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Application of augmented-space formalism to a problem of configuration averaging in the theory of unordered alloys with correlated disorder

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We present a method for calculating the electronic spectrum of a binary unordered alloy with short-range order (SRO). The method is based on a generalization of the augmented-space formalism in the case of correlated spatial disorder. A number of schemes for self-consistent calculation of the self-energy of the configurationally averaged Green's function are proposed. This approach guarantees a positive density of states (Herglotz property) for all values of the Cowley SRO parameter α. A merit of the method proposed is a correct limiting transition to the Green's function of the ordered alloy when the Cowley SRO parameter tends to the critical value. The approach is in agreement with the known approximations in the case of $\alpha=0$. As an illustration, a numerical analysis of self-consistent equations has been carried out for the case of one-dimensional Markov chain of atoms and for the case of the infinite-dimensional space.

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I. INTRODUCTION

In the present work, we study the problem of configuration averaging in the presence of spatial correlations that arises in calculating the macroscopic properties of unordered systems. This problem is urgent because in real systems the formation of physical properties is substantially influenced by the short-range ordering (SRO) effects. Among them one can mention the effect of the atomic ordering correlations on the quasiparticle spectrum in alloys, the influence of the charge- and spin-density correlations on the magnetic states of transition metals with itinerant electrons, the effect of SRO on the kinetic coefficients in disordered systems, and so on.

We should note that there is no universal principle for describing disordered systems, as fruitful as the Bloch theorem is for ideal crystals. When calculating approximately the Green's function one encounters standard difficulties connected with violation of the analytical properties of the averaged resolvent of the Hamiltonian that ensure a positive density of states. The coherent potential approximation[1] (CPA) first proposed by Soven is free of this shortcoming. However, the CPA is not able to take into account the effects of local ordering because of the single-site character of the averaging procedure performed within the framework of this method. A lot of attempts have been made to extend the CPA in order to consistently allow for the multiple scattering and SRO effects. We may refer to the molecular coherent potential approximation[2,3] (MCPA) and the embedded cluster method[4] (ECM).

In the MCPA the matrices of $n\times n$ size are introduced instead of the CPA single-site coherent potential and t matrix, which results in a matrix equation. In this framework one has to find n^2 parameters self-consistently. The attempts to reduce the number of self-consistent parameters and to make the self-energy translationally invariant lead to an approximate procedure of solving the self-consistent equations. As shown in Ref. 3, in such an approach, however, the Green's function may have branch points off the real axis on the complex plane, which does not agree with the required analytical properties and causes the sum-rule violation.

The method of the cluster embedded into an effective medium proposed in Refs. 4 and 5 is convenient for practical applications but is not a self-consistent approach. In realistic calculations the approximation for the effective medium is chosen in the simplest form and does not go beyond the single-site CPA framework.[5,6] For example, in calculations of the partial density of states (PDOS) such an approach is not fully consistent, as the accuracy of the effective medium approximation does not agree with the accuracy of the PDOS calculation in the embedded cluster. As it follows from the analysis performed in Ref. 7, in spite of the density of states peaks being situated at the expected positions on the energy axis, their width and shape are incorrect.

The traveling cluster approximation (TCA) proposed in Ref. 8 attempts to go beyond the single-site framework. The TCA holds the analytical properties of the averaged Green's function and takes into account the multiple-scattering effects without allowance for SRO. The numerical calculations performed in Refs. 7 and 9 have shown that the TCA reproduces much more accurately the fine structure of the impurity subband in the one-dimensional case than the ECM does.

Besides the above methods, the augmented-space formalism (ASF) has been developed by Mookerjee[10–12] for the problem of configuration averaging. It has received further development in Refs. 9 and 13 without, however, spatial correlations between the random variables. Based on the ASF, the authors of Refs. 9 and 13 proposed a generalization of the CPA that consistently takes into account multiple scattering within the limits of the ''maximum'' cluster and some approximations for the averaged resolvent that are controlled by a small parameter and have correct analytical properties.

Note, that the combination of the ASF with the ‘‘first-principles’’ methods for calculating the band structure allows the use of the ASF for realistic systems.[14,15]

For the problems with correlated disorder, the ASF has been used without any serious changes in Ref. 16. The authors expanded the averaged Green's function of a disordered alloy with SRO in terms of the averaged Green's function without SRO. Although the full expansion of the averaged Green's function is of the Herglotz-type, the truncation of the expansion results in a negative density of states for some energies the range of which increases with increasing the SRO parameter. A generalization of the ASF in the case of correlated disorder was proposed in Refs. 17 and 18. However, the operators of the random variables constructed in these works do not have the translation invariance of the corresponding crystal lattice and take into account the correlation effects only within the limits of one cluster. In our work, we propose a generalization of the ASF that is free of the above mentioned drawbacks and a scheme of self-consistent calculation of the averaged Green's function following the ideas of papers in Refs. 9 and 13.

We shall study the tight-binding model of a binary alloy with diagonal disorder. The Hamiltonian has the form

$$H(\{\epsilon_{\mathbf{n}}\})=\sum_{\mathbf{i}} |\mathbf{i}\rangle\epsilon_{\mathbf{i}}\langle\mathbf{i}|+\sum_{\mathbf{ij}} |\mathbf{i}\rangle V_{\mathbf{i-j}}\langle\mathbf{j}|, \tag{1.1}$$

where $|\mathbf{i}\rangle$ is the Wannier state at a site $\mathbf{i}$, the set $\{|\mathbf{i}\rangle\}$ is the complete orthogonal basis in a space Ψ. The configuration of the alloy is described by the set of random variables $\{\epsilon_{\mathbf{i}}\}$, where $\epsilon_{\mathbf{i}}$ assumes the value ϵ_A or ϵ_B depending on whether the site $\mathbf{i}$ is occupied by an atom of A or B type, respectively. The variables $\epsilon_{\mathbf{i}}$ are not independent for the alloy with SRO, i.e., $\epsilon_{\mathbf{i}}$ and $\epsilon_{\mathbf{j}}$ correlate at different sites of the lattice.

In a disordered system, it is the configurationally averaged properties that are of physical interest. For the Hamiltonian (1.1), the configurationally averaged Green's function is given by the relation

$$\overline{G}_{\mathbf{ij}}(\epsilon)=\int\int\cdots\int \langle\mathbf{i}|[\epsilon-H(\{\epsilon_{\mathbf{n}}\})]^{-1}|\mathbf{j}\rangle P(\{\epsilon_{\mathbf{n}}\})\prod_{\mathbf{n}} d\epsilon_{\mathbf{n}}, \tag{1.2}$$

where $P(\{\epsilon_{\mathbf{n}}\})$ is the joint probability density function for random variables and

$$\begin{aligned} P_{\epsilon_{\mathbf{i}}}(\epsilon)&=x\,\delta(\epsilon-\epsilon_A)+y\,\delta(\epsilon-\epsilon_B)\\ &=\int\int\cdots\int P(\{\epsilon_{\mathbf{n}}\})\prod_{\mathbf{n}\neq\mathbf{i}} d\epsilon_{\mathbf{n}} \end{aligned} \tag{1.3}$$

is the probability density of the random variable $\epsilon_{\mathbf{i}}$ at the fixed site. Here x and y are the concentrations of atoms of type A and B, respectively. The transfer matrix $V_{\mathbf{i-j}}$ in the Hamiltonian (1.1) is supposed to be nonrandom.

In Sec. II, we present a generalization of the ASF and the construction of a basis in the augmented space in the case of a one-dimensional chain of atoms whose configurations are determined by a first-order Markov process.[19] In Sec. III, a general scheme for self-consistent approximations of the resolvent averaged over configurations for such a chain is proposed. These approximations are based on the representation of the resolvent in the form of an infinity operator fraction. Next, the results obtained are extended to the case of the arbitrary correlation functions and space dimension. Also, it is shown that the theory yields a correct limiting transition to the Green's function of an ordered alloy if the Cowley SRO parameter tends to its critical values. Section IV is devoted to particular approximation schemes being the analogs of the CPA and TCA. We also present the results of a numerical study of the self-consistent equations. In Sec. V we summarize our results and say some words about possible applications of the proposed theory. The analytical details of calculations are presented in Appendices A, B, and C. Finally, in Appendix D, we prove that our approach does not violate analytical properties of the exactly averaged resolvent.

II. AUGMENTED-SPACE FORMALISM FOR AN ALLOY WITH SHORT-RANGE ORDER

In the ASF approach,[10,11] instead of direct averaging of the Green's function, one constructs a new Hamiltonian without disordered parameters defined on an augmented space. This new space can be represented as the direct product of the original Hilbert space by an auxiliary space that contains all possible configurations of the disordered system. For each random variable the self-conjugate operator determined on this auxiliary space is put into accordance. As it was shown by Mookerjee,[12] the physical background of this approach is the representation of these operators in terms of the creation and annihilation operators of pseudofermions. From this point of view, the problem of an electron moving in the random potential is equivalent to the problem of an electron interacting with the nonrandom fermion field, and the auxiliary space describing the configurations of an unordered alloy corresponds to the Fock space of pseudofermion states. From the same point of view, the motion of an electron in the Gaussian random field may be represented as an interaction of an electron with a bosonlike field.

A. Correlation functions of Markov type

To construct the ASF with allowance for the spatial correlations one should know the correlation functions of the products of random variables. Let us consider a one-dimensional A-B chain whose configuration is determined by a first-order Markov process.[19] Let $P(s_{\mathbf{i}}|s_{\mathbf{j}})$ be the probability of finding an atom of type $s_{\mathbf{i}}$ at site $\mathbf{i}$ provided that there is an atom of type $s_{\mathbf{j}}$ at site $\mathbf{j}$, and $P(s_{\mathbf{i}})$ be the probability of finding an atom $s_{\mathbf{i}}$ at site $\mathbf{i}$ that is equal to its concentration. Then the probability of the formation of a cluster with a given configuration is expressed as the product of pair conditional probabilities:

$$P_n(s_{\mathbf{l}_1},s_{\mathbf{l}_2},\ldots,s_{\mathbf{l}_n})=P(s_{\mathbf{l}_1})P(s_{\mathbf{l}_2}|s_{\mathbf{l}_1})P(s_{\mathbf{l}_3}|s_{\mathbf{l}_2})\cdots P(s_{\mathbf{l}_n}|s_{\mathbf{l}_{n-1}}), \tag{2.1}$$

where $l_1<l_2<\cdots<l_n$. The Cowley SRO parameter is defined as

$$\alpha=1-\frac{P^{AB}}{xy}, \tag{2.2}$$

where P^{AB} is the probability of the formation of an A-B pair at the neighboring sites. We shall suppose that A is an impurity atom, i.e., $x<y$. In the case of maximal repelling between atoms of different types, $P^{AB}=0$. In the opposite case of maximal attraction, $P^{AB}=x$. Hence, $0\leqslant P^{AB}\leqslant x$, $-x/y\leqslant\alpha\leqslant 1$. In the case of the absence of SRO, $P^{AB}=xy$, $\alpha=0$. The interval $0<\alpha<1$ corresponds to the repelling between the atoms A and B, the interval $-x/y<\alpha<0$ corresponds to their attraction. Using Eqs. (2.1) and (2.2), one can obtain the probability of an A-B pair forming at a distance n:

$$P_n^{AB}=xy(1-\alpha^n). \tag{2.3}$$

Hence, Eq. (2.1) is expressed in terms of x and α. Let

$$\overline{\epsilon}=x\epsilon_A+y\epsilon_B \tag{2.4}$$

be the averaged value of the energy at a site and

$$\xi_{\mathbf{i}}=\epsilon_{\mathbf{i}}-\overline{\epsilon}, \quad \overline{\xi_{\mathbf{i}}}=0 \tag{2.5}$$

be the energy shift at site **i**. Denote

$$\Delta\xi=(y-x)(\epsilon_A-\epsilon_B), \quad \Delta=\sqrt{xy}(\epsilon_A-\epsilon_B). \tag{2.6}$$

Since $\xi_{\mathbf{i}}$ assumes only two values $\xi_A=\epsilon_A-\overline{\epsilon}$ and $\xi_B=\epsilon_B-\overline{\epsilon}$, therefore $(\xi_{\mathbf{i}}-\xi_A)(\xi_{\mathbf{i}}-\xi_B)=0$, and

$$\xi_{\mathbf{i}}^2=(\Delta\xi)\xi_{\mathbf{i}}+\Delta^2. \tag{2.7}$$

We define the functions called ‘‘connected’’ correlation functions:

$$\langle\xi_{\mathbf{l}_1}\xi_{\mathbf{l}_2},\dots,\xi_{\mathbf{l}_n}\rangle_c=\Delta^2(\Delta\xi)^{n-2}\alpha^{l_n-l_1}, \quad n\geqslant 2, \tag{2.8}$$

$\langle\xi_{\mathbf{i}}\rangle_c=0$, hereafter $l_1<l_2<\cdots<l_n$, and according to Eq. (2.7) we do not consider the higher powers of $\xi_{\mathbf{i}}$. Then using Eqs. (2.1) and (2.3), one can show that any correlation function on the Markov chain can be represented in terms of ‘‘connected’’ functions. For example, leading correlation functions are given by the following expressions:

$$\begin{gathered}
\langle\xi_{\mathbf{l}_1}\xi_{\mathbf{l}_2}\rangle=\langle\xi_{\mathbf{l}_1}\xi_{\mathbf{l}_2}\rangle_c,\\
\langle\xi_{\mathbf{l}_1}\xi_{\mathbf{l}_2}\xi_{\mathbf{l}_3}\rangle=\langle\xi_{\mathbf{l}_1}\xi_{\mathbf{l}_2}\xi_{\mathbf{l}_3}\rangle_c,\\
\langle\xi_{\mathbf{l}_1}\xi_{\mathbf{l}_2}\xi_{\mathbf{l}_3}\xi_{\mathbf{l}_4}\rangle=\langle\xi_{\mathbf{l}_1}\xi_{\mathbf{l}_2}\rangle_c\langle\xi_{\mathbf{l}_3}\xi_{\mathbf{l}_4}\rangle_c+\langle\xi_{\mathbf{l}_1}\xi_{\mathbf{l}_2}\xi_{\mathbf{l}_3}\xi_{\mathbf{l}_4}\rangle_c,\\
\langle\xi_{\mathbf{l}_1}\xi_{\mathbf{l}_2}\xi_{\mathbf{l}_3}\xi_{\mathbf{l}_4}\xi_{\mathbf{l}_5}\rangle=\langle\xi_{\mathbf{l}_1}\xi_{\mathbf{l}_2}\xi_{\mathbf{l}_3}\rangle_c\langle\xi_{\mathbf{l}_4}\xi_{\mathbf{l}_5}\rangle_c+\langle\xi_{\mathbf{l}_1}\xi_{\mathbf{l}_2}\rangle_c\langle\xi_{\mathbf{l}_3}\xi_{\mathbf{l}_4}\xi_{\mathbf{l}_5}\rangle_c\\
+\langle\xi_{\mathbf{l}_1}\xi_{\mathbf{l}_2}\xi_{\mathbf{l}_3}\xi_{\mathbf{l}_4}\xi_{\mathbf{l}_5}\rangle_c,\\
\dots,
\end{gathered} \tag{2.9}$$

where $\langle\cdots\rangle$ means averaging over configurations. Now, we can formulate a general rule for calculating the correlation function of the nth order. One should separate a chain consisting of n atoms into the chains of smaller length taking away some edges in all possible ways. Each separation of a chain corresponds to a term in the correlation function that is equal to the product of the connected correlation functions of smaller order. Finally, we should add to the expression obtained the connected correlation function (2.8) of the nth order.

B. Construction of a basis in the augmented space in the case of a one-dimensional chain

Following the ASF,[10,11,13] we associate a real random value $\xi_{\mathbf{i}}$ (2.5) with a self-conjugate operator $\hat{\xi}_{\mathbf{i}}$ determined on an auxiliary space Φ, such that the range of the random value coincides with the spectrum of the corresponding operator. In the case of a binary alloy, $\xi_{\mathbf{i}}$ has a probability distribution given by Eq. (1.3), and Φ is a 2^N-dimensional vector space, where N is the number of the lattice sites. The complete orthonormalized basis $\{|s\rangle\}$ can be defined in the space Φ, where $s=(s_1,s_2,\dots,s_N)$ and $s_{\mathbf{i}}=A$ or B. Here the vector $|s\rangle$ is associated with one of the 2^N possible configurations ($s_{\mathbf{i}}=A$ if the site **i** is occupied by an atom of type A, and $s_{\mathbf{i}}=B$ otherwise). The vectors $\{|s\rangle\}$ are the eigenvectors for all $\hat{\xi}_{\mathbf{i}}$, so that

$$\hat{\xi}_{\mathbf{i}}|s\rangle=\xi_{\mathbf{i}}(s_{\mathbf{i}})|s\rangle, \tag{2.10}$$

$$\xi_{\mathbf{i}}(s_{\mathbf{i}})=\begin{cases}\epsilon_A-\overline{\epsilon}, & s_{\mathbf{i}}=A\\ \epsilon_B-\overline{\epsilon}, & s_{\mathbf{i}}=B.\end{cases}$$

According to this definition, the operators $\hat{\xi}_{\mathbf{i}}$ commutate with each other.

Let $f(\xi_{\mathbf{i}},\xi_{\mathbf{j}},\dots,\xi_{\mathbf{k}})$ be a function of random variables $\xi_{\mathbf{i}}$, $\xi_{\mathbf{j}},\dots,\xi_{\mathbf{k}}$. The operator associated with this function is defined as $\hat{f}=f(\hat{\xi}_{\mathbf{i}},\hat{\xi}_{\mathbf{j}},\dots,\hat{\xi}_{\mathbf{k}})$, and according to Eq. (2.10), $\langle s|\hat{f}|s\rangle$ is the value of f for a fixed configuration of atoms on a chain. Let $p(s)$ be the probability of the realization of configuration s. We define the ground state in Φ as

$$|vac\rangle=\sum_s \sqrt{p(s)}|s\rangle. \tag{2.11}$$

Then the value of f averaged over all configurations of a system is

$$\overline{f}=\langle vac|\hat{f}|vac\rangle. \tag{2.12}$$

Following the ideas of papers in Refs. 9 and 13, we construct a basis involving the vectors generated by $\hat{\xi}_{\mathbf{i}}$ when acting on $|vac\rangle$. It will be shown further that the configuration space Φ has a Fock-space structure:

$$\Phi=E_0\oplus E_1\oplus\cdots\oplus E_n\oplus\cdots. \tag{2.13}$$

Here E_0 is a one-dimensional subspace generated by $|vac\rangle$ (2.11). Next we define an N-dimensional subspace E_1 corresponding to single excitations as the span of the vectors

$$|\mathbf{i}\}=\Delta^{-1}\hat{\xi}_{\mathbf{i}}|vac\rangle, \tag{2.14}$$

which, unlike the case of independent random variables, are not orthogonal to each other. It follows from Eqs. (2.8) and (2.9) that the matrix of the scalar product of vectors (2.14) is $g_{ij}=\{\mathbf{i}|\mathbf{j}\}=\alpha^{|i-j|}$. The Fourier transform of g_{ij} is

$$g(q)=\frac{1}{N}\sum_{ij} g_{ij}\exp\{iq(i-j)\}=\frac{1-\alpha^2}{1+\alpha^2-2\alpha\cos q},$$

$$q\in[-\pi,\pi]. \tag{2.15}$$

If $|\alpha|<1$, then $g(q)>0$ (the matrix g_{ij} is positively defined), hence the vectors (2.14) are linearly independent and form a complete basis in E_1. Since $\overline{\xi_{\mathbf{i}}}=\{vac|\hat{\xi}_{\mathbf{i}}|vac\}=0$, E_1 is orthogonal to E_0.

Let $|\mathbf{i},\mathbf{j}\}$ $(i<j)$ be the basis vectors of E_2 that should be built up orthogonally to E_0 and E_1, therefore we require

$$\{vac|\mathbf{i},\mathbf{j}\}=0, \quad \{\mathbf{i}'|\mathbf{i},\mathbf{j}\}=0, \tag{2.16}$$

for all $\mathbf{i}'$ and $\mathbf{i}\neq\mathbf{j}$. Let

$$b_1|\mathbf{i},\mathbf{i+1}\}=[\hat{\xi}_{\mathbf{i+1}}\hat{\xi}_{\mathbf{i}}-a_0-a_1(\hat{\xi}_{\mathbf{i}}+\hat{\xi}_{\mathbf{i+1}})]|vac\}. \tag{2.17}$$

Since the vector $|\mathbf{i},\mathbf{i+1}\}$ has to satisfy the relations (2.16), and $|\mathbf{i}\}$ is defined by Eq. (2.14), we multiply $\{vac|$ and $\{vac|\hat{\xi}_{\mathbf{i}}$ from the left by Eq. (2.17) and, using Eqs. (2.8) and (2.9), we find

$$a_0=\Delta^2\alpha, \quad a_1=\Delta\xi\frac{\alpha}{1+\alpha}.$$

The coefficient b_1 in Eq. (2.17) can be found from the normalization condition $\{\mathbf{i},\mathbf{i+1}|\mathbf{i},\mathbf{i+1}\}=1$:

$$b_1^2=\Delta^4(1-\alpha^2)+\Delta^2(\Delta\xi)^2\frac{1-\alpha}{1+\alpha}\alpha. \tag{2.18}$$

Since $b_1^2>0$, from Eq. (2.18) we get the restriction on the Cowley parameter $-x/y<\alpha<1(x<y)$ that has been already mentioned. If $\alpha=1$ or $\alpha=-x/y$, then $b_1=0$. Bearing in mind that the correlation functions (2.8) and (2.9) are the powers of α, we can check that the vector $|\mathbf{i},\mathbf{i+1}\}$, built up according to Eq. (2.17), is orthogonal not only to $|\mathbf{i}\}$ and $|\mathbf{i+1}\}$, but to all other vectors $|\mathbf{j}\}\in E_1$. Besides, $\{\mathbf{i},\mathbf{i+1}|\mathbf{j},\mathbf{j+1}\}=0$ if $\mathbf{i}\neq\mathbf{j}$.

For an arbitrary vector $|\mathbf{i},\mathbf{i+n}\}$ we can write

$$b_n|\mathbf{i},\mathbf{i+n}\}=[\hat{\xi}_{\mathbf{i}}\hat{\xi}_{\mathbf{i+n}}-L_{n+1}^{(1)}(\hat{\xi}_{\mathbf{i}},\hat{\xi}_{\mathbf{i+1}},\dots,\hat{\xi}_{\mathbf{i+n}})]|vac\}. \tag{2.19}$$

Here $L_{n+1}^{(1)}$ is a first-degree polynomial in $(n+1)$ variables with $(n+2)$ arbitrary coefficients. We can find them demanding the vector $|\mathbf{i},\mathbf{i+n}\}$ to be orthogonal to $|vac\}$ and to the single excitations $|\mathbf{j}\}$ such that $i\leqslant j\leqslant i+n$. Using Eqs. (2.8) and (2.9) we get $(n+2)$ equations; b_n can be found using the normalization condition. Next, by direct verification, we make sure that the vector $|\mathbf{i},\mathbf{i+n}\}$ is constructed in such a way that is also orthogonal to $|\mathbf{j}'\}$, where $\mathbf{j}'\notin[i,i+n]$. Following that scheme we find that

$$b_2|\mathbf{i},\mathbf{i+2}\}=[\hat{\xi}_{\mathbf{i}}\hat{\xi}_{\mathbf{i+2}}-a_2^{(0)}-a_2^{(1)}(\hat{\xi}_{\mathbf{i}}+\hat{\xi}_{\mathbf{i+2}})-a_2^{(2)}\hat{\xi}_{\mathbf{i+1}}]|vac\},$$

where

$$a_2^{(0)}=\Delta^2\alpha^2, \quad a_2^{(1)}=\Delta\xi\frac{\alpha^2}{1+\alpha}, \quad a_2^{(2)}=\Delta\xi\alpha^2\frac{1-\alpha}{1+\alpha},$$

and

$$b_3|\mathbf{i},\mathbf{i+3}\}=[\hat{\xi}_{\mathbf{i}}\hat{\xi}_{\mathbf{i+3}}-a_3^{(0)}-a_3^{(1)}(\hat{\xi}_{\mathbf{i}}+\hat{\xi}_{\mathbf{i+3}})$$
$$-a_3^{(2)}(\hat{\xi}_{\mathbf{i+1}}+\hat{\xi}_{\mathbf{i+2}})]|vac\},$$

where

$$a_3^{(0)}=\Delta^2\alpha^3, \quad a_3^{(1)}=\Delta\xi\frac{\alpha^3}{1+\alpha}, \quad a_3^{(2)}=\Delta\xi\alpha^3\frac{1-\alpha}{1+\alpha},$$

and so on. We define the subspace E_2 as a span of the vectors $\{|\mathbf{i},\mathbf{i+n}\}\}$ given by Eq. (2.19). Under the restriction $-x/y<\alpha<1$, one can prove that the set of vectors (2.19) is a complete (but nonorthogonal) basis in E_2. In this case, for the pairs of vectors $|\mathbf{i},\mathbf{j}\}$ $(j>i)$ and $|\mathbf{l},\mathbf{m}\}$ $(m>l)$ we have

$$\{\mathbf{i},\mathbf{j}|\mathbf{l},\mathbf{m}\}=0, \quad j\leqslant l,$$

$$\{\mathbf{i},\mathbf{j}|\mathbf{l},\mathbf{m}\}=\frac{b_{j-l}^2}{b_{j-i}b_{m-l}}\alpha^{l-i}\alpha^{m-j}, \quad i\leqslant l<j\leqslant m, \tag{2.20}$$

$$\{\mathbf{i},\mathbf{j}|\mathbf{l},\mathbf{m}\}=\frac{b_{m-l}}{b_{j-i}}\alpha^{l-i}\alpha^{j-m}, \quad i\leqslant l<m\leqslant j.$$

In the general case, we shall assume that the subspace E_n is a span of the vectors

$$|\sigma_n(\mathbf{l})\rangle=|\mathbf{l}_1,\mathbf{l}_2,\dots,\mathbf{l}_n\}, \tag{2.21}$$

where σ_n is the configuration of a cluster, $\mathbf{l}$ is the location of its center of gravity, $l_1<l_2<\cdots<l_n$. By analogy with Eq. (2.19), we write

$$b_{\sigma_n}|\mathbf{l}_1,\mathbf{l}_2,\dots,\mathbf{l}_n\}=[\hat{\xi}_{\mathbf{l}_1}\hat{\xi}_{\mathbf{l}_2}\cdots\hat{\xi}_{\mathbf{l}_n}$$
$$-L_{l_n-l_1+1}^{(n-1)}(\hat{\xi}_{\mathbf{l}_1},\hat{\xi}_{\mathbf{l}_1+1},\hat{\xi}_{\mathbf{l}_1+2},\dots,\hat{\xi}_{\mathbf{l}_n})]|vac\}. \tag{2.22}$$

Here $L_k^{(n-1)}(\xi_1,\xi_2,\dots,\xi_k)$, $n\leqslant k$ is a $(n-1)$-th degree polynomial in k variables of the form

$$L_k^{(n-1)}(\xi_1,\xi_2,\dots,\xi_k)$$
$$=c_0^{(n)}+\sum_{i=1}^{k}c_i^{(n)}\xi_i+\sum_{1\leqslant i<j\leqslant k}c_{ij}^{(n)}\xi_i\xi_j+\cdots$$
$$+\sum_{1\leqslant i_1<i_2<\cdots<i_{n-1}\leqslant k}c_{i_1i_2\cdots i_{n-1}}^{(n)}\xi_{i_1}\xi_{i_2}\cdots\xi_{i_{n-1}}. \tag{2.23}$$

The coefficients of the polynomial (2.23) are determined by the condition that the vector $|\sigma_n(\mathbf{l})\rangle$ is orthogonal to any vector defined on the cluster $\sigma_m(\mathbf{l}')\subseteq\{\mathbf{l}_1,\mathbf{l}_2,\dots,\mathbf{l}_n\}(m<n)$, and by relations (2.7), (2.8), and (2.9). The vector $|\sigma_n(\mathbf{l})\rangle$ built up in such a way proves to be orthogonal to any vector $|s\rangle\in E_0\oplus E_1\oplus\cdots\oplus E_{n-1}$. The vectors $|\sigma_n(\mathbf{l})\rangle$ and $|\sigma_n'(\mathbf{l}')\rangle$ are orthogonal for different clusters $\sigma_n(\mathbf{l})$ and $\sigma_n'(\mathbf{l}')$ if they do not overlap. Relations (2.20) are a particular case of this rule.

In the ASF representation the Hamiltonian (1.1) has the form[13]:

$$\mathcal{H}=\sum_{\mathbf{i}} |\mathbf{i}\rangle\langle\mathbf{i}|\otimes\hat{\xi}_{\mathbf{i}}+\sum_{\mathbf{ij}} |\mathbf{i}\rangle(\overline{\epsilon}\delta_{\mathbf{ij}}+V_{\mathbf{i-j}})\langle\mathbf{j}|\otimes\hat{I}, \qquad (2.24)$$

where $\hat{I}$ is the unit operator in Φ. The Hamiltonian (2.24) acts on the augmented space $\Psi\otimes\Phi$, $|\mathbf{i}\rangle\in\Psi$, which as before has a Fock-space structure:

$$\Psi\otimes\Phi=E^{(0)}\oplus E^{(1)}\oplus\cdots\oplus E^{(n)}\oplus\cdots,$$

where $E^{(n)}=\Psi\otimes E_n$. We denote a basis vector in $E^{(n)}$:

$$|\mathbf{i+l},\sigma_n(\mathbf{l})\rangle=|\mathbf{i+l}\rangle\otimes|\sigma_n(\mathbf{l})\rangle. \qquad (2.25)$$

Here $\mathbf{i}$ is the location of an electron with respect to the center of gravity of a cluster $\sigma_n(\mathbf{l})$ ($\mathbf{i}\equiv 0$ if $n=0$). According to Eq. (2.22),

$$\mathrm{Im}\,\hat{\xi}_{\mathbf{i}}(E_n)\subseteq E_{n-1}\oplus E_n\oplus E_{n+1},$$

where $\mathrm{Im}\,\hat{\xi}_{\mathbf{i}}(E_n)$ is the image of E_n under the mapping $\hat{\xi}_{\mathbf{i}}$. Therefore, the Hamiltonian (2.24) has a three-diagonal block form in the basis (2.25):

$$\mathcal{H}_{nm}=\mathcal{H}_n\delta_{nm}+\Delta_n\delta_{n+1,m}+\Delta_n^{+}\delta_{n-1,m}, \qquad (2.26)$$

where $\mathcal{H}_{nm}=P_n\mathcal{H}P_m$, $\Delta_n=P_n\mathcal{H}P_{n+1}$, and $P_n(n\geqslant 0)$ is the orthogonal projector onto $E^{(n)}$.

III. CONFIGURATION AVERAGING OF THE RESOLVENT

A. Representation of the resolvent as a continued fraction in the case of Markov-type correlations

In the ASF framework the problem of finding the Green's function (1.2) reduces to calculating the projection $G_0(\epsilon)=P_0[1/(\epsilon-\mathcal{H})]P_0$ of the resolvent of the Hamiltonian (2.24) onto a subspace $E^{(0)}$. According to Eq. (2.12), we have

$$G_0(\epsilon)=\sum |\mathbf{l},\sigma_0(\mathbf{l})\rangle\overline{G}_{\mathbf{lm}}(\epsilon)\langle\mathbf{m},\sigma_0(\mathbf{m})|. \qquad (3.1)$$

For further calculations it is convenient to define a basis $\{|\chi[\sigma_n(\mathbf{l})]\rangle\}$ in Φ that is dual to $\{|\sigma_n(\mathbf{l})\rangle\}$ (2.21), (2.22), such that

$$\langle\chi[\sigma_n(\mathbf{l})]|\sigma_m'(\mathbf{l}')\rangle=\delta_{\sigma\sigma'}\delta_{nm}\delta_{\mathbf{ll}'}.$$

Then in the augmented space $\Psi\otimes\Phi$ a basis $|\mathbf{i+l},\chi[\sigma_n(\mathbf{l})]\rangle=|\mathbf{i+l}\rangle\otimes|\chi[\sigma_n(\mathbf{l})]\rangle$ dual to the basis (2.25) is generated:

$$\langle\mathbf{i+l},\chi[\sigma_n(\mathbf{l})]|\mathbf{j+l}',\sigma_m'(\mathbf{l}')\rangle=\delta_{\sigma\sigma'}\delta_{nm}\delta_{\mathbf{ll}'}\delta_{\mathbf{ij}}.$$

We next introduce the Fourier transform:

$$|\mathbf{i},\sigma_n,\mathbf{q}\rangle=\frac{1}{\sqrt{N}}\sum_{\mathbf{l}} |\mathbf{i+l},\sigma_n(\mathbf{l})\rangle\exp\{-i\mathbf{ql}\}, \qquad \mathbf{q}\in[-\pi,\pi]$$

$$|\chi(\mathbf{i},\sigma_n,\mathbf{q})\rangle=\frac{1}{\sqrt{N}}\sum_{\mathbf{l}} |\mathbf{i+l},\chi[\sigma_n(\mathbf{l})]\rangle\exp\{-i\mathbf{ql}\}, \qquad (3.2)$$

$$\langle\chi(\mathbf{i},\sigma_n,\mathbf{q})|\mathbf{j},\sigma_m',\mathbf{q}'\rangle=\delta_{\sigma\sigma'}\delta_{nm}\delta_{\mathbf{ij}}\delta_{\mathbf{qq}'},$$

$$\langle\mathbf{i},\sigma_n,\mathbf{q}|\mathbf{j},\sigma_m',\mathbf{q}'\rangle=\delta_{\mathbf{qq}'}\delta_{nm}\exp\{i\mathbf{q}(\mathbf{j-i})\}\langle\sigma_n(\mathbf{i})|\sigma_m'(\mathbf{j})\rangle.$$

Then the Hamiltonian (2.24) has the form

$$\mathcal{H}=\sum_{\mathbf{q}} \mathcal{H}(\mathbf{q}), \qquad \mathcal{H}(\mathbf{q})=\mathcal{H}_{vc}(\mathbf{q})+\mathcal{U}(\mathbf{q}),$$

$$\begin{aligned}\mathcal{H}_{vc}(\mathbf{q})=&|\mathbf{0},\sigma_0,\mathbf{q}\rangle(\overline{\epsilon}+V(\mathbf{q}))\langle\mathbf{0},\sigma_0,\mathbf{q}|\\&+\sum_{\mathbf{i},\,\mathbf{j},\sigma_n,n\geqslant 1} |\mathbf{i},\sigma_n,\mathbf{q}\rangle(\overline{\epsilon}\delta_{\mathrm{ij}}+V_{\mathbf{i-j}})\langle\chi(\mathbf{j},\sigma_n,\mathbf{q})|,\end{aligned} \qquad (3.3)$$

$$V(\mathbf{q})=\frac{1}{N}\sum_{\mathbf{ij}} V_{\mathbf{i-j}}\exp\{i\mathbf{q}(\mathbf{i-j})\},$$

$$\begin{aligned}\mathcal{U}(\mathbf{q})=&\sum_{\mathbf{i},\mathbf{d},\sigma_n,\sigma_m'} |\mathbf{i},\sigma_n,\mathbf{q}\rangle\exp\{i\mathbf{qd}\}\xi^{(0)}_{\sigma_n(\mathbf{i})\sigma_m'(\mathbf{i+d})}\\&\times\langle\chi(\mathbf{i+d},\sigma_m',\mathbf{q})|,\end{aligned}$$

where $\xi^{(0)}_{\sigma_n(\mathbf{i})\sigma_m'(\mathbf{i+d})}=\langle\chi[\sigma_n(\mathbf{i})]|\hat{\xi}_{\mathbf{0}}|\sigma_m'(\mathbf{i+d})\rangle$, $\mathbf{d}$ is the vector connecting the centers of gravity of clusters $\sigma_n(\mathbf{i})$ and $\sigma_m'(\mathbf{i+d})$, $\mathcal{H}_{vc}(\mathbf{q})$ is the Hamiltonian of the "virtual" crystal, $\mathcal{U}(\mathbf{q})$ is the representation of the random potential.

Let us introduce the orthogonal projectors onto the spaces $E_{\mathbf{q}}^{(n)}$:

$$P_{\mathbf{n}}^{\mathbf{q}}=\sum_{\mathbf{i},\sigma_n} |\mathbf{i},\sigma_n,\mathbf{q}\rangle\langle\chi(\mathbf{i},\sigma_n,\mathbf{q})|. \qquad (3.4)$$

Using Eq. (3.4), we can rewrite Eq. (3.1) in the form[13]

$$G_0(\epsilon,\mathbf{q})=\frac{1}{\epsilon-\mathcal{H}_0(\mathbf{q})-\Sigma_0(\epsilon,\mathbf{q})}, \qquad (3.5)$$

where

$$\mathcal{H}_0(\mathbf{q})=P_0^{\mathbf{q}}\mathcal{H}(\mathbf{q})P_0^{\mathbf{q}}, \qquad Q_0^{\mathbf{q}}=1-P_0^{\mathbf{q}},$$

$$\Sigma_0(\epsilon,\mathbf{q})=P_0^{\mathbf{q}}\mathcal{H}(\mathbf{q})Q_0^{\mathbf{q}}\frac{1}{\epsilon-Q_0^{\mathbf{q}}\mathcal{H}(\mathbf{q})Q_0^{\mathbf{q}}}Q_0^{\mathbf{q}}\mathcal{H}(\mathbf{q})P_0^{\mathbf{q}}. \qquad (3.6)$$

Proceeding the projection, we write $\Sigma_0(\epsilon,\mathbf{q})$ in the form of a continued fraction[13]:

$$\Sigma_0(\epsilon,\mathbf{q})=\Delta_0(\mathbf{q})\frac{1}{\epsilon-\mathcal{H}_1-\Delta_1(\mathbf{q})\dfrac{1}{\epsilon-\mathcal{H}_2(\mathbf{q})-\ddots\;\Delta_{n-1}(\mathbf{q})\dfrac{1}{\epsilon-\mathcal{H}_n(\mathbf{q})-\Sigma_n(\epsilon,\mathbf{q})}\Delta^+_{n-1}(\mathbf{q})}\Delta^+_1(\mathbf{q})}\Delta^+_0(\mathbf{q}), \tag{3.7}$$

where $\mathcal{H}_n(\mathbf{q})=P_n^{\mathbf{q}}\mathcal{H}(\mathbf{q})P_n^{\mathbf{q}}$, $\Delta_n(\mathbf{q})=P_n^{\mathbf{q}}\mathcal{U}(\mathbf{q})P_{n+1}^{\mathbf{q}}$, and the projectors $P_n^{\mathbf{q}}$ are defined by Eq. (3.4).

It is impossible to calculate analytically the formally exact expression (3.7) because it is determined by infinite-dimensional matrices. In contrast to the paper in Ref. 13, problems arise already on the first ''level'' of the fraction. Therefore, it is convenient to choose a special orthogonal basis in each space $E_{\mathbf{q}}^{(n)}$. Next we write $|\sigma_{\mathbf{n}}(\mathbf{i}),\mathbf{q}\rangle=|\mathbf{l}_1,\mathbf{l}_2,\ldots,\mathbf{l}_n,\mathbf{q}\rangle$ instead of $|\mathbf{i},\sigma_n,\mathbf{q}\rangle$, where, as before in Eq. (2.21), $\sigma_n(\mathbf{i})=\{\mathbf{l}_1,\mathbf{l}_2,\ldots,\mathbf{l}_n\}$ denotes a cluster of $\sigma_{\mathbf{n}}$, and $\mathbf{i}$ is its center of gravity. Let us construct an orthogonal basis for $n=1$:

$$|\psi_0,\mathbf{q}\rangle=|\mathbf{0},\mathbf{q}\rangle,$$

$$|\psi_m,\mathbf{q}\rangle=(1-\alpha^2)^{-1/2}(|\mathbf{m},\mathbf{q}\rangle-|\mathbf{m-1},\mathbf{q}\rangle\alpha\exp\{iq\}), \tag{3.8}$$

$$|\psi_{-m},\mathbf{q}\rangle=(1-\alpha^2)^{-1/2}(|\mathbf{-m},\mathbf{q}\rangle-|-\mathbf{m+1},\mathbf{q}\rangle\alpha\times\exp\{-iq\}),\quad m>0.$$

In the subspace $E_{\mathbf{q}}^{(2)}$ the orthogonal basis can be defined as

$$|\psi_{m,m+1},\mathbf{q}\rangle=|\mathbf{m},\mathbf{m+1},\mathbf{q}\rangle,$$

$$|\psi_{m,m+2},\mathbf{q}\rangle=(1-2\mu^2)^{-1/2}(|\mathbf{m},\mathbf{m+2},\mathbf{q}\rangle-|\mathbf{m},\mathbf{m+1},\mathbf{q}\rangle\mu\exp\{iq/2\}-|\mathbf{m+1},\mathbf{m+2},\mathbf{q}\rangle\mu\exp\{-iq/2\}),$$

$$|\psi_{m,m+3},\mathbf{q}\rangle=(1-\lambda^2-\eta^2)^{-1/2}(|\mathbf{m},\mathbf{m+3},\mathbf{q}\rangle-|\mathbf{m},\mathbf{m+2},\mathbf{q}\rangle\lambda\exp\{iq/2\}-|\mathbf{m+1},\mathbf{m+3},\mathbf{q}\rangle\lambda\exp\{-iq/2\}+\eta|\mathbf{m+1},\mathbf{m+2},\mathbf{q}\rangle),$$

$$\ldots .$$

Here $\mu=\alpha b_1/b_2$, $\lambda=\alpha b_2/b_3$, $\eta=\alpha b_1/b_3$, the coefficients b_1, b_2, b_3 are defined by Eqs. (2.18) and (2.19). Using the scalar products (2.20), an arbitrary basis vector $|\psi_{m,m+k},\mathbf{q}\rangle$ can be obtained by orthogonalizing $|\mathbf{m},\mathbf{m+k},\mathbf{q}\rangle$ to each of the double excitation vectors from the segment $[m,m+k]$.

A similar statement is also valid for the subspace $E_{\mathbf{q}}^{(n)}(n>2)$. We shall denote the vectors of the orthonormal basis in $E_{\mathbf{q}}^{(n)}$ by $|\psi_{\sigma_n(\mathbf{i})},\mathbf{q}\rangle$, where $\sigma_n(\mathbf{i})=\{\mathbf{l}_1,\mathbf{l}_2,\ldots,\mathbf{l}_n\}$. An arbitrary basis vector $|\psi_{\sigma_n(\mathbf{i})},\mathbf{q}\rangle$ can be obtained by orthogonalization of the vector $|\sigma_n(\mathbf{i}),\mathbf{q}\rangle$ to all n-fold excitations belonging to $[l_1 l_n]$.

Let us now consider the matrix components of the random potential $\mathcal{U}(\mathbf{q})$. Let $\mathcal{U}_n(\mathbf{q})=P_n^{\mathbf{q}}\mathcal{U}(\mathbf{q})P_n^{\mathbf{q}}$. According to Eq. (2.26), the Hamiltonian (3.3) has a three-diagonal block form, hence,

$$\mathcal{U}(\mathbf{q})=\sum_{n\geqslant1}\mathcal{U}_n(\mathbf{q})+\sum_{n\geqslant0}[\Delta_n(\mathbf{q})+\Delta_n^+(\mathbf{q})]. \tag{3.9}$$

The matrix components of the operator (3.9) can be calculated using the relation

$$\langle\mathbf{j},\sigma_n,\mathbf{q}|\mathcal{U}(\mathbf{q})|\mathbf{i},\sigma'_m,\mathbf{q}\rangle=\langle\sigma_n(\mathbf{j})|\hat{\xi}_{\mathbf{0}}|\sigma'_m(\mathbf{i})\rangle\exp\{i\mathbf{q}(\mathbf{i-j})\};$$

then

$$\langle\mathbf{0},\sigma_0,\mathbf{q}|\Delta_0(\mathbf{q})|\psi_m,\mathbf{q}\rangle=\delta_{m,0}\Delta. \tag{3.10}$$

The random potential $\mathcal{U}_1(\mathbf{q})$ is diagonal in the basis (3.8) of the subspace $E_{\mathbf{q}}^{(1)}$:

$$\langle\psi_0,\mathbf{q}|\mathcal{U}_1(\mathbf{q})|\psi_0,\mathbf{q}\rangle=\Delta\xi, \tag{3.11}$$

$$\langle\psi_m,\mathbf{q}|\mathcal{U}_1(\mathbf{q})|\psi_k,\mathbf{q}\rangle=\delta_{mk}\Delta\xi\frac{\alpha^{|m|}}{1+\alpha},\quad m\neq0.$$

In the case of uncorrelated disorder ($\alpha=0$), the nonzero matrix components of $\Delta_1(\mathbf{q})$ are written as[13]:

$$\langle\psi_m,\mathbf{q}|\Delta_1(\mathbf{q})|\psi_{0,m},\mathbf{q}\rangle=\Delta\exp\{-iqm/2\},\quad m\neq0. \tag{3.12}$$

In the case of $\alpha\neq0$, the constant Δ in Eq. (3.12) is replaced by another constant. For example,

$$\langle\psi_1,\mathbf{q}|\Delta_1(\mathbf{q})|\psi_{0,1},\mathbf{q}\rangle=\Delta^{-1}(1-\alpha^2)^{-1/2}b_1\exp\{-iq/2\}, \tag{3.13}$$

$$\langle\psi_{-1},\mathbf{q}|\Delta_1(\mathbf{q})|\psi_{0,-1},\mathbf{q}\rangle=\Delta^{-1}(1-\alpha^2)^{-1/2}b_1\exp\{iq/2\},$$

where $b_1>0$ is defined by Eq. (2.18). Since the vectors $|\psi_{m,m+k},\mathbf{q}\rangle$ are builtup by means of orthogonalization of the vectors of type (2.19), for $\alpha\neq0$, the matrix components $\langle\psi_k,\mathbf{q}|\Delta_1(\mathbf{q})|\psi_{m,k},\mathbf{q}\rangle$, $\langle\psi_{-k},\mathbf{q}|\Delta_1(\mathbf{q})|\psi_{-m,-k},\mathbf{q}\rangle$, where $0<m<k$, are also nonzero and tend to zero as $\alpha\to0$. The other matrix components of $\Delta_1(\mathbf{q})$ are equal to zero.

In the subspace $E_{\mathbf{q}}^{(2)}$, the random potential $\mathcal{U}_2(\mathbf{q})$ is diagonal for the clusters of unit length:

$$\langle\psi_{m,m+1},\mathbf{q}|\mathcal{U}_2(\mathbf{q})|\psi_{k,k+1},\mathbf{q}\rangle=\delta_{mk}\frac{\Delta\xi}{1+\alpha}\alpha^m, \tag{3.14}$$

$$\langle \psi_{-m,-m-1},\mathbf{q}|\mathcal{U}_2(\mathbf{q})|\psi_{-k,-k-1},\mathbf{q}\rangle=\delta_{mk}\frac{\Delta\xi}{1+\alpha}\alpha^{|m|},$$

$$m\geqslant 0.$$

It is not difficult to see that in the general case the matrix components

$$\langle \psi_{n,n+m},\mathbf{q}|\mathcal{U}_2(\mathbf{q})|\psi_{k,k+l},\mathbf{q}\rangle\neq 0$$

and decrease as powers of α like Eq. (3.14).

We can analyze in the same way the matrix components of operators $\Delta_n(\mathbf{q})(n\geqslant 2)$ and $\mathcal{U}_n(\mathbf{q})(n>2)$. For example, in the absence of SRO, on the mth ''level'' of the continued fraction the random potential has the form[13]:

$$\mathcal{U}_m(\mathbf{q})=\sum_{\mathbf{i}\in\sigma_m}|\mathbf{i},\sigma_m,\mathbf{q}\rangle\Delta\xi\langle\mathbf{i},\sigma_m,\mathbf{q}|,\quad(\alpha=0).$$

In the case of $\alpha\neq 0$ the matrix components of the kind $\langle\psi_{\sigma_m(\mathbf{l})},\mathbf{q}|\mathcal{U}_m(\mathbf{q})|\psi_{\sigma'_m(\mathbf{l}')},\mathbf{q}\rangle$ decrease as powers of α with increasing distance between the site **0** and the cluster centers of gravity **l** and **l’**.

For particular calculations, one has to use an approximation scheme. Let us select a cluster σ_n with n sites, the scattering on which will be exactly taken into account. We shall call it the ''maximum'' cluster $\sigma_n^{\max}$. Define in $E_{\mathbf{q}}^{(1)}\oplus E_{\mathbf{q}}^{(2)}\oplus\cdots\oplus E_{\mathbf{q}}^{(n)}$ a subspace $L_{\mathbf{q}}=L_{\mathbf{q}}^{(1)}\oplus L_{\mathbf{q}}^{(2)}\oplus\cdots\oplus L_{\mathbf{q}}^{(n)}$, where $L_{\mathbf{q}}^{(m)}$ is a span of the vectors $|\mathbf{i},\sigma_m,\mathbf{q}\rangle$ such that $\mathbf{i}\cup\sigma_m\subseteq\sigma_n^{\max}(m\leqslant n)$. It follows from Eq. (2.22) that $\mathcal{U}(\mathbf{q})$ maps $L_{\mathbf{q}}$ onto $L_{\mathbf{q}}\oplus E_{\mathbf{q}}^{(0)}$. Let $T_m^{\mathbf{q}}$ be an orthogonal projector onto the subspace $L_{\mathbf{q}}^{(m)}$ and

$$T^{\mathbf{q}}=\sum_{m=1}^{n}T_m^{\mathbf{q}}$$

be an orthogonal projector onto $L_{\mathbf{q}}$. In terms of these, the nonconsistent approximation consists in the following substitution:

$$\mathcal{U}(\mathbf{q})\Rightarrow T^{\mathbf{q}}\mathcal{U}(\mathbf{q})T^{\mathbf{q}+}+\Delta_0(\mathbf{q})+\Delta_0^{+}(\mathbf{q}),\tag{3.15}$$

i.e., the action of $\mathcal{U}(\mathbf{q})$ is restricted to the subspace $L_{\mathbf{q}}\oplus E_{\mathbf{q}}^{(0)}$. After substitution (3.15), the operators $\Delta_m(\mathbf{q})$ and $\mathcal{U}_m(\mathbf{q})(m\leqslant n)$ have nonzero matrix components for a finite number of clusters, therefore the inversion of matrices in Eq.(3.7) can be performed analytically.

Following the paper in Ref. 13, to construct self-consistent approximations we define the operators

$$\Sigma^{\mathrm{eff}}(\epsilon,\mathbf{q})=\sum_{\mathbf{i},\mathbf{j},\sigma_n,n\geqslant 1}|\mathbf{i},\sigma_n,\mathbf{q}\rangle\Sigma_{\mathbf{i}-\mathbf{j}}(\epsilon)\langle\chi(\mathbf{j},\sigma_n,\mathbf{q})|,\tag{3.16}$$

$$\mathcal{H}^{\mathrm{eff}}(\epsilon,\mathbf{q})=\mathcal{H}_{vc}(\mathbf{q})+\Sigma^{\mathrm{eff}}(\epsilon,\mathbf{q}),$$

where $\Sigma_{\mathbf{i}-\mathbf{j}}(\epsilon)$ is the Fourier transform of $\Sigma_0(\epsilon,\mathbf{q})$. According to Eq. (3.15), we replace the random potential in Eq. (3.3) by a potential the action of which is restricted to $L_{\mathbf{q}}\oplus E_{\mathbf{q}}^{(0)}$. Further, on each ''level'' of the continued fraction we make the substitution:

$$\Sigma_m(\epsilon,\mathbf{q})\Rightarrow T_m^{\mathbf{q}}\Sigma_m(\epsilon,\mathbf{q})T_m^{\mathbf{q}+}+S_m^{\mathbf{q}}\Sigma^{\mathrm{eff}}(\epsilon,\mathbf{q})S_{\mathbf{m}}^{\mathbf{q}+},\tag{3.17}$$

where

$$S_m^{\mathbf{q}}=P_m^{\mathbf{q}}-T_m^{\mathbf{q}}$$

is a projector onto the orthogonal complement to $L_{\mathbf{q}}^{(m)}$ in the subspace $E_{\mathbf{q}}^{(m)}$. We also define a projector

$$S^{\mathbf{q}}=\sum_{m=1}^{n}S_m^{\mathbf{q}}.$$

The substitution (3.17) means that we exactly take into account the scattering on all clusters $\sigma_m\subseteq\sigma_n^{max}(m\leqslant n)$. The contribution of other configurations is taken into account by means of effective medium. As a result, at every ''level'' of the continued fraction the summation is going over a finite set of clusters. Although the matrices in the continued fraction are infinite with respect to **i, j**, their inversion may be performed analytically. In the particular case of $\alpha=0$, we come to the approximation suggested in the Ref. 9.

When the parameter α is not small, it is more efficient to restrict the random potential with consideration for the magnitude of α, instead of substitution (3.15). Namely, on the mth ''level'' of the continued fraction we define the orthogonal projectors $R_m^{\mathbf{q}}$ onto a finite subspace of vectors $\{|\psi_{\sigma_m(\mathbf{l})},\mathbf{q}\rangle\}$ such that the matrix components $\langle\psi_{\sigma_m(\mathbf{l})},\mathbf{q}|\mathcal{U}_m(\mathbf{q})|\psi_{\sigma'_m(\mathbf{l}')},\mathbf{q}\rangle$ have the order of α not greater than p ($p>0$ is an integer). In this case we should make the following substitution:

$$\mathcal{U}(\mathbf{q})\Rightarrow\sum_{m=1}^{n}R_m^{\mathbf{q}}\mathcal{U}_m(\mathbf{q})R_m^{\mathbf{q}}+\sum_{m=1}^{n}[T_m^{\mathbf{q}}\Delta_m(\mathbf{q})T_{m+1}^{\mathbf{q}}$$
$$+T_{m+1}^{\mathbf{q}}\Delta_m^{+}(\mathbf{q})T_m^{\mathbf{q}}]+\Delta_0(\mathbf{q})+\Delta_0^{+}(\mathbf{q}).$$

B. The ASF and the averaging of the resolvent in the cases of arbitrary correlations and space dimension

Let us consider how to extend the above theory to the cases of arbitrary correlations and space dimension. In the general case, the Cowley parameter α is not unique. For an unordered binary alloy we have a set of parameters α_n that characterize the pair-correlation function. For the nth coordination shell α_n is defined by an expression similar to Eq. (2.2):

$$\alpha_n=1-\frac{P_n^{AB}}{xy},$$

here P_n^{AB} is the probability of the formation of an AB pair at a distance equal to the radius of the nth coordination shell. Other correlation functions are determined by their own sets of parameters. Although these correlation functions remain unknown for real systems, a few parameters may be extracted from the experiment. To formulate the theory, it is not necessary to know all the correlation functions. For example, to obtain an approximation like the TCA, which will be discussed in details in Sec. IV A, in calculating the matrix components on the second ''level'' of the continued fraction one has to know only the correlation functions up to the fifth, inclusive. Therefore, we should either know the required correlation functions or suggest a kind of model correlation that would approximate those of the real system.

In the general case, we shall not separate the space Φ into subspaces E_n which are orthogonal to each other, because their construction according to formulas (2.22) and (2.23) is valid only in the case of Markov-type correlations. Let, as before, the basis vector $|vac\rangle$ (2.11) generate a one-dimensional subspace E_0. Define the vectors $|\sigma_m(\mathbf{l})\rangle$, $m>0$, which are orthogonal to $|vac\rangle$, as follows

$$c_{\sigma_m}|\sigma_m(\mathbf{l})\rangle=\left(\prod_{\mathbf{i}\in\sigma_m(\mathbf{l})}\hat{\xi}_{\mathbf{i}}\right)|vac\rangle+a_{\sigma_m}|vac\rangle, \tag{3.18}$$

where the coefficient a_{σ_m} is determined from the condition $\langle vac|\sigma_m(\mathbf{l})\rangle=0$, and the constant c_{σ_m} is determined from the normalization condition of the vector $|\sigma_m(\mathbf{l})\rangle$. Adding the electron functions to Eq. (3.18) as in Eq. (2.25), we get a set of vectors $|\mathbf{i}+\mathbf{l},\sigma_n(\mathbf{l})\rangle$ that form a complete basis in $\Psi\otimes\Phi$. The Hamiltonian $\mathcal{H}$ acting on the augmented space $\Psi\otimes\Phi$, in the site representation has as before the form (2.24). Using Eq. (3.2) and making the Fourier transform, we rewrite the Hamiltonian $\mathcal{H}(\mathbf{q})$ in the form (3.3). Let $E_{\mathbf{q}}^{(0)}$ be a one-dimensional subspace generated by the vector $|\mathbf{0},\sigma_0,\mathbf{q}\rangle$, and $E_{\mathbf{q}}$ be a span of vectors $\{|\mathbf{i},\sigma_m,\mathbf{q}\rangle\}$ such that $\sigma_m\subseteq\sigma_n^{max}(m>0)$, i.e., $E_{\mathbf{q}}$ is a space of clusters the scattering on which is exactly taken into account. Let $P_0^{\mathbf{q}}$ be an orthogonal projector onto the subspace $E_{\mathbf{q}}^{(0)}$, $P^{\mathbf{q}}$ be an orthogonal projector onto $E_{\mathbf{q}}$, $Q_0^{\mathbf{q}}=1-P_0^{\mathbf{q}}$, $Q^{\mathbf{q}}=1-P_0^{\mathbf{q}}-P^{\mathbf{q}}$. Introduce also the operators,

$$\Delta_0(\mathbf{q})=P_0^{\mathbf{q}}\mathcal{U}(\mathbf{q})Q_0^{\mathbf{q}},\quad \Delta_*(\mathbf{q})=P^{\mathbf{q}}\mathcal{U}(\mathbf{q})Q^{\mathbf{q}},$$

$$\mathcal{H}_*(\mathbf{q})=P^{\mathbf{q}}\mathcal{H}(\mathbf{q})P^{\mathbf{q}}.$$

The averaged Green's function $G_0(\epsilon,\mathbf{q})$ of the Hamiltonian (1.1) is defined by the expression (3.5). Since the subspaces corresponding to clusters with different numbers of sites are not orthogonal to each other, the representation of the self-energy in the form of a continued fraction is not convenient. Therefore, we write the exact expression for $\Sigma_0(\epsilon,\mathbf{q})$ as follows:

$$\Sigma_0(\epsilon,\mathbf{q})=\Delta_0(\mathbf{q})\,\frac{1}{\epsilon-\mathcal{H}_*(\mathbf{q})-\Sigma_*(\epsilon,\mathbf{q})}\,\Delta_0^+(\mathbf{q}), \tag{3.19}$$

where

$$\Sigma_*(\epsilon,\mathbf{q})=\Delta_*(\mathbf{q})\,\frac{1}{\epsilon-Q^{\mathbf{q}}\mathcal{H}(\mathbf{q})Q^{\mathbf{q}}}\,\Delta_*^+(\mathbf{q}). \tag{3.20}$$

Let $T^{\mathbf{q}}$ be an orthogonal projector onto a subspace $L_{\mathbf{q}}$ of vectors $|\mathbf{i},\sigma_m,\mathbf{q}\rangle$, such that $\mathbf{i}\cup\sigma_m\subseteq\sigma_n^{max}(m>0)$. According to Eqs. (3.18) and (3.3), the operator $\mathcal{U}(\mathbf{q})$ maps the subspace $L_{\mathbf{q}}$ onto $L_{\mathbf{q}}\oplus E_{\mathbf{q}}^{(0)}$. Since $\mathcal{U}(\mathbf{q})$ is Hermitian, it follows from Eq. (3.20) that

$$T^{\mathbf{q}}\Sigma_*(\epsilon,\mathbf{q})=\Sigma_*(\epsilon,\mathbf{q})T^{\mathbf{q}}=0. \tag{3.21}$$

Consider some possible approximations for $\Sigma_0(\epsilon,\mathbf{q})$. Let us make in the Hamiltonian (3.3) the substitution (3.15) and put $\Sigma_*(\epsilon,\mathbf{q})=0$ in Eq. (3.19). Then we get a nonconsistent approximation. For a self-consistent approximation, besides the restriction of the random potential to $L_{\mathbf{q}}\oplus E_{\mathbf{q}}^{(0)}$, one should make the substitution in Eq. (3.19) satisfying the rule (3.21):

$$\Sigma_*(\epsilon,\mathbf{q})\Rightarrow S^{\mathbf{q}}\Sigma^{\mathrm{eff}}(\epsilon,\mathbf{q})S^{\mathbf{q}}, \tag{3.22}$$

where

$$S^{\mathbf{q}}=P^{\mathbf{q}}-T^{\mathbf{q}},$$

and $\Sigma^{\mathrm{eff}}(\epsilon,\mathbf{q})$ is defined by Eq. (3.16). For the case of Markov correlations, the scheme proposed is the same as the approximation discussed above, and it transforms into the approximation suggested in Ref. 9 if there is no SRO. Since the subspace $L_{\mathbf{q}}$ contains a finite set of clusters, the inversion of the matrices in Eq. (3.19) may be performed analytically. The details of such calculations are presented in Appendix A, the case of the one-dimensional chain is discussed in Sec. IV A and in Appendices B and C.

The ASF was generalized to the case of off-diagonal disorder in Ref. 9. A similar generalization is also possible in case of SRO within the framework of the above proposed scheme. For an example, in the case of a one-dimensional chain with Markov-type correlations we will have the five-diagonal Hamiltonian determined on the augmented space. The expression (3.7) for the self-energy in the form of continued fraction is valid only for the case of diagonal disorder. However, the general approximation scheme (3.15), (3.19), and (3.22) does not imply such restriction.

C. Limiting cases of the ordered alloy

The representation of the resolvent proposed above has the advantage of providing correct limiting transition to the Green's function of the ordered alloy if the SRO parameter tends to its critical values. Consider, for example, a two-dimensional square lattice and define a two-site correlation function as follows

$$g_{\mathbf{r}_1\mathbf{r}_2}=\langle\hat{\xi}_{\mathbf{r}_1}\hat{\xi}_{\mathbf{r}_2}\rangle=\Delta^2\alpha^{\|\mathbf{r}_1-\mathbf{r}_2\|}, \tag{3.23}$$

where $\|\mathbf{r}_1-\mathbf{r}_2\|=|x_1-x_2|+|y_1-y_2|$, $|\alpha|<1$ is the the Cowley parameter. Then, for $\alpha=1$, the alloy separates into two subsystems containing the atoms of A or B type only. For $x=0.5$, $\alpha=-1$, the atoms A alternate with the atoms B in staggered order. In these cases the exact Green's functions are known and we can compare them with our expressions.

In the case of $\alpha=\pm1$, for the Fourier transform of the matrix $g_{\mathbf{r}_1\mathbf{r}_2}$ (3.23) we get the formulas:

$$g(\mathbf{q})=(2\pi)^2\sum_{\mathbf{g}}\ \delta(\mathbf{q}+\mathbf{g}),\quad \alpha=1, \tag{3.24}$$

$$g(\mathbf{q})=(2\pi)^2\sum_{\mathbf{g}}\ \delta(\mathbf{q}+\mathbf{Q}+\mathbf{g}),\quad \alpha=-1,$$

here the summation goes over all vectors $\mathbf{g}$ of the reciprocal lattice, $\mathbf{Q}=(\pi,\pi)$ (the lattice constant $a=1$). We denote by $|(nk),\mathbf{q}\rangle=|\mathbf{i},\mathbf{q}\rangle$ a basis in the Fourier representation of the subspace corresponding to single-site excitations. We can orthogonalize this basis using Eq. (3.23);

$$|\phi_{(00)},\mathbf{q}\rangle=|\mathbf{0},\mathbf{q}\rangle,$$

$$|\phi_{(nk)},\mathbf{q}\rangle=(1-\alpha^2)^{-1}(|(nk),\mathbf{q}\rangle-\alpha\exp\{iq_2\}|(n,k-1),\mathbf{q}\rangle-\alpha\exp\{iq_1\}|(n-1,k),\mathbf{q}\rangle+\alpha^2\exp\{iq_1+iq_2\}|(n-1,k-1),\mathbf{q}\rangle),$$

$$n>0,k>0,\quad(q_1,q_2)=\mathbf{q}. \tag{3.25}$$

For other n and k, we have the similar formulas. For $n=0$ or $k=0$, the orthogonal basis is defined according to Eq. (3.8).

Associate the transfer matrix $V_{\mathbf{i-j}}$ with an operator $V_{\mathbf{q}}$ acting on the augmented space as defined by Eq. (3.16). Since the vectors corresponding to multiple excitations can be orthogonalized to the vectors $|\phi_{(nk)},\mathbf{q}\rangle$, in the case of $\alpha=\pm 1$ it is sufficient to examine only the matrix components of the kind $\langle\mathbf{0},\mathbf{q}|V_{\mathbf{q}}|\phi_{(nk)},\mathbf{q}\rangle$. Using Eqs. (A5) (3.24) and (3.25), we obtain

$$\tilde{V}_{00}(\mathbf{q})=\langle\mathbf{0},\mathbf{q}|V_{\mathbf{q}}|\mathbf{0},\mathbf{q}\rangle=V(\mathbf{q}),\quad\alpha=1,$$

$$\tilde{V}_{00}(\mathbf{q})=\langle\mathbf{0},\mathbf{q}|V_{\mathbf{q}}|\mathbf{0},\mathbf{q}\rangle=V(\mathbf{q+Q}),\quad\alpha=-1, \tag{3.26}$$

$$\langle\mathbf{0},\mathbf{q}|V_{\mathbf{q}}|\phi_{(nk)},\mathbf{q}\rangle\rightarrow\frac{1-\alpha}{1+\alpha}V(\mathbf{q})\exp\{iq_1n+iq_2k\}\rightarrow 0,\quad(\alpha\rightarrow 1),$$

$$\langle\mathbf{0},\mathbf{q}|V_{\mathbf{q}}|\phi_{(nk)},\mathbf{q}\rangle\rightarrow\frac{1+\alpha}{1-\alpha}V(\mathbf{q+Q})\exp\{i(q_1+\pi)n+i(q_2+\pi)k\}\rightarrow 0,\quad(\alpha\rightarrow -1).$$

Therefore the matrix $\mathcal{H}_{*}(\mathbf{q})$ is factorized in the limiting cases, and for the averaged Green's function we have the expression

$$G_0(\epsilon,\mathbf{q})=\frac{1}{\epsilon-\overline{\epsilon}-V(\mathbf{q})-\Sigma_0(\epsilon,\mathbf{q})}, \tag{3.27}$$

$$\Sigma_0(\epsilon,\mathbf{q})=\frac{\Delta^2}{\epsilon-\overline{\epsilon}-\tilde{V}_{00}(\mathbf{q})-\Delta\xi},$$

where the constants Δ, $\Delta\xi$, and $\overline{\epsilon}$ are defined by Eqs. (2.6) and (2.4).

In the case of $\alpha=1$, the expression for the averaged resolvent has the form

$$G_0(\epsilon,\mathbf{q})=\frac{x}{\epsilon-\epsilon_A-V(\mathbf{q})}+\frac{y}{\epsilon-\epsilon_B-V(\mathbf{q})},$$

and coincides with the exact Green's function of the alloy separated into two subsystems with weights x and y.

In the case of $\alpha=-1$, using Eq. (3.26) for the diagonal matrix component of the averaged resolvent we obtain the expression

$$\overline{G}_{00}(\epsilon)=\frac{1}{(2\pi)^2}\int d\mathbf{q}\frac{\epsilon-\overline{\epsilon}-V(\mathbf{q+Q})}{(\epsilon-\epsilon_A)(\epsilon-\epsilon_B)-(\epsilon-\overline{\epsilon})[V(\mathbf{q})+V(\mathbf{q+Q})]+V(\mathbf{q})V(\mathbf{q+Q})},$$

which coincides, for $x=0.5$, with the exact expression for the Green's function of the ideal crystal with a staggered arrangement of the A and B atoms.

IV. ANALYSIS OF THE SELF-CONSISTENT EQUATIONS FOR THE SELF-ENERGY

A. TCA-like approximation

As an example of the suggested approximation scheme (3.15), (3.17) for the self-energy, consider a one-dimensional Markov chain, put $n=2$, and choose a pair of nearest neighbors as the maximum cluster $\sigma_2^{\max}=\sigma_2$. On the second ''level'' of the continued fraction the vectors $|i,\sigma_2,q\rangle$ are orthogonal to each other. As noted above in Sec. III B, on the first ''level'' of the continued fraction the basis $\{|i,\sigma_1,q\rangle\}$ is not orthogonal, therefore it is convenient to perform all subsequent calculations using the orthonormalized basis $\{|\psi_m,q\rangle\}$ defined by expressions (3.8). Denote by $\tilde{A}_{ij}(q)=\langle\psi_i,q|A_q|\psi_j,q\rangle$ the matrix components of a translation-invariant operator of the kind (3.16). It is shown in Appendix B that using the formulas (3.8) of transformation of the basis, the matrix components $\tilde{A}_{ij}(q)$ can be expressed via the convolution:

$$\langle i,q|A_q|j,q\rangle=\sum_k\langle i,q|k,q\rangle A_{k-j}=\frac{1}{2\pi}\int_{-\pi}^{\pi}dp\,g(p-q)A(p)\exp\{ip(j-i)\}, \tag{4.1}$$

where integration is over the first Brillouin zone (the lattice constant $a=1$), $A(p)$ is the Fourier transform of the matrix A_{i-j}, and $g(q)$ is determined by Eq. (2.15). Carrying out the substitution of Eqs. (3.15) and (3.17) into Eq. (3.7) and in view of Eq. (3.10), we get

$$\Sigma_0(\epsilon,q)=\Delta^2\left\langle\psi_0,q\left|G_1^{\text{eff}}(\epsilon,q)\frac{1}{1-W_1(\epsilon,q)G_1^{\text{eff}}(\epsilon,q)}\right|\psi_0,q\right\rangle, \tag{4.2}$$

$$W_1(\epsilon,q)=\sum_{ij}|\psi_i,q\rangle W_{ij}^{\sigma_1}(\epsilon,q)\langle\psi_j,q|,$$

$$G_1^{\mathrm{eff}}(\epsilon,q)=[\epsilon-\mathcal{H}_1^{\mathrm{eff}}(\epsilon,q)]^{-1}.$$

The nonzero matrix components $W_{ij}^{\sigma_1}(\epsilon,q)$ have the form:

$$W_{ij}^{\sigma_1}(\epsilon,q)=\delta_{ij}\omega_i+\Sigma_{ij}^{\sigma_1}(\epsilon,q)-\tilde{\Sigma}_{ij}(\epsilon,q),\quad i,j\in\sigma,$$
$$W_{ij}^{\sigma_1}(\epsilon,q)=-\tilde{\Sigma}_{ij}(\epsilon,q),\quad i\in\sigma,\quad j\notin\sigma. \tag{4.3}$$

Here $\sigma=\{-1,0,1\}$, $\omega_0=\Delta\xi$, $\omega_1=\omega_{-1}=\alpha\Delta\xi/(1+\alpha)$; in the case of $i\notin\sigma$, $j\in\sigma$, $W_{ij}^{\sigma_1}(\epsilon,q)$ is defined in the same way as in Eq. (4.3) with rearrangement of indices i and j. The matrix components $\Sigma_{ij}^{\sigma_1}(\epsilon,q)$ in the first expression of Eq. (4.3) are nonzero for $i,j\neq 0$. Using Eq. (3.13), they can be determined by an expression similar to Eq. (4.2):

$$\Sigma_{ij}^{\sigma_1}(\epsilon,q)=b^2\exp\{iq(j-i)/2\}\left\langle i/2,\sigma_2,q\left|G_2^{\mathrm{eff}}(\epsilon,q)\frac{1}{1-W_2(\epsilon,q)G_2^{\mathrm{eff}}(\epsilon,q)}\right|j/2,\sigma_2,q\right\rangle,$$
$$b^2=\frac{b_1^2}{\Delta^2(1-\alpha^2)}, \tag{4.4}$$
$$W_2(\epsilon,q)=\sum_{ij}|i,\sigma_2,q\rangle W_{ij}^{\sigma_2}(\epsilon,q)\langle j,\sigma_2,q|,\qquad G_2^{\mathrm{eff}}(\epsilon,q)=[\epsilon-\mathcal{H}_2^{\mathrm{eff}}(\epsilon,q)]^{-1}.$$

Here $\sigma_2=\{-1/2,1/2\}$, $W_{ij}^{\sigma_2}(\epsilon,q)=0$, if $i,j\notin\sigma_2$, otherwise

$$W_{ij}^{\sigma_2}(\epsilon,q)=v_0\delta_{ij}-\Sigma_{i-j}(\epsilon),\quad v_0=\frac{\Delta\xi}{1+\alpha}.$$

With appropriate rearrangement of rows and columns of the matrices in Eqs. (4.2) and (4.4), their inversion can be performed analytically (see Appendix C). As a result, we obtain a self-consistent nonlinear integral equation that should be solved numerically. In the absence of SRO ($\alpha=0$), the approximation suggested coincides with the TCA.[8,9]

The approximation considered correctly takes into account the scattering on all pairs of nearest neighbors, the scattering on the other clusters is taken into account by means of the effective medium. As shown in Ref. 13, in the case of $\alpha=0$ it is a successive approximation in terms of (a/R_0) and $\exp\{-a/l_0\}$, where a is the lattice constant, R_0 is the effective damping length of the transfer integral $V_{\mathbf{i}-\mathbf{j}}$, and l_0 is of the order of the mean free path of an electron. From the analysis in Sec. III A, it follows that in the presence of SRO α is an additional small parameter.

We have carried out a numerical analysis of the self-consistent Eqs. (4.2), (4.3) and (4.4) for the following values of the model parameters of the Hamiltonian (1.1): $\epsilon_A=-\epsilon_B=2.5$; $V_{\mathbf{i}-\mathbf{j}}=1.0$, if **i, j** are the nearest neighbors, and $V_{\mathbf{i}-\mathbf{j}}=0$ otherwise. The concentration of impurity atoms (of A type) was $x=0.1$ and $x=0.5$. Such parameters determine the most interesting range of strong scattering and high concentrations. There is a gap between the impurity and host bands, the former being in the energy range from -4.5 to -0.5, the latter in the range from 0.5 to 4.5. At $x=0.1$ the changes occurring in the host band are small as compared to the ideal crystal ($x=0$) and at $x=0.5$ the bands are symmetric with respect to $\epsilon=0$. So we can examine the energy range (0.5;4.5) corresponding to the impurity band. For comparison of the theoretical results with the ''exact'' ones, numerical analysis of the distribution of eigenvalues of the random Hamiltonian (1.1) has been carried out. The histograms in Figs. 2 and 3 correspond to a fixed lattice containing 10^6 atoms. In the one-dimensional case, such an analysis is simple and reduces to calculating the number of zeroes of eigenfunctions of the Hamiltonian.[21]

The central peak in Fig. 1 close to $\epsilon=\epsilon_A$ corresponds mainly to the states localized on the A-B pairs, and two satellite peaks correspond primarily to the bonding and antibonding states localized on the A-A pairs. Their contribution to the total density of states is proportional to $P^{AA}=x(x+\alpha y)$, where P^{AA} is the probability of the formation of an A-A pair at the nearest-neighbor sites. The weight of the central subband is $\sim P^{AB}=xy(1-\alpha)$. The curves in Fig. 1 demonstrate the correct behavior under changes of the Cowley parameter. The case of $\alpha>0$ (thin solid curve) corresponds to the situation of effective attraction between the atoms of the same type. The weight of the satellite subbands increases as compared to the case of the absence of SRO because of the increase in the number of A-A pairs. The weight of the central subband, on the contrary, decreases. For $\alpha<0$ (dashed line), we have the opposite situation of effective repulsion between the atoms of the same type.

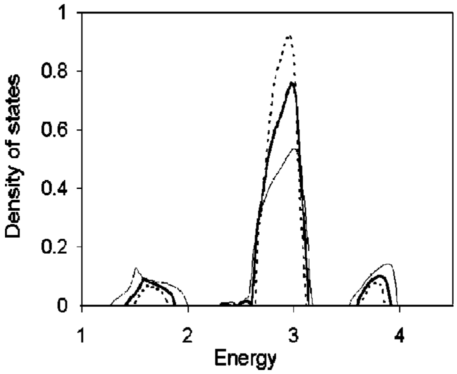
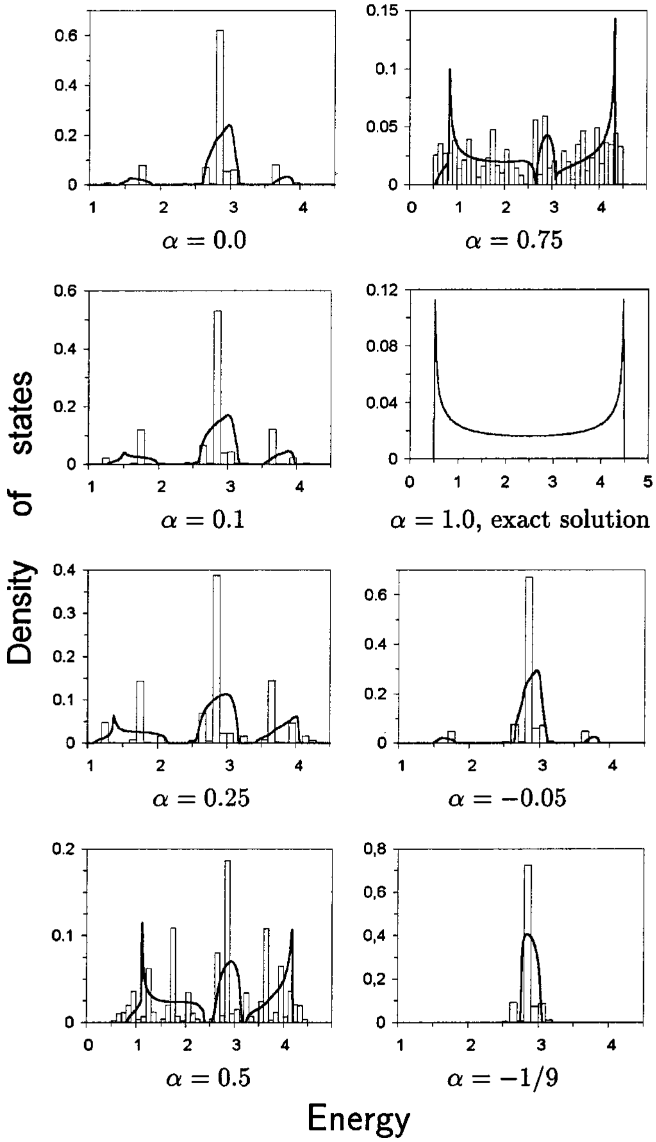


FIG. 1. Density of states in the impurity band of a disordered Markov chain for $x=0.1$, $\epsilon_A=-\epsilon_B=2.5$, $V=1.0$, $\alpha=0$ (thick line), $\alpha=0.1$ (thin line), $\alpha=-0.05$ (dashed line).



$\alpha = 0.0$ $\alpha = 0.75$

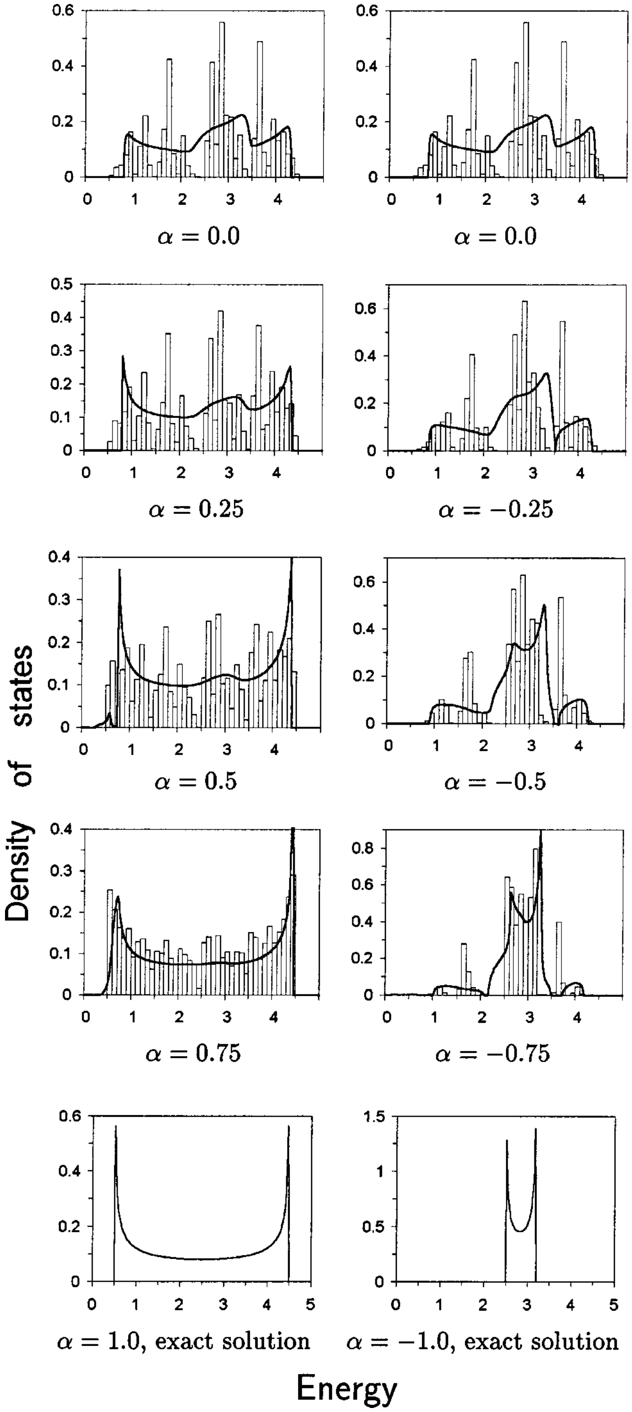
$\alpha = 0.1$ $\alpha = 1.0$, exact solution

$\alpha = 0.25$ $\alpha = -0.05$

$\alpha = 0.5$ $\alpha = -1/9$

FIG. 2. Density of states in the impurity band of a disordered Markov chain for $x=0.1$, $\epsilon_A=-\epsilon_B=2.5$, $V=1.0$.

In Fig. 2 the density of states at $x=0.1$ and different values of the SRO parameter calculated using the self-consistent equations are compared with the ''exact'' results for a chain containing 10^6 atoms. The theoretical curves reproduce fairly well the main peculiarities of the histograms, the density of states being positive over the whole range of the SRO parameter variation. For $\alpha>0$, the density of states evolves towards the exact solution $(\alpha=1)$ corresponding to total segregation of the alloy. The case of $\alpha=-1/9$ corresponds to the critical point of maximal repelling between the atoms of the same kind. In the approximation considered, the relative weight of the satellite subbands is defined by the matrix components of the projectors $\Delta_1(\mathbf{q})$, $\Delta_1^+(\mathbf{q})$ (3.13), which are equal to zero for $\alpha=-x/y$. The contribution of other configurations, except for the A-A pairs, is of order x^3, and for $x=0.1$, it is not observed on the histogram corresponding to the ''exact'' solution.



$\alpha = 0.0$ $\alpha = 0.0$

$\alpha = 0.25$ $\alpha = -0.25$

$\alpha = 0.5$ $\alpha = -0.5$

$\alpha = 0.75$ $\alpha = -0.75$

$\alpha = 1.0$, exact solution $\alpha = -1.0$, exact solution

FIG. 3. Density of states in the impurity band of a disordered Markov chain for $x=0.5$, $\epsilon_A=-\epsilon_B=2.5$, $V=1.0$.

Figure 3 presents the density of states at $x=0.5$ for positive $(0<\alpha<1)$ and negative $(-1<\alpha<0)$ SRO parameters, when two limiting cases of the chain ordering are possible. Since at $x=0.5$ the contribution of the cluster configurations, the scattering on which is taken into account by means of the effective medium, is rather large $(\sim x^3)$, our approximation does not reproduce completely the fine structure of the subband in the case of $\alpha=0$. In order to obtain a better agreement with the histogram, it is necessary to take into account the clusters larger than a pair of nearest neighbors. However, the calculated density of states agrees reasonably well with the histograms when α tends to its critical values.

B. CPA-like approximation

In this section we shall consider the simplest self-consistent single-site approximation which extends the CPA (Ref. 1) to the case of correlated disorder. In the general self-consistent scheme proposed in Sec. III B, this approximation corresponds to the choice of a single site of the lattice as the maximum cluster ($\sigma^{\max}=\sigma_1$). Using Eqs. (A2) and (A3) and the relations similar to Eq. (C4), we get the self-consistent integral equation for the self-energy:

$$\Sigma_0(\epsilon,\mathbf{q})=\frac{\Delta^2\tilde{G}^{\mathrm{eff}}_{00}(\epsilon,\mathbf{q})}{[1+\tilde{I}_{00}(\epsilon,\mathbf{q})]^2-[(\Delta\xi)+\tilde{\Sigma}_{00}(\epsilon,\mathbf{q})+\tilde{J}_{00}(\epsilon,\mathbf{q})]\tilde{G}^{\mathrm{eff}}_{00}(\epsilon,\mathbf{q})},\tag{4.5}$$

where

$$\begin{aligned}\tilde{\Sigma}_{00}(\epsilon,\mathbf{q})&=\frac{1}{(2\pi)^d}\int d\mathbf{p}\,g(\mathbf{p}-\mathbf{q})\Sigma_0(\epsilon,\mathbf{p}),\\ \tilde{G}^{\mathrm{eff}}_{00}(\epsilon,\mathbf{q})&=\frac{1}{(2\pi)^d}\int d\mathbf{p}\,g(\mathbf{p}-\mathbf{q})G_0(\epsilon,\mathbf{p}),\\ \tilde{I}_{00}(\epsilon,\mathbf{q})&=\frac{1}{(2\pi)^d}\int d\mathbf{p}\,g(\mathbf{p}-\mathbf{q})\Sigma_0(\epsilon,\mathbf{p})G_0(\epsilon,\mathbf{p}),\\ \tilde{J}_{00}(\epsilon,\mathbf{q})&=\frac{1}{(2\pi)^d}\int d\mathbf{p}\,g(\mathbf{p}-\mathbf{q})\Sigma_0^2(\epsilon,\mathbf{p})G_0(\epsilon,\mathbf{p}).\end{aligned}\tag{4.6}$$

Here the integration is over the first Brillouin zone of the lattice, d is the space dimension, $g(\mathbf{q})$ is the Fourier transform of the two-site correlation function:

$$g(\mathbf{q})=\frac{1}{N}\sum_{\mathbf{ij}}g_{\mathbf{ij}}\exp\{i\mathbf{q}(\mathbf{i}-\mathbf{j})\},\tag{4.7}$$

$$g_{\mathbf{ij}}=\Delta^{-2}\langle\hat{\xi}_{\mathbf{i}}\hat{\xi}_{\mathbf{j}}\rangle.$$

In the absence of spatial correlations in the alloy, $g_{\mathbf{ij}}=\delta_{\mathbf{ij}}$, and Eqs. (4.5) and (4.6) lead to the CPA in the form of Onodera and Toyozawa:[22]

$$\Sigma(\epsilon)=\frac{\Delta^2G^{\mathrm{eff}}_{00}(\epsilon)}{1-[\Delta\xi-\Sigma(\epsilon)]G^{\mathrm{eff}}_{00}(\epsilon)},$$

where $G^{\mathrm{eff}}_{00}(\epsilon)$ is the diagonal matrix component of the resolvent of the effective Hamiltonian in the site representation.

It should be noted that in the presence of SRO, in contrast to the CPA, the approximation (4.5) leads to spatial dispersion of the self-energy. In the limit of ''strong'' correlations, $g(\mathbf{p})$ has the form (3.24) and for the self-energy we have the expression (3.27) corresponding to the Green's function of the ordered alloy.

Let us consider the omitted terms in Eq. (4.5) connected with SRO. For this purpose, in the subspace of single-site excitations that form the subspace $L_{\mathbf{q}}$ in our case (see Sec. III B), it is convenient to introduce an orthonormalized basis $\{|\phi_{\mathbf{i}},\sigma_1,\mathbf{q}\rangle\}$. Such a basis can be built up by orthogonalizing the basis $\{|\mathbf{i},\sigma_1,\mathbf{q}\rangle\}$ similar to the formula (3.25), where $|\phi_{\mathbf{0}},\sigma_1,\mathbf{q}\rangle=|\mathbf{0},\sigma_1,\mathbf{q}\rangle$. Let us assume that the vectors corresponding to multiple excitations are orthogonalized to the subspace $L_{\mathbf{q}}$. In virtue of the restriction (3.15), in the subspace of single-site excitations there remains the only matrix component of the random potential $\langle\mathbf{0},\sigma_1,\mathbf{q}|\mathcal{U}(\mathbf{q})|\mathbf{0},\sigma_1,\mathbf{q}\rangle=\Delta\xi$. As follows from Eq. (4.6), in the approximation considered, only the two-site correlation function should be known. For the analysis of the omitted terms, one has to consider the matrix components of a random potential of the kind $\langle\phi_{\mathbf{i}},\sigma_1,\mathbf{q}|\mathcal{U}(\mathbf{q})|\phi_{\mathbf{j}},\sigma_1,\mathbf{q}\rangle$, which can be calculated using a three-site correlation function. As an example, consider a simple cubic lattice in d-dimensional space and define the correlation functions as follows:

$$\begin{gathered}\langle\hat{\xi}_{\mathbf{i}}\hat{\xi}_{\mathbf{j}}\rangle=\Delta^2g_{\mathbf{ij}}=\Delta^2\alpha^{\|\mathbf{i}-\mathbf{j}\|},\quad|\alpha|<1,\\ \|\mathbf{i}-\mathbf{j}\|=\sum_{n=1}^{d}|i_n-j_n|,\\ \langle\hat{\xi}_{\mathbf{i}}\hat{\xi}_{\mathbf{j}}\hat{\xi}_{\mathbf{k}}\rangle=\Delta^2(\Delta\xi)\alpha^p,\quad p=\sum_{n=1}^{d}m_n,\\ m_n=\max\{|i_n-j_n|,|i_n-k_n|,|j_n-k_n|\}.\end{gathered}\tag{4.8}$$

Then the orthonormalized basis $\{|\phi_{\mathbf{i}},\sigma_1,\mathbf{q}\rangle\}$ can be constructed as in (3.25) and the restriction of the random potential to the subspace $L_{\mathbf{q}}$ has the form:

$$\langle\phi_{\mathbf{i}},\sigma_1,\mathbf{q}|\mathcal{U}(\mathbf{q})|\phi_{\mathbf{j}},\sigma_1,\mathbf{q}\rangle=\delta_{\mathbf{ij}}(\Delta\xi)\frac{\alpha^{\|\mathbf{i}\|}}{(1+\alpha)^d}.$$

As follows from the matrix components of the random potential, the omitted terms in Eqs. (4.5)–(4.7) are small in parameter α. Moreover, for a translation-invariant operator $V_{\mathbf{q}}$ of the kind in Eq. (3.16), one can obtain the relations similar to Eq. (3.26):

$$\begin{aligned}\langle\mathbf{0},\sigma_1,\mathbf{q}|V_{\mathbf{q}}|\phi_{\mathbf{i}},\sigma_1,\mathbf{q}\rangle\rightarrow&\left(\frac{1-\alpha}{1+\alpha}\right)^{d/2}V(\mathbf{q})\\ &\times\exp\left\{i\sum_{n=1}^{d}q_ni_n\right\}\rightarrow0\quad(\alpha\rightarrow1),\end{aligned}$$

$$\langle \mathbf{0},\sigma_1,\mathbf{q}|V_{\mathbf{q}}|\phi_{\mathbf{i}},\sigma_1,\mathbf{q}\rangle \to \left(\frac{1+\alpha}{1-\alpha}\right)^{d/2} V(\mathbf{q+Q}) \times \exp\left\{ i\sum_{n=1}^{d}(q_n+\pi)i_n\right\}\to 0$$

$$(\alpha\to -1),$$

$$\mathbf{Q}=(\pi,\dots,\pi).$$

Using the inversion formulas for block matrices and calculating the expression (3.19), we come to the result that in the limit of ‘‘strong’’ correlations, when $\alpha\to 1$ or $\alpha\to -1$, the correction to the exact solution (3.27) is of the order of $(1-|\alpha|)^d$.

The numerical analysis of the self-consistent Eq. (4.5) becomes much easier if we choose the two-site correlation function in the form (4.8) and consider the limit of the infinite space dimension ($d=\infty$). According to Eq. (2.15), for the Fourier transform of $g_{\mathbf{ij}}$ we have

$$g(\mathbf{q})=\prod_{n=1}^{d} g(q_n)=\prod_{n=1}^{d}\left(\frac{1-\alpha^2}{1+\alpha^2-2\alpha\cos q_n}\right). \qquad (4.9)$$

We assume the components of the transfer matrix $V_{\mathbf{i-j}}$ in the Hamiltonian (1.1) to be different from zero and equal to V only for the pairs of nearest neighbors. It is known that in order to obtain the nontrivial result in the case of $d=\infty$, one should overdetermine the parameter V as $V=V^*/\sqrt{d}$, where V^* is a finite magnitude. Then the dispersion law of the Hamiltonian of the virtual crystal has the form:

$$\epsilon_{\mathbf{k}}=\bar{\epsilon}+\frac{b}{\sqrt{d}}\sum_{n=1}^{d}\cos k_n, \quad b=2V^*.$$

To solve the integral equation (4.5), let us assume that the function $\Sigma_0(\epsilon,\mathbf{q})$ has the form

$$\Sigma_0(\epsilon,\mathbf{q})=\Sigma(\epsilon,\mu), \quad \mu=\frac{1}{\sqrt{d}}\sum_{n=1}^{d}\cos q_n. \qquad (4.10)$$

Here $\Sigma(\epsilon,\mu)$ is an unknown function of μ. If this assumption is true, it is necessary that the functional dependence of the form (4.10) should also be valid for all functions in Eq. (4.6). We shall prove it by obtaining $\tilde{G}_{00}^{\mathrm{eff}}(\epsilon,\mathbf{q})$. Using Eq. (4.9), we get

$$\tilde{G}_{00}^{\mathrm{eff}}(\epsilon,\mathbf{q})=\frac{1}{(2\pi)^d}\int \frac{1}{\epsilon-\bar{\epsilon}-\frac{b}{\sqrt{d}}\sum_{n=1}^{d}\cos p_n-\Sigma_0(\epsilon,\mathbf{p})} \times\prod_{n=1}^{d} g(q_n-p_n)dp_n$$

$$=\int_{-\infty}^{+\infty}\frac{\rho(z,\mathbf{q})}{\epsilon-\bar{\epsilon}-bz-\Sigma(\epsilon,z)}dz, \qquad (4.11)$$

where

$$\rho(z,\mathbf{q})=\frac{1}{(2\pi)^d}\int \delta\left(z-\frac{1}{\sqrt{d}}\sum_{n=1}^{d}\cos p_n\right) \times\prod_{n=1}^{d} g(q_n-p_n)\,dp_n.$$

The probability density $\rho(z,\mathbf{q})$ can be found easily. Since

$$\frac{1}{2\pi}\int_{-\pi}^{\pi} g(q_n-p_n)\,dp_n=1,$$

we can consider the integration variables p_n as independent random variables distributed on the segment $[-\pi,\pi]$ with probability density $(1/2\pi)g(q_n-p_n)$. Then $\rho(z,\mathbf{q})$ is the probability density of the random variable $z=(1/\sqrt{d})\Sigma_{n=1}^{d}\cos p_n$. Therefore, by virtue of the central limit theorem, using Eq. (4.9) we get

$$\rho(z,\mathbf{q})=\frac{1}{\sqrt{\pi(1-\alpha^2)}}\exp\left[-\frac{(z-\alpha\mu)^2}{1-\alpha^2}\right],$$

$$\mu=\frac{1}{\sqrt{d}}\sum_{n=1}^{d}\cos q_n.$$

The functional dependence of such a form allows us to write $\tilde{G}_{00}^{\mathrm{eff}}(\epsilon,\mathbf{q})=\tilde{G}^{\mathrm{eff}}(\epsilon,\mu)$, where

$$\tilde{G}^{\mathrm{eff}}(\epsilon,\mu)=\frac{1}{\sqrt{\pi(1-\alpha^2)}}\int_{-\infty}^{+\infty}\frac{\exp\left[-\frac{(z-\alpha\mu)^2}{1-\alpha^2}\right]}{\epsilon-\bar{\epsilon}-bz-\Sigma(\epsilon,z)}dz. \qquad (4.12)$$

Thus, we have proved that the functional dependence $\tilde{G}_{00}^{\mathrm{eff}}(\epsilon,\mathbf{q})$ on $\mathbf{q}$ has the form (4.10). For the diagonal matrix component of the averaged resolvent we have the expression:

$$\bar{G}_{00}(\epsilon)=\frac{1}{\sqrt{\pi}}\int_{-\infty}^{+\infty}\frac{e^{-\mu^2}\,d\mu}{\epsilon-\bar{\epsilon}-b\mu-\Sigma(\epsilon,\mu)}.$$

Here $\Sigma(\epsilon,\mu)$ satisfies the integral equation:

$$\Sigma(\epsilon,\mu) =\frac{\Delta^2\tilde{G}^{\mathrm{eff}}(\epsilon,\mu)}{[1+\tilde{I}(\epsilon,\mu)]^2-[(\Delta\xi)+\tilde{\bar{\Sigma}}(\epsilon,\mu)+\tilde{J}(\epsilon,\mu)]\tilde{G}^{\mathrm{eff}}(\epsilon,\mu)}, \qquad (4.13)$$

where $\tilde{\bar{\Sigma}}(\epsilon,\mu)$, $\tilde{I}(\epsilon,\mu)$, $\tilde{J}(\epsilon,\mu)$ are defined by integrals similar to Eq. (4.12) according to Eq. (4.6).

The equation (4.13) for the self-energy can be easily solved numerically. Calculations are carried out for the following values of the Hamiltonian (1.1): $\epsilon_A=-\epsilon_B=1.0$, $b=2V^*=1.0$. Figure 4 shows the density of states for the impurity concentration $x=0.2$ and $\alpha>0$. Figure 5 presents the density of states for $x=0.5$ and $\alpha<0$. The dashed line in the figures corresponds to the CPA ($\alpha=0$). The thin solid

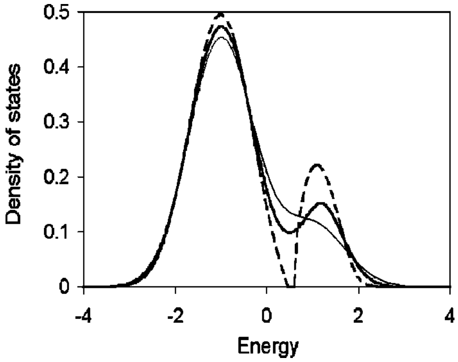


FIG. 4. Density of states of the unordered alloy at $d=\infty$ for $x=0.2$, $\epsilon_A=-\epsilon_B=1.0$, $b=2V^*=1.0$, $\alpha=0$ (dashed line, CPA), $\alpha=0.5$ (thick line), $\alpha=1.0$ (thin line).

line ($\alpha=0.5$ and $\alpha=-0.5$) demonstrates the evolution of the density of states from the case of a completely unordered alloy to the ordered system.

V. CONCLUSION

In this paper we have considered the problem of calculating the electronic spectrum of a binary unordered alloy with correlated diagonal disorder. For configuration averaging of the one-particle Green's function we have proposed a method which, in the framework of the ASF, allowed us to take into account the correlations of random variables. The suggested method, as compared to other approaches, has the advantage of using the translation invariance when defining the basis in the augmented space. We have demonstrated the method of constructing such a basis in the case of the one-dimensional chain, on which the spatial correlations of random variables are determined by a first-order Markov process. In contrast to the case of uncorrelated disorder, this basis is not orthogonal.

Using the ASF, we have obtained the formally exact expression for the translation-invariant self-energy operator of the averaged Green's function. In the case of the one-dimensional Markov chain, the self-energy is presented as a continued operator fraction. The general schemes of non- and self-consistent approximations for the self-energy operator have been proposed. They can be applied in the space of any dimension if the necessary correlation functions are known. The considered scheme leads to consistent allowance for multiple scattering in the limits of a chosen maximum cluster. In the simplest case we have obtained an extended variant of the CPA that takes into account the SRO effects.

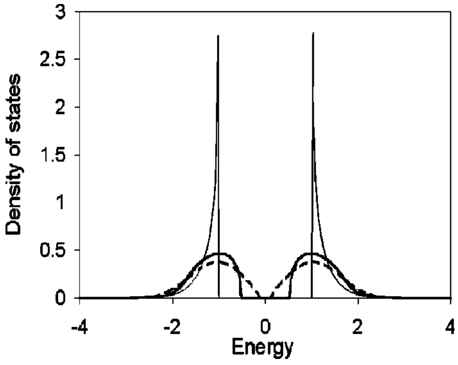


FIG. 5. Density of states of the unordered alloy at $d=\infty$ for $x=0.5$, $\epsilon_A=-\epsilon_B=1.0$, $b=2V^*=1.0$, $\alpha=0$ (dashed line, CPA), $\alpha=-0.5$ (thick line), $\alpha=-1.0$ (thin line).

An analysis of the approximations suggested shows that, in addition to the small parameters of the theory developed in Ref. 13, in our approach the expansion is also performed in small parameters α and $(1-|\alpha|)^d$ (d is the space dimension, α is the Cowley parameter). The approximations ensure a correct limiting transition to the Green's function of the ordered alloy when the Cowley parameter tends to its critical values. For $\alpha=0$ we have obtained the expressions of the known approximations.[9,13] Analysis of the analytical properties of the approximations shows that they are of Herglotz-type and do not result in a negative density of states for all values of the SRO parameter in the whole energy range.

We have also carried out numerical analysis of the self-consistent equations for a chain and for the case of the infinite-dimensional space. The results obtained are in reasonable agreement with the histograms and their qualitative behavior adequately reflects the dependence of the spectrum on the SRO parameter.

As mentioned at the end of Sec. III A, the ASF can be generalized to the case of off-diagonal disorder. Additionally, within the ASF one can obtain the exact expression for the one-particle density of states for a cluster of fixed size and configuration.[7] In our approach, the partial density of states depending on the arrangement of impurity atoms in the nearest neighborhood calculated in the general approximation scheme, will automatically incorporate the SRO.

The tight-binding model of an unordered alloy with diagonal disorder represents the simplest example of a disordered system. However, the solution of this problem may be used as a necessary foundation for realistic calculations of the electronic structure of unordered alloys with SRO. Particular attention must be paid to the CPA+SRO expression in Sec. IV B (4.5). It is easily seen that this equation contains familiar functions that do not involve the ASF terms. Besides, the method proposed can be used for comparative assessment of different techniques that do not possess a thorough mathematical foundation.

For realistic calculations of the electronic structure of disordered alloys Kudrnovský and Drchal[23,24] have combined the CPA with the first-principles tight-binding muffin-tin orbitals (TB–LMTO) method.[25,26] To represent the Green's function of the system in this approach one should find the auxiliary Green's function of some tight-binding Hamiltonian. The disorder leads to the existence of random off-diagonal elements in the auxiliary Hamiltonian. However, by using the localized TB–LMTO representation (also called β representation) we can reduce the Hamiltonian to the one with diagonal disorder only and then use the CPA. A similar scheme may be used to allow for the SRO effects. While taking account of the angular moment in the ASF approach, we deal with the finite matrices whose elements are labeled by orbital indices L and L' instead of scalar numbers in the Fourier representation, and with a matrix equation instead of the CPA+SRO relation (4.5). The two-site correlation function $g(\mathbf{q})$ arising in this equation can be reconstructed from the Cowley SRO parameters α_n by means of the Fourier transform (2.15) (the experimental Cowley SRO parameters are found from the x-ray diffraction[27]).

Of crucial importance for describing the magnetic properties of transition-metal alloys is the allowance for spatial spin correlations[28] that may be carried out within our extended version of the CPA.

Another problem is connected with taking into account the spatial correlations in the arrangement of electrons with different spin directions within the Hubbard model. This allowance for spatial correlations brings one beyond the scope of the ''Hubbard-III'' (or alloylike) approximation.[29] In this case we should consider some correlation functions with intrinsic SRO parameters, and then, by analogy with the variational Gutzwiller's method,[30] minimize the ground-state energy over the SRO parameters.

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APPENDIX A

In this appendix we show how to calculate the expression (3.19) for the self-energy operator. Carrying out the substitution of Eqs. (3.15) and (3.22) into Eq. (3.19), we write the equation for $\Sigma_0(\epsilon,\mathbf{q})$:

$$\Sigma_0(\epsilon,\mathbf{q})=\Delta^2\left\langle \mathbf{0},\sigma_1,\mathbf{q}\left| G_*(\epsilon,\mathbf{q})\frac{1}{1-W_*(\epsilon,\mathbf{q})G_*^{\mathrm{eff}}(\epsilon,\mathbf{q})}\right|\mathbf{0},\sigma_1,\mathbf{q}\right\rangle, \tag{A1}$$

where

$$G_*^{\mathrm{eff}}(\epsilon,\mathbf{q})=[\epsilon-\mathcal{H}_*^{\mathrm{eff}}(\epsilon,\mathbf{q})]^{-1},$$

$$W_*(\epsilon,\mathbf{q})=W_*^{(1)}+W_*^{(3)}+W_*^{(3)T},$$

$$W_*^{(1)}=T^{\mathbf{q}}[\mathcal{U}(\mathbf{q})-\Sigma^{\mathrm{eff}}(\epsilon,\mathbf{q})]T^{\mathbf{q}},$$

$$W_*^{(3)}=-S^{\mathbf{q}}\Sigma^{\mathrm{eff}}(\epsilon,\mathbf{q})T^{\mathbf{q}},\quad W_*^{(3)T}=-T^{\mathbf{q}}\Sigma^{\mathrm{eff}}(\epsilon,\mathbf{q})S^{\mathbf{q}}.$$

We define also the operators

$$G_*^{\mathrm{eff}(1)}=T^{\mathbf{q}}G_*^{\mathrm{eff}}(\epsilon,\mathbf{q})T^{\mathbf{q}},\quad G_*^{\mathrm{eff}(2)}=S^{\mathbf{q}}G_*^{\mathrm{eff}}(\epsilon,\mathbf{q})S^{\mathbf{q}},$$

$$G_*^{\mathrm{eff}(3)}=S^{\mathbf{q}}G_*^{\mathrm{eff}}(\epsilon,\mathbf{q})T^{\mathbf{q}},\quad G_*^{\mathrm{eff}(3)T}=T^{\mathbf{q}}G_*^{\mathrm{eff}}(\epsilon,\mathbf{q})S^{\mathbf{q}}.$$

The superscript T here designates the transposition operation.

Then, using the inversion formulae for block matrices,[20] one can show that $\Sigma_0(\epsilon,\mathbf{q})$ in Eq. (A1) is defined as

$$\Sigma_0(\epsilon,\mathbf{q})=\Delta^2\langle\mathbf{0},\sigma_1,\mathbf{q}|D^{-1}|\mathbf{0},\sigma_1,\mathbf{q}\rangle, \tag{A2}$$

where D is the operator mapping the subspace $L_{\mathbf{q}}$ (see Sec. III B) onto itself:

$$D=\Gamma^{-1}-W_*^{(1)}-W_*^{(3)T}G_*^{\mathrm{eff}(2)}W_*^{(3)}, \tag{A3}$$

$$\Gamma^{-1}=(1-W_*^{(3)T}G_*^{\mathrm{eff}(3)})(G_*^{\mathrm{eff}(1)})^{-1}(1-G_*^{\mathrm{eff}(3)T}W_*^{(3)}).$$

For further calculations it is convenient to choose in the subspace $L_{\mathbf{q}}$ the orthonormalized basis $\{|\psi_{\sigma_m(\mathbf{i})},\mathbf{q}\rangle\}$, where $\mathbf{i}\cup\sigma_m\subseteq\sigma_n^{max}(m>0)$, which can be obtained by orthogonalization of the basis $\{|\mathbf{i},\sigma_m,\mathbf{q}\rangle\}$, as in the case of the Markov-type correlations in Sec. III A. Consider also the operators:

$$\Sigma^{\mathrm{eff}}(\epsilon,\mathbf{q}),\quad G^{\mathrm{eff}}(\epsilon,\mathbf{q})=[\epsilon-\mathcal{H}^{\mathrm{eff}}(\epsilon,\mathbf{q})]^{-1}, \tag{A4}$$

$$I(\epsilon,\mathbf{q})=G^{\mathrm{eff}}(\epsilon,\mathbf{q})\Sigma^{\mathrm{eff}}(\epsilon,\mathbf{q}),$$

$$J(\epsilon,\mathbf{q})=\Sigma^{\mathrm{eff}}(\epsilon,\mathbf{q})G^{\mathrm{eff}}(\epsilon,\mathbf{q})\Sigma^{\mathrm{eff}}(\epsilon,\mathbf{q}).$$

Then the calculation of Eqs. (A2), (A3) reduces to multiplication and inversion of the finite matrices composed from the matrix components of the operators (A4) in the orthonormalized basis. The matrix components $\langle\psi_{\sigma_n(\mathbf{i})},\mathbf{q}|A_{\mathbf{q}}|\psi_{\sigma'_m(\mathbf{j})},\mathbf{q}\rangle$, [$A_{\mathbf{q}}$ is one of the operators (A4) of the kind (3.16)] can be expressed by the convolution

$$\langle\mathbf{i},\sigma_n,\mathbf{q}|A_{\mathbf{q}}|\mathbf{j},\sigma'_m,\mathbf{q}\rangle$$

$$=\frac{1}{(2\pi)^d}\int d\mathbf{p}\,g^{\sigma_n\sigma'_m}(\mathbf{p}-\mathbf{q})A(\mathbf{p})\exp\{i\mathbf{p}(\mathbf{j}-\mathbf{i})\}. \tag{A5}$$

Here $A(\mathbf{p})$ is the Fourier transform of the matrix $A_{\mathbf{i}-\mathbf{j}}$, and $g^{\sigma_n\sigma'_m}(\mathbf{p}-\mathbf{q})$ is the Fourier transform of the matrix of the scalar products of the vectors defined by Eq. (3.18):

$$g_{\mathbf{ij}}^{\sigma_n\sigma'_m}=\langle\sigma_n(\mathbf{i})|\sigma'_m(\mathbf{j})\rangle. \tag{A6}$$

Integration in Eq. (A5) is over the first Brillouin zone, d is the space dimension. As a result, we obtain the integral equation defining $\Sigma_0(\epsilon,\mathbf{q})$.

For more details, see also Sec. IV A and Appendices B and C, where we discuss the one-dimensional case.

APPENDIX B

Let $d=1$ and the translation-invariant operator A_q has the form similar to Eq. (3.16):

$$A_q=\sum_{i,j}\sum_{\sigma_n,n\geqslant 1}|i,\sigma_n,q\rangle A_{i-j}\langle\chi(j,\sigma_n,q)|. \tag{B1}$$

Then on the first ''level'' of the continued fraction the matrix components

$$\tilde{A}_{ij}(q)=\langle\psi_i,q|A_q|\psi_j,q\rangle,$$

$(i,j=0,\pm 1)$ are expressed in terms of the matrix components $\langle i,q|A_q|j,q\rangle$ (B1) (in what follows we omit the index q for simplicity):

$$\tilde{A}_{00}=\langle 0|A|0\rangle,$$

$$\tilde{A}_{01}=\tilde{A}_{-10}=\frac{1}{\sqrt{1-\alpha^2}}[\langle 0|A|1\rangle-\alpha e^{iq}\langle 0|A|0\rangle],$$

$$\tilde{A}_{0-1}=\tilde{A}_{10}=\frac{1}{\sqrt{1-\alpha^2}}[\langle 1|A|0\rangle-\alpha e^{-iq}\langle 0|A|0\rangle],$$

$$\tilde{A}_{11}=\tilde{A}_{-1-1}=\frac{1+\alpha^2}{1-\alpha^2}\langle 0|A|0\rangle$$
$$-\frac{\alpha}{1-\alpha^2}[e^{iq}\langle 1|A|0\rangle+e^{-iq}\langle 0|A|1\rangle],$$

$$\tilde{A}_{1-1}=\frac{1}{1-\alpha^2}[\langle 1|A|-1\rangle+\alpha^2e^{-2iq}\langle 0|A|0\rangle$$
$$-2\alpha e^{-iq}\langle 1|A|0\rangle],$$

$$\tilde{A}_{-11}=\frac{1}{1-\alpha^2}[\langle -1|A|1\rangle+\alpha^2e^{2iq}\langle 0|A|0\rangle$$
$$-2\alpha e^{iq}\langle -1|A|0\rangle].$$

APPENDIX C

In this Appendix we present the details of calculation of expressions (4.2), (4.3), and (4.4). As shown in Appendix A, it is convenient to present the matrices $G_n^{\rm eff}(\epsilon,q)$ and $W_n(\epsilon,q)$ $(n=1,2)$ in a block form by rearrangement of the rows and columns:

$$\begin{bmatrix} G_n^{\rm eff(1)} & G_n^{{\rm eff}(3)T} \\ G_n^{\rm eff(3)} & G_n^{\rm eff(2)} \end{bmatrix},\quad \begin{bmatrix} W_n^{\rm eff(1)} & W_n^{{\rm eff}(3)T} \\ W_n^{\rm eff(3)} & 0 \end{bmatrix},$$

where for $n=1$: $[A_1^{(1)}]_{ij}$, $i,j\in\sigma$; $[A_1^{(3)}]_{ij}$, $i\notin\sigma$, $j\in\sigma$; $[A_1^{(2)}]_{ij}$, $i,j\notin\sigma$ (here the matrix components of the operators are calculated in the orthogonal basis), and for $n=2$: $[A_2^{(1)}]_{ij}$, $i,j\in\sigma_2$; $[A_2^{(3)}]_{ij}$, $i\notin\sigma_2$, $j\in\sigma_2$; $[A_2^{(2)}]_{ij}$, $i,j\notin\sigma_2$. The symbol T denotes the transposition operation. The operator A_q may be presented in a block form through the projector operators:

$$A_n^{(1)}=T_n^qA_qT_n^q,\quad A_n^{(2)}=S_n^qA_qS_n^q,$$

$$A_n^{(3)}=S_n^qA_qT_n^q,\quad A_n^{(3)T}=T_n^qA_qS_n^q,$$

where the projectors T_n^q and S_n^q are defined in Sec. III A. This representation allows all necessary transformations in Eqs. (4.2) and (4.4) using the inversion formulas of block matrices.[20] To define $\Sigma_0(\epsilon,q)$ one should calculate one component of the matrix that is inverse to the following matrix:

$$D=\begin{bmatrix} A_1 & B_1^T & 0 \\ B_1 & C_1 & S_1 \\ 0 & S_1^+ & A_2 \end{bmatrix}, \tag{C1}$$

$$\Sigma_0(\epsilon,q)=\Delta^2\langle\psi_0,q|D^{-1}|\psi_0,q\rangle.$$

Here, according to Eqs. (3.13) and (3.15), S_1 is the matrix of the operator

$$T^q\Delta_1(q)T^q$$
$$=\sum_{n=\pm 1}|\psi_n,q\rangle\Delta^{-1}(1-\alpha^2)^{-1/2}b_1e^{-iqn/2}\langle\psi_{0,n},q|,$$

$$\begin{bmatrix} A_n & B_n^T \\ B_n & C_n \end{bmatrix}=\Gamma_n^{-1}-W_n^{(1)}-W_n^{(3)T}G_n^{\rm eff(2)}W_n^{(3)}, \tag{C2}$$

$$\Gamma_n^{-1}=(1-W_n^{(3)T}G_n^{\rm eff(3)})[G_n^{\rm eff(1)}]^{-1}(1-G_n^{{\rm eff}(3)T}W_n^{(3)}).$$

The diagonal blocks in Eq. (C2) have the following dimensions: $A_1(1\times 1)$ (the central site **0** forming the cluster σ_1), $C_1(2\times 2)$ (two nearest neighbors **1 −1**), $A_2\,(2\times 2)$ (two sites forming the cluster σ_2). Therefore, a rank of the matrix D is equal to 5.

For calculation (C2) it is convenient to define the following operators:[13]

$$G^{\rm eff}(\epsilon,q)=[\epsilon-\mathcal{H}(\epsilon,q)]^{-1},\quad I(\epsilon,q)=G^{\rm eff}(\epsilon,q)\Sigma^{\rm eff}(\epsilon,q), \tag{C3}$$

$$J(\epsilon,q)=\Sigma^{\rm eff}(\epsilon,q)G^{\rm eff}(\epsilon,q)\Sigma^{\rm eff}(\epsilon,q).$$

Using the formula $S_n^q=P_n^q-T_n^q$, where P_n^q is the orthogonal projector onto the subspace $E_q^{(n)}$ (see Sec. III A), one can obtain that

$$W_n^{(3)T}G_n^{\rm eff(2)}W_n^{(3)}=J_n^{(1)}-I_n^{(1)}\Sigma_n^{\rm eff(1)}-\Sigma_n^{\rm eff(1)}I_n^{(1)}$$
$$+\Sigma_n^{\rm eff(1)}G_n^{\rm eff(1)}\Sigma_n^{\rm eff(1)}, \tag{C4}$$

$$\Gamma_n^{-1}=(1+I_n^{(1)}-\Sigma_n^{\rm eff(1)}G_n^{\rm eff(1)})[G_n^{\rm eff(1)}]^{-1}(1+I_n^{(1)}$$
$$-G_n^{\rm eff(1)}\Sigma_n^{\rm eff(1)}).$$

Then in case of $n=2$, the involutions in Eq. (C2) are expressed in terms of matrices of order (2×2), which are defined by matrix components of operators (C3):

$$\Sigma_{i-j}(\epsilon)=\frac{1}{2\pi}\int_{-\pi}^{\pi}dq\Sigma_0(\epsilon,q)\exp\{-iq(i-j)\},$$

$$G_{i-j}^{\rm eff}(\epsilon)=\frac{1}{2\pi}\int_{-\pi}^{\pi}dq\,G_0(\epsilon,q)\exp\{-iq(i-j)\},$$

$$I_{i-j}(\epsilon)=\frac{1}{2\pi}\int_{-\pi}^{\pi}dq\,\Sigma_0(\epsilon,q)G_0(\epsilon,q)\exp\{-iq(i-j)\},$$

$$J_{i-j}(\epsilon)=\frac{1}{2\pi}\int_{-\pi}^{\pi}dq\Sigma_0^2(\epsilon,q)G_0(\epsilon,q)\exp\{-iq(i-j)\},$$

where $i,j=\pm 1/2$. In case of $n=1$, the matrices of order (3×3) in the expressions (C2) are formed from the magnitudes $\tilde{\Sigma}_{ij}(\epsilon,q)$, $\tilde{G}_{ij}(\epsilon,q)$, $\tilde{I}_{ij}(\epsilon,q)$, $\tilde{J}_{ij}(\epsilon,q)$ $(i,j=0,\pm 1)$, which are the matrix components of the operators (C3) in the orthogonal basis (see Appendix B).

APPENDIX D: ANALYTICAL PROPERTIES OF THE RESOLVENT AND ITS APPROXIMATIONS

The resolvent of the self-conjugate operator $\mathcal{H}$ has the properties[31]

$$G^{+}(\epsilon)=G(\epsilon^{*}),\quad G(\epsilon_1)-G(\epsilon_2)=(\epsilon_2-\epsilon_1)G(\epsilon_1)G(\epsilon_2). \tag{D1}$$

As follows from Eq. (D1), the anti-Hermitian part of the resolvent has a fixed sign (the Herglotz property). In contrast to $G(\epsilon)$, $G_0(\epsilon)$ does not satisfy the second relation in Eq. (D1). Nevertheless, due to the condition $P_0G(\epsilon)G^{+}(\epsilon)P_0 \geqslant 0$, $G_0(\epsilon)$ is of Herglotz type.

Any approximation of the resolvent $G_0(\epsilon)$ such that

$$G_0^{+}(\epsilon)=G_0(\epsilon^{*}), \tag{D2}$$

$$G_0(\epsilon_1)-G_0(\epsilon_2)=(\epsilon_2-\epsilon_1)G_0(\epsilon_1)\Phi(\epsilon_1,\epsilon_2)G_0(\epsilon_2),$$

where $\Phi(\epsilon_1,\epsilon_2)$ is an operator analytical function of two variables and $\Phi(\epsilon,\epsilon^{*})\geqslant 0$, has the anti-Hermitian part of fixed sign, i.e.,

$$G_0(\epsilon)-G_0^{+}(\epsilon)=(\epsilon^{*}-\epsilon)G_0(\epsilon)\Phi(\epsilon,\epsilon^{*})G_0^{+}(\epsilon).$$

The nonconsistent approximations for $\Sigma_0(\epsilon,\mathbf{q})$, obtained by breaking the continued fraction on the mth ''level'' satisfy the condition (D2) and have correct analytical properties.

We prove that the self-consistent scheme (3.15), (3.17) in the case of one-dimensional chain and the scheme (3.15), (3.22) for the general case provide the equation for $\Sigma_0(\epsilon,\mathbf{q})$ satisfying the condition (D2). Denote

$$G_{*}(\epsilon,\mathbf{q})=[\epsilon-P^{\mathbf{q}}\mathcal{H}_{vc}(\mathbf{q})P^{\mathbf{q}+}-T^{\mathbf{q}}\mathcal{U}(\mathbf{q})T^{\mathbf{q}+}-S^{\mathbf{q}}\Sigma^{\mathrm{eff}}(\epsilon,\mathbf{q})S^{\mathbf{q}+}]^{-1},$$

where the projectors $T^{\mathbf{q}}$, $S^{\mathbf{q}}$, and $P^{\mathbf{q}}$ have been defined in Sec. III A and Sec. III B, $\Sigma^{\mathrm{eff}}(\epsilon,\mathbf{q})$ has the form (3.16). Then, using Eqs. (3.7) and (3.19), we write

$$G_0(\epsilon,\mathbf{q})-G_0(\epsilon^{*},\mathbf{q})=(\epsilon^{*}-\epsilon)G_0(\epsilon,\mathbf{q})\left(1+\frac{\Delta\Sigma_0(\mathbf{q})}{\epsilon^{*}-\epsilon}\right)G_0^{+}(\epsilon,\mathbf{q}), \tag{D3}$$

$$\Delta\Sigma_0(\mathbf{q})=\Delta_0(\mathbf{q})G_{*}(\epsilon,\mathbf{q})(\epsilon^{*}-\epsilon+S^{\mathbf{q}}\Delta\Sigma^{\mathrm{eff}}(\mathbf{q})S^{\mathbf{q}+})G_{*}^{+}(\epsilon,\mathbf{q})\Delta_0^{+}(\mathbf{q}),$$

where $\Delta\Sigma_0(\mathbf{q})=\Sigma_0(\epsilon,\mathbf{q})-\Sigma_0(\epsilon^{*},\mathbf{q})$, $\Delta\Sigma^{\mathrm{eff}}(\mathbf{q})=\Sigma^{\mathrm{eff}}(\epsilon,\mathbf{q})-\Sigma^{\mathrm{eff}}(\epsilon^{*},\mathbf{q})$. Consider further an abstract vector space Θ, where we choose the complete orthonormalized basis $\{|\phi(\mathbf{l},\sigma)\rangle\}$. Here $\sigma\subseteq\sigma_n^{max}$, $\sigma\neq\sigma_0$, and the index $\mathbf{l}$ goes over all sites of the lattice. Denote by $|\phi(\mathbf{q},\sigma)\rangle$ the Fourier transforms of $|\phi(\mathbf{l},\sigma)\rangle$. Then

$$S^{\mathbf{q}}\Delta\Sigma^{\mathrm{eff}}(\mathbf{q})S^{\mathbf{q}+}=\sum_{\mathbf{p}} S^{\mathbf{q}}K^{\mathbf{q}}\Delta\Sigma_0(\mathbf{p})\hat{g}^{-1}(\mathbf{p},\mathbf{q})K^{\mathbf{q}+}S^{\mathbf{q}+}, \tag{D4}$$

where

$$K^{\mathbf{q}}=\sum_{\mathbf{l},\sigma\subseteq\sigma_n^{max}}|\mathbf{l},\sigma,\mathbf{q}\rangle\langle\phi(\mathbf{l},\sigma)|,$$

and $\hat{g}^{-1}(\mathbf{p},\mathbf{q})$ is the inverse operator to

$$\hat{g}(\mathbf{p},\mathbf{q})=\sum_{\sigma,\sigma'\subseteq\sigma_n^{max}}|\phi(\mathbf{p},\sigma\rangle)g^{\sigma\sigma'}(\mathbf{p}-\mathbf{q})\langle\phi(\mathbf{p},\sigma')|,$$

here $g^{\sigma\sigma'}(\mathbf{p}-\mathbf{q})$ is the Fourier transform of the matrix of scalar products (A6). Since the matrix of scalar products is positively definite, the operator $\hat{g}^{-1}(\mathbf{p},\mathbf{q})$ is positively definite, too. From the structure of Eqs. (D3) and (D4) it follows that any iteration of Eq. (D3) is of the Herglotz-type if the initial condition is Herglotz. If the iteration process is convergent, then in the limit we get the resolvent with required analytical properties.

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

[2] M. Tsukada, J. Phys. Soc. Jpn. **32**, 1475 (1972).

[3] W. H. Butler, Phys. Rev. B **8**, 4499 (1973).

[4] A. Gonis and J. W. Garland, Phys. Rev. B **16**, 2424 (1977).

[5] A. Gonis, G. M. Stocks, W. H. Butler, and H. Winter, Phys. Rev. B **29**, 555 (1984).

[6] H. Chacham, E. G. da Silva, D. Guenzburger, and D. E. Ellis, Phys. Rev. B **35**, 1602 (1987); Li Zhiqiang, Luo Helie, and Lai Wuyan, J. Phys.: Condens. Matter **3**, 6649 (1991).

[7] A. K. Arzhnikov, L. V. Dobysheva, and S. G. Novokshonov, Phys. Met. Metallogr. **76**, 427 (1993).

[8] R. Mills and P. Ratanavararaksa, Phys. Rev. B **18**, 5291 (1978).

[9] T. Kaplan, P. L. Leath, L. J. Gray, and H. M. Diehl, Phys. Rev. B **21**, 4230 (1980).

[10] A. Mookerjee, J. Phys. C **6**, 1340 (1973).

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

[12] A. Mookerjee, J. Phys. C **8**, 1524 (1975); **8**, 2688 (1975).

[13] A. K. Arzhnikov, L. V. Dobysheva, and S. G. Novokshonov, J. Phys.: Condens. Matter **3**, 9015 (1991); **3**, 9025 (1991).

[14] A. Mookerjee, J. Phys. F **17**, 1511 (1987); S. S. Rajput, S. S. A. Razee, R. Prasad, and A. Mookerjee, J. Phys.: Condens. Matter **2**, 2653 (1990).

[15] S. S. A. Razee and R. Prasad, Phys. Rev. B **48**, 1361 (1993).

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

[17] T. Kaplan and L. J. Gray, J. Phys. C **9**, L483 (1976).

[18] A. Mookerjee and R. Prasad, Phys. Rev. B **48**, 17 724 (1993).

[19] W. Feller, *An Introduction to Probability Theory and Its Applications* (Wiley, New York; Chapman & Hall, Ltd., London, 1966), Vol. I.

[20] F. R. Gantmacher, *Theory of Matrices* (Chelsea, Bronx, NY, 1959), Vols. I and II.

[21] P. Dean, Proc. R. Soc. London, Ser. A **260**, 262 (1961); Rev. Mod. Phys. **44**, 127 (1972).

[22] Y. Onodera and Y. Toyozawa, J. Phys. Soc. Jpn. **24**, 341 (1968)

[23] J. Kudrnovský, V. Drchal, and J. Mašek, Phys. Rev. B **35**, 2487 (1987).

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

[25] O. K. Andersen, O. Jepsen, and M. Šob, in *Electronic Structure and Its Applications*, edited by M. Yussoff, Springer Lecture

Notes in Physics Vol. 283 (Springer, Berlin, 1987).

[26] O. K. Andersen and O. Jepsen, Phys. Rev. Lett. **53**, 2571 (1984).

[27] *Local Atomic Arrangements Studied by X-Ray Diffraction*, edited by J. B. Cohen and J. E. Hilliard (Gordon and Breach, New York, 1966).

[28] Y. Kakehashi, Prog. Theor. Phys. Suppl. **101**, 105 (1990).

[29] J. Hubbard, Proc. R. Soc. London, Ser. A **281**, 401 (1964)

[30] M. C. Gutzwiller, Phys. Rev. Lett. **10**, 159 (1963); Phys. Rev. **137**, A1728 (1965).

[31] M. Reed and B. Simon, *Methods of Morden Mathematical Physics. 1. Functional Analysis* (Academic Press, New York, 1972).