-1}|j;F\rangle(xF_1+F_2)] + xy\langle i;F_i|\tilde{A}^{-1}|j;F_j\rangle F_1 , \quad (58)$$

where

$$\bar{\bar{F}} = x^2F^{AA}+y^2F^{BB}+xyF^{AB}+xyF^{BA} . \quad (59)$$

The matrix elements of $\tilde{A}^{-1}$ appearing in Eq. (58) can be determined by the partitioning technique discussed above. The element $\langle i;F|\tilde{A}^{-1}|j;F_j\rangle$ falls on the E_{12} block of Eq. (44), and with the help of Eqs. (45), (47), and (49) we can write

$$\langle i;F|\tilde{A}^{-1}|j;F_j\rangle \equiv X^{ij}_1 = -\sum_k T^{ik}_{\text{eff}}\omega\langle k;F_k|\mathcal{A}_2^{-1}|j;F_j\rangle . \quad (60)$$

Using Eq. (50) in Eq. (60) one finally gets

Substituting Eqs. (58), (60), (61), and (64) into Eq. (32), we get

$$\langle G_{\mathrm{NSD}}(\mathbf{r},\mathbf{r}')\rangle = \mathrm{Tr}\{T^{ij}\bar{\bar{F}} + (xy)^{1/2}[X_1^{ij}(xF_1+F_3) + X_2^{ij}(xF_1+F_2)] + xyX_3^{ij}F_1\} \ . \tag{66}$$

The configuration-averaged DOS and the charge density for the alloy are given by

$$\langle n(E)\rangle = -\frac{1}{\pi}\mathrm{Im}\int_{\Omega_i}\langle G_{\mathrm{SD}}(\mathbf{r}_i,\mathbf{r}_i)\rangle d\mathbf{r}_i \tag{67}$$

and

$$\langle \rho(\mathbf{r})\rangle = -\frac{1}{\pi}\mathrm{Im}\int_{-\infty}^{E_F}\langle G_{\mathrm{SD}}(\mathbf{r},\mathbf{r})\rangle d\mathbf{r} \ . \tag{68}$$

The average Green's function (site-diagonal form) by the restricted-averaging method (RAM) is given by

$$[G_{\mathrm{SD}}(\mathbf{r},\mathbf{r}')]_{\mathrm{RAM}} = \mathrm{Tr}(xD^A T_{\mathrm{eff}}^{00} F^A + yD^B T_{\mathrm{eff}}^{00} F^B) - \sum_L [xZ_L^A(\mathbf{r})J_L^A(\mathbf{r}') + yZ_L^B(\mathbf{r})J_L^B(\mathbf{r}')] \ , \tag{69}$$

where

$$D^\alpha = [I + T_{\mathrm{eff}}^{00}(C^\alpha - C_{\mathrm{eff}})]^{-1} \ . \tag{70}$$

Note that, for a general cluster size, Eqs. (53) and (69) are quite different. However, for a one-atom cluster, Eq. (53) reduces exactly to Eq. (69), thus giving the correct limit.

IV. RESULTS AND DISCUSSION

We have applied this formulation to a one-dimensional muffin-tin alloy model A_xB_y (Ref. 9). Various expressions regarding the wave functions, the scattering matrices, and the method of calculating the path operators for this model are presented in detail in Appendix B of Ref. 4. We have implemented the KKR-CCPA for a two-atom cluster on this model. The form of KKR-CCPA equations that can be used directly on the computer are given in Appendix A of Ref. 4. The lattice parameters ($a=6.00$ a.u.) and the muffin-tin radii ($r_m=2.25$ a.u.) of the two components of the alloy are taken to be identical. The depth of the two constituent potentials are $V_0^A=-0.3$ Ry and $V_0^B=-0.5$ Ry, respectively.

In Fig. 1(a) we show the averaged DOS calculated by the present method and that of Ref. 4 for $x=0.1$. We observe that in the first band there is no apparent difference between the two results. However, in the second band, which is due to A-type impurities,[10] the present calculation shows two peaks around $E=-0.13$ Ry and -0.10 Ry in contrast to a single peak around $E=-0.13$ Ry in the DOS of Ref. 4. Also, we note that

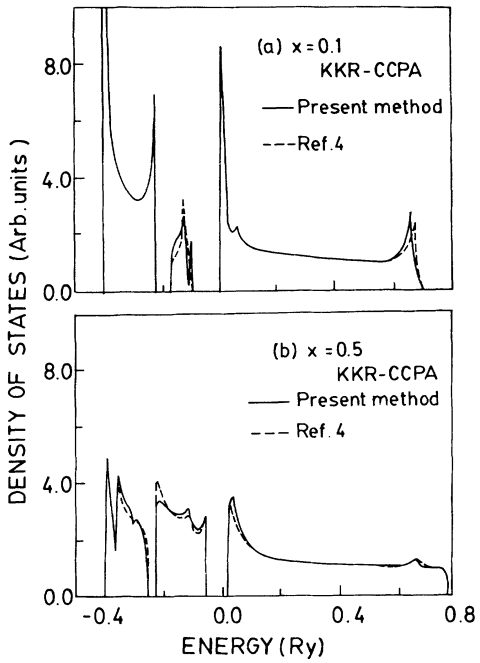

FIG. 1. Averaged density of states for the one-dimensional muffin-tin alloy for (a) $x=0.1$ and (b) $x=0.5$, calculated by the present method (solid line) and that of Ref. 4 (dashed line).

in the third band the peak around $E=0.68$ Ry is slightly shifted towards the lower-energy region in the present calculation. In Fig. 1(b) we show the averaged DOS of the present calculation and that of the restricted-averaging method (Ref. 4) for $x=0.5$. In this case we observe that, apart from the differences in the respective heights of the peaks, the results of the two calculations are more or less the same. But, nevertheless, there is a small but observable dip around $E=-0.30$ Ry in the present calculation, which is absent in the DOS calculated by the method of Ref. 4.

V. CONCLUSION

We have calculated the configuration-averaged Green's function exactly within the KKR-CCPA, while the corresponding expression in Ref. 4 is an approximated one. For a general cluster size these two expressions yield different results. However, for a one-atom cluster both expressions are identical, thus giving the correct limit. We calculated the averaged DOS for the one-dimensional alloy using these two methods. We found only small differences between the two results except for the impurity band of the dilute alloy.

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