Cluster generalization of the coherent-potential approximation on the basis of projection formalism in augmented space: I. Theoretical analysis of different approximations

A K Arzhnikov, L V Dobisheva and S G Novokshonov

Physics-Technical Institute, Academy of Sciences of USSR, Ural Branch, 132 Kirov Street, SU-426001 Izhevsk, USSR

Abstract. The problem of the electron spectrum of a substitutional binary alloy with diagonal disorder is considered. The general scheme of direct approximations with correct analytical properties on the basis of the self-energy representation as an operator continued fraction is proposed. The interpretation of the approximations obtained and the analysis of corrections to them in terms of the Edwards diagrams are given. The scheme proposed is shown to lead to the well-known approximations.

1. Introduction

In the present work the model of a binary substitutional alloy with diagonal disorder with Hamiltonian given by

$$H = \sum_i |i\rangle \xi_i \langle i| + \sum_{i,j} |i\rangle V_{ij} \langle j| \tag{1}$$

is studied. In (1), $|i\rangle$ specifies the state-vector localized at the site i ($\{|i\rangle\}$ is assumed to generate a complete orthonormal basis for the lattice with N sites). $\{\xi_i\}$ is a set of independent random variables with distribution

$$P_{\xi_i}(\mathscr{E}) = c\delta(\mathscr{E} - \mathscr{E}_1) + (1 - c)\delta(\mathscr{E} - \mathscr{E}_2) \tag{2}$$

where c is the concentration of atoms of kind 1. Finally, the interatomic hopping integrals V_{ij} in (1) are assumed to be non-random.

The configurational averaging problem arising while calculating the macroscopic quantities of disordered systems with Hamiltonian (1) has existed for a long time. Among a variety of different approaches to solve the problem, methods based on multiple-scattering theory are of great importance. The coherent-potential approximation (CPA) [1] was the first successful result obtained within the framework of such an approach. Another paper [2] helped to elucidate its meaning. It showed that the CPA is the first approximation in the self-energy expansion in powers of the small parameter (a/R_0), where a is the lattice constant and R_0 is the characteristic action radius of hopping. Different generalizations aimed at self-consistent calculation of electron scattering by

pairs of atoms ran up against certain difficulties of both computational and fundamental character [3]. Only in 1978 did Mills and Ratanavararaksa [4] obtain a self-consistent expression for the self-energy, called the travelling-cluster approximation (TCA), which on the one hand takes into account the scattering by nearest-neighbour pairs and on the other satisfies the *herglotz* conditions

$$\Sigma(E - i\varepsilon) = \Sigma^*(E + i\varepsilon) \qquad \text{Im } \Sigma(E - i\varepsilon) \geqslant 0 \qquad \varepsilon > 0. \qquad (3)$$

However, systematic constructions of the cluster generalizations of the CPA (CCPA) became possible on the basis of the augmented-space (AS) formalism proposed in [8, 9]. In the 1980s this approach was widely used for solving different tasks in the theory of disordered alloys. Papers [5, 7] were devoted to the CCPA in the single-electron states theory; in [5, 6, 16] this task was considered for the vibrational states of disordered alloys. In [17, 18] the generalization of the CPA was conducted for dynamic disorder. Recently the cluster generalization of the CPA was included in the Korringa–Kohn–Rostoker (KKR) scheme [19, 20]. In [8] the AS formalism was used in the theory of conductivity in disordered alloys. At the same time a number of problems are not settled, for example the nature of the approximation under consideration, the dependence on the dimensionality of space and the coordination number are not clear.

The present paper is devoted to investigation of the cluster generalizations of the CPA on the basis of projection formalism in augmented space, elucidation of their correlation with the CPA and TCA, and their interpretation in terms of the Edwards diagrams [3].

2. Projection formalism in augmented space

The representation of the real random quantity ξ through the self-conjugate operator $\hat{\xi}$ acting in an auxiliary space Ω is the basis of the augmented-space (AS) formalism. We will not dwell on the introduction of the AS and interpretation of the random variables in the AS, these questions being discussed at length in [9–11]. We designate

$$|0\rangle = c^{1/2}|\omega_1\rangle + (1 - c)^{1/2}|\omega_2\rangle$$
$$|1\rangle = c^{1/2}|\omega_2\rangle - (1 - c)^{1/2}|\omega_1\rangle. \qquad (4)$$

Here $|\omega_1\rangle$, $|\omega_2\rangle$ are eigenvectors of the operator $\hat{\xi}$, corresponding to the eigenvalues $\mathscr{E}_1$, $\mathscr{E}_2$. The vector $|0\rangle$ is chosen so that

$$\langle 0|f(\hat{\xi})|0\rangle = \langle f(\xi)\rangle \qquad (5)$$

where $\langle \ldots \rangle$ means the configurational averaging. Following the conventional terminology the states $|0\rangle$ and $|1\rangle$ will be referred to as ground and excited, respectively. The matrix elements of operator $\hat{\xi}$ in basis (4) are

$$\xi_{00} = \bar{\xi} = c\mathscr{E}_1 + (1 - c)\mathscr{E}_2$$

$$\xi_{11} = \tilde{\xi} = (1 - c)\mathscr{E}_1 + c\mathscr{E}_2 \qquad (6)$$

$$\xi_{10} = \xi_{01} = \xi' = [c(1 - c)]^{1/2}(\mathscr{E}_2 - \mathscr{E}_1).$$

Passing to the AS representation by rules described in [9–11], we rewrite the Hamiltonian (1) in the form

$$\mathscr{H} = \sum_i |i\rangle \hat{I}_1 \otimes \hat{I}_2 \otimes \ldots \otimes \hat{\xi}_i \otimes \ldots \otimes \hat{I}_N \langle i| + \sum_{i,j} |i\rangle V_{ij} \hat{I}_1 \otimes \hat{I}_2 \otimes \ldots \otimes \hat{I}_N \langle j|. \tag{7}$$

Here

$$\hat{I}_i = \sum_\alpha |\alpha_i\rangle\langle\alpha_i| \qquad \hat{\xi}_i = \sum_{\alpha,\beta} |\alpha_i\rangle \xi_{\alpha\beta} \langle\beta_i| \tag{8}$$

where $\alpha, \beta = 0, 1$. We designate

$$|i + l, \sigma_n(l)\rangle = |i + l\rangle |\alpha_1\rangle |\alpha_2\rangle \ldots |\alpha_N\rangle \tag{9}$$

where σ_n is a set containing n sites with $|\alpha_k\rangle = |1_k\rangle$—the AS degrees of freedom being excited; l is the radius vector of the set σ_n centre of mass; i is the radius vector of the site where the electron state is localized, which is measured relative to the centre of mass of the set σ_n. The set of vectors (9) forms a complete orthonormal system in AS. Note that with $n = 0$ in (9) and hereafter one should set $i \equiv 0$ in order to avoid multiple summation of the corresponding states in AS.

Now let us pass to the momentum representation, performing the Fourier transform of the state vectors (9) on the cluster σ_n centre coordinates:

$$|i, \sigma_n, q\rangle = \frac{1}{\sqrt{N}} \sum_l |i + l, \sigma_n(l)\rangle \exp(-iql). \tag{10}$$

It is not hard to make certain that the vector set (10) is complete and orthonormal like (9). The Hamiltonian (7) in this basis looks like

$$\mathscr{H} = \sum_q \mathscr{H}_q = \sum_q [\mathscr{H}^{vc}(q) + \mathscr{U}(q)]$$

$$\mathscr{H}^{vc}(q) = |0, \sigma_0, q\rangle H(q) \langle 0, \sigma_0, q| + \sum_{\substack{i,j,\sigma_n \\ n \geqslant 1}} |i, \sigma_n, q\rangle H_{ij} \langle j, \sigma_n, q|$$

$$\tag{11}$$

$$\mathscr{U}(q) = \sum_{\substack{\sigma_n, n \geqslant 0 \\ i \notin \sigma_n, i \cup \sigma_n = \sigma_{n+1}}} [|i, \sigma_n, q\rangle \xi' \exp(-iqd)\langle i - d, \sigma_{n+1}, q| + \text{HC}]$$

$$+ \sum_{\substack{\sigma_n, n \geqslant 1 \\ i \in \sigma_n}} |i, \sigma_n, q\rangle (\bar{\xi} - \tilde{\xi})\langle i, \sigma_n, q|.$$

Here

$$H(q) = \frac{1}{N} \sum_{ij} H_{ij} \exp[iq(i - j)] \tag{12}$$

$$H_{ij} = \xi \delta_{ij} + V_{ij}$$

HC means the term that is Hermitian conjugate to the last one; $\mathscr{H}^{vc}(q)$ represents the Hamiltonian of the virtual crystal; $\mathscr{U}(q)$ is the random potential; d is the cluster centre displacement due to the transition from σ_n to $\sigma_{n+1} = \sigma_n \cup \{i\}$ ($d = i/(n + 1)$); i and $i - d$ in $\mathscr{U}(q)$ are radius vectors of one and the same lattice site measured relative to the centres of the cluster σ_n and σ_{n+1} respectively.

In the AS formalism the problem of the configurational averaging of the Hamiltonian (1) resolvent $(E - H)^{-1}$ according to (5) comes to the calculation of the diagonal matrix element of the Hamiltonian $\mathcal{H}_q$ (11) resolvent on the ground-state vectors (10)

$$\langle G_q(E) \rangle = \frac{1}{N} \sum_{i,j} \langle\!\langle i | 1/(E-H)|j \rangle\!\rangle \exp[iq(i-j)] = (0, \sigma_0, q | 1/(E - \mathcal{H}_q) | 0, \sigma_0, q) \tag{13}$$

in other words to the calculation of the projection

$$G_0(E, q) = P_0 \frac{1}{E - \mathcal{H}_q} P_0 \tag{14}$$

where the projection operators are determined by

$$P_n = \sum_{\sigma_n} P_{\sigma_n} = \sum_{i, \sigma_n} |i, \sigma_n, q)(i, \sigma_n, q|. \tag{15}$$

It is easy to ascertain that all properties of the orthogonal projectors are valid

$$P_n P_m = P_n \delta_{nm'} \qquad P_n^+ = P_n \qquad \sum_n P_n = I. \tag{16}$$

Using the projection technique in AS we rewrite (14) as

$$G_0(E, q) = \frac{1}{E - \mathcal{H}_0(q) - \Sigma_0(E, q)} \tag{17}$$

where

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

$$\Sigma_0(E, q) = P_0 \mathcal{H}_q Q_0 \frac{1}{E - Q_0 \mathcal{H}_q Q_0} Q_0 \mathcal{H}_q P_0. \tag{18}$$

Taking into account the three-diagonality of the Hamiltonian (11) in the index n

$$\mathcal{H}_{nm}(q) = P_n \mathcal{H}_q P_m = \mathcal{H}_n(q)\delta_{nm} + \Delta_n(q)\delta_{n+1.m} + \Delta_n^+(q)\delta_{n-1.m}$$

$$\mathcal{H}_n(q) = P_n \mathcal{H}_q P_n \qquad \Delta_n(q) = P_n \mathcal{H}_q P_{n+1} \tag{19}$$

the expression for $\Sigma_0(E, q)$ (18) may be presented as the finite operator continued fraction

$$\Sigma_0(E, q) = \Delta_0(q) \cfrac{1}{E - \mathcal{H}_1(q) - \Delta_1(q)\cfrac{1}{E - \mathcal{H}_2(q) - }\Delta_1^+(q)} \Delta_0^+(q)$$

$$\vdots$$

$$- \Delta_{m-1}(q)\frac{1}{E - \mathcal{H}_m(q) - \Sigma_m(E, q)}\Delta_{m-1}^+(q). \tag{20}$$

This representation is the initial one for approximate calculations of resolvent (13), (14).

The representation of the Green function in the continued-fraction form with the help of the projection formalism was known long ago [21]. Various versions of this approach are based on the possibility of the choice of such an orthogonal basis in which the Hamiltonian matrix is a three-diagonal one (19).
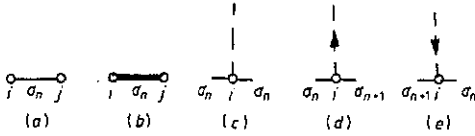
Figure 1. Elements of the diagram series:
(a) $|i, \sigma_n, q) G_{ij}^{vc}(E)(j, \sigma_n, q|$;
(b) $|i, \sigma_n, q) G_{ij}^{eff}(E)(j, \sigma_n, q|$;
(c) $|i, \sigma_n, q)(\xi - \bar{\xi})(i, \sigma_n, q|$;
(d) $|i, \sigma_n, q)\xi' \exp(-iqd)(i - d, \sigma_{n+1}, q|$;
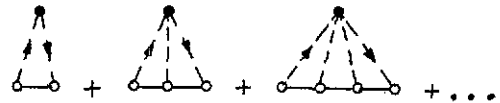(e) $|i - d, \sigma_{n+1}, q)\xi' \exp(iqd)(i, \sigma_n, q|$.

Figure 2. Diagram series of the single-site approximation of $\Sigma_0(E, q)$.
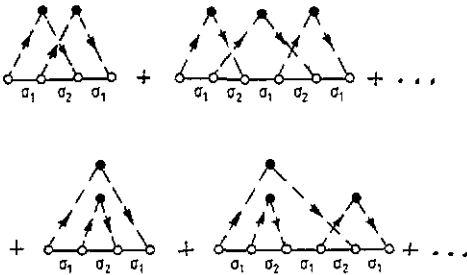

Figure 3. Diagrams depicting first corrections to the ATMA.

In [17, 18] the generalization of the CPA on the basis of projection formalism in the AS was considered for the lattice with arbitrary diagonal, including dynamic disorder. To solve similar problems it is sufficient to determine properly the inner degrees-of-freedom space at each site. From this point of view the representation of $\Sigma^{CPA}(E)$ as an infinite continued fraction obtained in [17, 18] can be obtained from the common expression (20), which is formally exact.

3. Analysis and discussion of different approximations

Expression (20), obtained in the previous section, is a branched operator continued fraction. For a better understanding of subsequent approximations consider in detail its structure. As appears from (15) and (19)

$$\mathcal{H}_n(q) = \mathcal{H}_n^{vc}(q) + \mathcal{U}_n(q) = \sum_{\sigma_n} \mathcal{H}_{\sigma_n}(q) = \sum_{\sigma_n} [\mathcal{H}_{\sigma_n}^{vc}(q) + \mathcal{U}_{\sigma_n}(q)]$$

$$\mathcal{H}_{\sigma_n}(q) = P_{\sigma_n} \mathcal{H}_q P_{\sigma_n} = \sum_{i,j} |i, \sigma_n, q) H_{ij}(j, \sigma_n, q| + \sum_{i \in \sigma_n} |i, \sigma_n, q)(\xi - \bar{\xi})(i, \sigma_n, q| \qquad (21)$$

$\mathcal{H}_{\sigma_n}$ can be interpreted as a Hamiltonian of a virtual crystal containing n defects in sites of the cluster σ_n. $\mathcal{H}_n(q)$ is diagonal in the clusters σ_n unlike the operators $\Delta_n(q)$ describing the transitions between the clusters σ_n and σ_{n+1}.

A sequence of simplest approximations for (20) can be obtained supposing $\Sigma_n(E, q) = 0$ at the nth level. In this case the quantity $\delta = c(1 - c)[(\mathscr{C}_1 - \mathscr{C}_2)/w]^2$ is actually the small parameter (w is the width of the virtual crystal band). First unvanishing corrections to the approximation will be proportional to δ^{n+1}. In order to make sure of this and to compare the approximations obtained we will expand the nth approaching
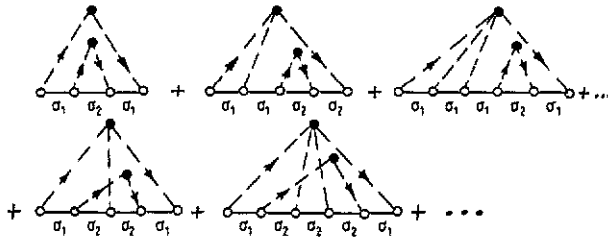
Figure 4. Series corresponding to the third structural diagram in figure 3.

fraction for $\Sigma_0(E, q)$ in a power series of δ and $\bar{\xi} - \bar{\xi}$. This expansion can be conveniently expressed by diagrams, the main elements of which are represented in figure 1.

Setting in (20) $n = 1$ and $\Sigma_1(E, q) = 0$, we get the expression for $\Sigma_0(E, q)$ which conforms to the diagram series in figure 2. This approximation evidently coincides with the well known averaged t-matrix approximation (ATMA) [3, 4, 12]. The next non-self-consistent approximation is obtained as a result of the truncation of the continued fraction (20) at the second level $(n = 2, \Sigma_2(E, q) = 0)$. It is easily seen that the sum of all possible diagrams shown in figure 3 contributes to the approximation considered along with the diagram series in figure 2.

Below, diagrams of such type will be referred to as 'skeleton', assuming each of them to be a sum of all diagrams of the following type: every triangle formed by directed lines is supplemented by any number of undirected ones gathering in its vertex (figure 4 shows the series corresponding to the third diagram in figure 3). The diagrams of figure 3 containing intersecting lines of interaction obviously correspond to the coherent scattering processes on pairs of sites. Thus the conclusion can be inferred that the truncation of the continued fraction (20) at the nth level $(\Sigma_n(E, q) = 0)$ allows one to take account of multiple scattering by the clusters of n excited sites. In diagram terms it means the sum of the contributions of all diagrams with cluster indices not exceeding n.

The dependence of $\Sigma_0(E, q)$ on the quasi-momentum is formed by the products of the exponential factors of the type $\exp(\pm i\, qd)$ involved in $\Delta_n(q)$ ((11), (19)). These products evidently look like $\exp[iq(l - m)]$, where $m - l$ is the vector connecting the centres of mass of the extreme left and right clusters in the diagram describing the scattering process of interest. Hence in the sum of all the terms containing one and the same phase multiplier the coefficient of $\exp[iq(l - m)]$ has the meaning of the self-energy matrix element in the site representation $\Sigma_0(E, l - m)$. Taking this into consideration the diagram series can be considered as depicted in the coordinate space ignoring the dependence on the quasi-momentum.

The corrections for site multiple filling as stated above are automatically taken into account in the self-energy approximations by continued fractions. This is important because their consideration in direct calculations of the electron spectrum moments of higher orders may be quite laborious [3, 12]. In diagram terms it means the prohibition of two or more lines with the same orientation, belonging to a site. Analytically this manifests itself as the absence of the transition operator $|i, \sigma_n, q\rangle\langle j, \sigma_{n+1}, q|$ when $i \in \sigma_n$ in the Hamiltonian (11).

It should also be noted that the approximations of $\Sigma_0(E, q)$ by the approaching continued fractions satisfy the *herglotz* conditions (3). Testing the first one is not hard, and the validity of the second one is proved with the help of the identity

$$\Sigma_n(E,q) - \Sigma_n^+(E,q) = \Delta_n(q)G_{n+1}(E,q)[\Sigma_{n+1}(E,q) - \Sigma_{n+1}^+(E,q)]G_{n+1}^+(E,q)\Delta_n^+(q)$$

$$(22)$$

where $G_n(E,q) = [E - \mathcal{H}_n(q) - \Sigma_n(E,q)]^{-1}$.

The usage of the non-self-consistent approximations suggested above is possible only up to $n = 2$, $\Sigma_2(E,q) = 0$, since beginning from the second level the number of different configurations of clusters σ_n becomes infinite. As a result the problem of inverting matrices of infinite rank arises while calculating the nth approaching fraction (20). It can be avoided when approximating $\Sigma_0(E,q)$ by the figured approaching fractions used in the theory of the branched continued fractions [14]. For this purpose it is necessary to choose a set of clusters $\{\sigma_n\}$ without those that involve each other; this choice depends on from which sets of sites the scattering is taken into account in the approximation. The clusters σ_n which below will be called 'maximum' generate a family of sets $\{\sigma_m; m \leqslant n, \sigma_m \subseteq \sigma_n\}$. The approaching continued fraction approximating $\Sigma_0(E,q)$ (20) is obtained when retaining in operators $\Delta_m(q)$ (19) only those terms which correspond to transitions within this family of sets. The branches of the figured approaching fraction are generally truncated at different levels unlike the nth approaching fraction with all branches being truncated at the nth level. The approximation obtained in such a manner obviously fulfils the *herglotz* conditions as well.

Let, for example, a nearest-neighbour pair σ_2 be chosen as the maximum cluster in a one-dimensional chain. It generates the family consisting of one set $\{\sigma_1, \sigma_2\}$. Replacing now in (20) the operators $\Delta_m(q)$ by the truncated ones according to the above rule, we obtain the figured approaching fraction describing the non-self-consistent TCA [4]. This approximation coincides with the sum of all diagrams of the type shown in figures 2 and 3 with σ_2 being only a nearest-neighbour pair. Let us estimate the order of the terms omitted in the TCA. For instance, the sum corresponding to the first skeleton diagram in figure 3 is proportional to $(G_{ij}^{vc}/G_{00}^{vc})^3(\Sigma^{(0)}/\xi')^2$, where $\Sigma^{(0)}$ is the self-energy calculated in the ATMA. It is of the same order in the parameter $(\Sigma^{(0)}/\xi')^2$ not depending on the distance between the sites $i, j \in \sigma_2$, but its contribution to $\Sigma_0(E,q)$ and also to the density of states depending on $|i - j|$ reaches a maximum in different energy regions. As $|i - j|$ increases the region of the main contribution of the states bonded on the pair of sites $\sigma_2 = \{i, j\}$ shifts to the impurity band centre [13], where the single-site states are of main importance. These arguments allow us to substantiate the non-self-consistent approximations with $\delta \ll 1$ considered above.

But the self-consistent approximations of $\Sigma_0(E,q)$ have a greater region of application. To construct them we define the following operators:

$$\Sigma_n^{\text{eff}}(E,q) = \sum_{\sigma_n} \Sigma_{\sigma_n}^{\text{eff}}(E,q) = \sum_{i,j,\sigma_n} |i, \sigma_n, q\rangle \Sigma_{ij}^{\text{eff}}(E)\langle j, \sigma_n, q|$$

$$\mathcal{H}_n'(E,q) = \mathcal{H}_n(q) + \Sigma_n^{\text{eff}}(E,q) \qquad (23)$$

$$\mathcal{H}_n^{\text{eff}}(E,q) = \mathcal{H}_n^{vc}(q) + \Sigma_n^{\text{eff}}(E,q)$$

$\mathcal{H}_n(q)$ and $\mathcal{H}_n^{vc}(q)$ are defined in (21). Then the expression for $\Sigma_0(E,q)$ can be represented as

$$\Sigma_0(E,q) = \Delta_0(q) \frac{1}{E - \mathcal{H}_1'(E,q) - \Delta\Sigma_1(E,q)} \Delta_0^+(q)$$

$$\Delta\Sigma_n(E,q) = \Delta_n(q) \frac{1}{E - \mathcal{H}_{n+1}'(q) - \Delta\Sigma_{n+1}(E,q)} \Delta_n^+(q) - \Sigma_n^{\text{eff}}(E,q) \qquad (24)$$

$$= \sum_{i,j,\sigma_n,\sigma_n'} |i, \sigma_n, q\rangle [\Sigma_{ij}^{\sigma_n \sigma_n'}(E,q) - \delta_{\sigma_n \sigma_n'}\Sigma_{ij}^{\text{eff}}(E)]\langle j, \sigma_n', q|.$$
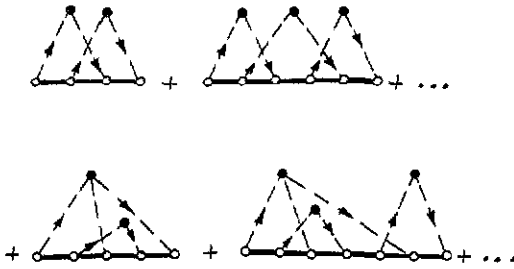
Figure 5. Diagrams depicting first corrections to the CPA.

These expressions are equivalent to (20) and result from it by adding and subtracting $\Sigma_n^{\text{eff}}(E, q)$ at every level. To analyse and compare different approximations, we expand the continued fraction (24) in a power series of the displacements from $\mathcal{H}^{\text{eff}}(E, q)$ and represent it by diagrams obtained from those depicted in figure 1, by replacing thin electron lines with the bold ones corresponding to matrix elements of the resolvent of the effective Hamiltonian (23).

The simplest scheme of self-consistency is obtained if at $n = 1$ we put in (24)

$$\Sigma_{ij}^{\sigma_n \sigma'_n}(E, q) = \delta_{\sigma_n \sigma_n} \Sigma_{ij}^{\text{eff}}(E) \qquad i \notin \sigma_n, j \notin \sigma'_n. \tag{25}$$

In this case the dependence on the quasi-momentum in the equation obtained vanishes and after some algebra the equation can be reduced to the CPA one of Onodera and Toyozawa [15]

$$\Sigma^{\text{eff}}(E) = \frac{(\xi')^2 G_{00}^{\text{eff}}(E)}{1 - [\bar{\xi} - \xi - \Sigma^{\text{eff}}(E)] G_{00}^{\text{eff}}(E)} \tag{26}$$

where

$$G_{ij}^{\text{eff}}(E) = \frac{1}{N} \sum_q \frac{\exp[-i\, q(i - j)]}{[E - H(q) - \Sigma^{\text{eff}}(E, q)]}. \tag{27}$$

This approximation corresponds to the diagram series in figure 2, where thin electron lines are replaced by bold ones. Here we do not show the compensating diagrams [3], which are concerned with the corrections for multiple filling of sites. They appear due to conserving some of the matrix elements $\Sigma_{ij}^{\text{eff}}(E)$ after performing substitution (25) in (24), namely those matrix elements which satisfy at least one of the conditions: $i \in \sigma_n$ or $j \in \sigma'_n$. This compensation mechanism should also remain in self-consistent generalizations considered below and will not be discussed in the following.

We obtain the first unvanishing corrections to the CPA performing substitution (25) in (24) at the second level. The series of skeleton diagrams corresponding to these corrections is depicted in figure 5. Distinct undirected dotted lines in the two last diagrams mean that the corresponding series do not contain the terms cancelling in self-consistent approaches due to compensation. They include, for instance, the first three diagrams of figure 4. Thus, as one should expect, the corrections to the CPA begin with the diagrams with single-intersected directed interaction lines.

As in the case of non-self-consistent cluster approximations the substitution (25) can be made for each n, that is the procedure of self-consistency at the nth level of the continued fraction (24) can be performed. That leads to taking into account all the

diagrams with cluster indices not exceeding n. But in contrast to the non-self-consistent case the corrections to the self-consistent approximation always start with the skeleton diagrams, each of them containing at least one n-fold-intersected directed line of interaction. As shown in [2], they make a contribution to the self-energy proportional to $(a/R_0)^m$. The exponent m depends on the space dimensionality and the level number n, so in the three-dimensional case $m = 4n + 2$, and in the one-dimensional case $m = n + 1$, that is, the proposed scheme of self-consistency in the three-dimensional case yields the $(n - 1)$th approximation in the small parameter $(a/R_0)^4$. Unfortunately its practical realization runs up against the same difficulties that have already been discussed just after formula (22). A variant of approximation by figured continued fractions has been proposed as well, which can easily be generalized to the self-consistent scheme. The desired approximation is obtained when making the substitution (25) in (24) at all levels of the continued fraction, but only for those i, j which satisfy at least one of the conditions $i \cup \sigma_m \notin \sigma_n$ or $j \cup \sigma_m' \notin \sigma_n$. Here σ_m, σ_m' and σ_n are clusters from the family of sets, which defines the structure of the continued fraction and has been discussed when constructing an analogous non-self-consistent approximation. As a result we obtain the CPA generalization where scattering by *all clusters of the family of sets under consideration* is taken into account.

A well known self-consistent TCA [4, 5] for a linear chain is obtained if substitution (25) is made at the first two levels of (24) for all i, j satisfying at least one of the conditions $i \cup \sigma_1 \notin \sigma_2$ or $j \cup \sigma_1 \notin \sigma_2$, where σ_2 is the nearest-neighbour pair. The first corrections to the self-consistent TCA are described by the diagrams in figure 5, where σ_2 is not the nearest-neighbour pair. Their order-of-magnitude estimation has already been conducted when discussing the corrections to the non-self-consistent TCA. In the self-consistent case the TCA receives better substantiation. Really, in addition to the above estimations the additional smallness parameter appears here [3], $G_{ij}^{\mathrm{eff}}(E) \sim \exp[-|i - j|/l_0(E)]$, where $l_0(E)$ is the mean free path of the electron. For example, the relative correction to the TCA brought by the diagram in figure 3 in the case of next-nearest-neighbour pair scattering is proportional to the coefficient $\exp[-3a/l_0(E)]$. The appearance of this additional small parameter is the main argument for self-consistent approximations in comparison with analogous non-self-consistent ones.

4. Conclusions

Thus with the help of the projection formalism in the AS the electron self-energy in the binary alloy model (1) can be presented as an operator continued fraction (20). Proceeding from this expression the paper proposes a general scheme of approximations of $\Sigma_0(E, q)$ based on the usage of figured approaching fractions as approximants of the branched continued fractions [14].

The approach used in this work has a number of advantages. First, in terms of the projection formalism the corrections for multiple filling are taken into account automatically. This allows one to avoid a tedious combinatorial analysis of diagram series, which becomes boundless when out of the single-site approximation. Secondly, the approximations built on the basis of figured approaching fractions satisfy the *herglotz* conditions (3). The proof is conducted by analogy with [11].

A discussion of both non-self-consistent and self-consistent variants of the approximation scheme proposed has been conducted. Their interpretation in terms of Edwards

diagram is given. This allows us to compare the approximations obtained with those known earlier and also to control the order of the terms omitted.

The corrections to the approaching continued fractions truncated at the nth level are shown to be proportional to the parameter $\{c(1 - c)[(\mathscr{E}_1 - \mathscr{E}_2)/w]^2\}^{n+1}$ in the non-self-consistent approximation and to the parameter $(a/R_0)^m$ in the self-consistent one. At $n = 1$ these approximations coincide with the ATMA and CPA respectively. The applicability condition of the self-consistent approaches for the three-dimensional case obtained in that way is that the inequality, analogous to those obtained in [2],

$$\left(\frac{a}{R_0}\right)^6 \left[c(1 - c)\left(\frac{w}{E - E_0}\right)^{1/2}\right] < 1 \tag{28}$$

should be true, where E_0 is the spectrum boundary nearest to E, calculated in the approximation under consideration. In other words, like the CPA, the self-consistent approximations proposed here for $\Sigma_0(E, q)$ become inapplicable near the spectrum boundaries. If we take into account that the CPA is a variant of the mean-field theory [2], then the self-consistent approximation based on the figured approaching continued fraction takes into consideration the fluctuations in all clusters σ_m the scattering on which is considered exactly. In this case the small parameter of the approximation is $\exp[-r/l_0(E)]$, where r is the maximum distance between the sites of the omitted cluster. Taking account of fluctuations expands the spectrum boundaries especially in the impurity band and according to (28) the energy range where this approximation is valid. In the one-dimensional case with allowance for scattering only on nearest-neighbour pairs our results coincide with the TCA [4, 5].

References

[1] Soven P 1967 *Phys. Rev.* **156** 809
[2] Vedjaev A V 1977 *Teor Mat. Fiz.* **31** 392
[3] Elliott R J, Krumhansl J A and Leath P L 1974 *Rev. Mod. Phys.* **46** 465
[4] Mills R and Ratanavararaksa P 1978 *Phys. Rev.* B **18** 5291
[5] Kaplan T, Leath P L, Gray L J and Diehl H W 1980 *Phys. Rev.* B **21** 4230
[6] Yousuff M and Mookerjee A 1984 *J. Phys. C: Solid State Phys.* **17** 1009
[7] Kumar V, Mookerjee A and Srivastava V K 1982 *J. Phys. C: Solid State Phys.* **15** 1939
[8] Mookerjee A and Thakur P K 1988 *Phys. Rev.* B **38** 3798
[9] Mookerjee A 1973 *J. Phys. C: Solid State Phys.* **6** 1340
[10] Mookerjee A 1973 *J. Phys. C: Solid State Phys.* **6** L205
[11] Arzhnikov A K and Novokshonov S G 1990 *Teor. Mat. Fiz.* **84** 128
[12] Ehrenreich H and Schwartz L M 1976 *Solid State Physics* vol 31, ed H Ehrenreich, F Seitz and D Turnbull (New York: Academic) p 150
[13] Lifshitz I M 1964 *Usp. Fiz. Nauk* **83** 617
[14] Skorobogat'ko V Ja 1983 *Teorija wetwjaschikhsja tzepnykh drobej i ee primenenie v vychislitel'noj matematike* (Moskva: Nauka)
[15] Onodera Y and Toyozawa Y 1968 *J. Phys. Soc. Japan* **24** 341
[16] Singh R P and Mookerjee A 1985 *J. Phys. C: Solid State Phys.* **18** 4677
[17] Paquet D and Leroux-Hugon P 1984 *Phys. Rev.* B **29** 593
[18] Mookerjee A 1990 *J. Phys.: Condens. Matter* **2** 897
[19] Mookerjee A 1987 *J. Phys. F: Met. Phys.* **17** 1511
[20] Mookerjee A *et al* 1990 *J. Phys.: Condens. Matter* **2** 2653
[21] Mori H 1965 *Prog. Theor. Phys.* **33** 423