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An augmented-space recursion in the k -space representation

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Abstract. We present here a technique for the calculation of configurationally averaged quantities in the reciprocal k -space representation, such as the spectral function and complex band structures. We apply the technique to AgPd alloys in conjunction with the tight-binding linearized muffin-tin orbital basis. We also indicate why the same technique is ideal for application to the more accurate screened KKR and allows us to go beyond the single-site coherent potential approximation and include multi-site effects such as short-ranged ordering and local lattice distortions due to size mismatch of the constituent atoms.

1. Introduction

In a recent letter [1] we introduced a computationally feasible technique for the calculation of configuration-averaged quantities, such as the density of states, for disordered binary alloys. We indicated that the technique allowed us to take into account coherent scattering from more than one site and consequently deal with effects such as short-ranged ordering [2] and essential off-diagonal disorder due to local lattice distortions arising out of size mismatch of constituents. Since a central part of the technique required the use of the recursion method [3], it was essential first to represent the Hamiltonian in a basis in which the representation is *sparse*. For this reason we chose to illustrate our method within the tight-binding linearized muffin-tin orbital (TB-LMTO) basis. Two aspects remained unsatisfactory. First, many physical properties require us to examine configuration averages of quantities which are expressed in terms of reciprocal space (k -space) representations, for example, spectral functions, if we want to compare with angle-resolved photoemission experimental data, or complex band structures, momentum densities and *fuzzy* Fermi surfaces which are probed in Compton scattering and positron annihilation experiments. Calculation of response functions also require configuration-averaged k -space Green functions $[G(k, z)]_{av}$. Second, there are often objections raised against the TB-LMTO itself, particularly against the most localized (the so-called β) representation. The objections are related to the approximations involved, as we worked with the first-order β Hamiltonian. It would be therefore desirable if we extended the augmented-space recursion to overcome both these aspects. This is the main motivation behind the present work.

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It should be noted that recursion in the k -space representation was carried out earlier on non-crystalline and disordered materials [4]. The novelty of the present work is the use of recursion in augmented space.

2. Formulation

Let us address the first drawback of our previous formulation. We shall start from the most localized TB-LMTO, first-order β representation of the alloy Hamiltonian:

$$\begin{aligned} \mathcal{H} &= \sum_{RL} C_{RL} \mathcal{P}_R \otimes \mathcal{P}_L + \sum_{RL} \sum_{R'L' \neq RL} \Delta_{RL}^{1/2} S_{RL,R'L'} \Delta_{R'L'}^{1/2} \mathcal{T}_{RR'} \otimes \mathcal{T}_{LL'} \\ C_{RL} &= \hat{C}_L^A n_R + \hat{C}_L^B (1 - n_R) \\ \hat{C}_L^\lambda &= C_L^\lambda + \Delta_L^\lambda S_{RL,RL} \\ \Delta_{RL}^{1/2} &= (\Delta^A)_L^{1/2} n_R + (\Delta^B)_L^{1/2} (1 - n_R) \\ \mathcal{P}_R \otimes \mathcal{P}_L &= |RL\rangle\langle RL| \\ \mathcal{T}_{RR'} \otimes \mathcal{P}_{LL'} &= |RL\rangle\langle R'L'| \quad RL \neq R'L'. \end{aligned} \tag{1}$$

The \mathcal{P} and \mathcal{T} are projection and translation operators in the space Φ spanned by the tight-binding basis $\{|RL\rangle\}$ and n_R is a random occupation variable which takes the value 1 if the muffin-tin labelled by R is occupied by an A-type atom, and is 0 otherwise.

In the case where the disorder is *homogeneous*, i.e. if the probability distribution of the random variables $\{n_R\}$ is independent of R , configuration-averaged quantities are lattice translationally symmetric. This is generally the case for bulk properties in homogeneous alloys, but can break down, for instance, near the surface because of surface segregation which leads to an inhomogeneous concentration profile. This translation symmetry leads to

$$\begin{aligned} [\langle k, L | \mathcal{G}(z) | k', L' \rangle]_{av} &= \bar{G}(k, z)_{LL'} \delta(k - k') \\ \mathcal{G}(z) &= (z\mathcal{I} - \mathcal{H})^{-1} \end{aligned}$$

which is the resolvent of the Hamiltonian. This is a random operator in the space Φ .

The configuration average may now be expressed within the augmented-space formalism as follows:

$$[\langle k, L | \mathcal{G}(z) | k', L' \rangle]_{av} = \langle k, L \otimes \{\emptyset\} | (z\tilde{\mathcal{I}} - \tilde{\mathcal{H}})^{-1} | k', L' \otimes \{\emptyset\} \rangle. \tag{2}$$

The augmented-space formalism has been discussed in detail in several previous communications [5]. We refer the readers to these publications and summarize here the main results.

The probability density of the random variables n_R is written as

$$p(n_R) = x\delta(n_R - 1) + y\delta(n_R) = (-1/\pi) \Im m \langle \uparrow_R | (n_R \mathcal{I} - \mathcal{M}_R)^{-1} | \uparrow_R \rangle \tag{3}$$

where x and y are the concentrations of the constituents A and B with $x + y = 1$; \mathcal{M}_R is an operator in the space of configurations ψ_R of the variable n_R . This is of rank 2 and is spanned by the *states* $\{|\uparrow_R\rangle, |\downarrow_R\rangle\}$:

$$\mathcal{M}_R = x\mathcal{P}_\uparrow^R + y\mathcal{P}_\downarrow^R + \sqrt{xy} (\mathcal{T}_{\uparrow\downarrow}^R + \mathcal{T}_{\downarrow\uparrow}^R). \tag{4}$$

$\tilde{\mathcal{H}}$ is an operator which is constructed out of \mathcal{H} by replacing all the random variables n_R by the corresponding operators \mathcal{M}_R . It is an operator in the augmented space $\Psi = \Phi \otimes \prod_R \psi_R$. The configuration space $\prod_R \psi_R = \Psi$ is of rank 2^N if there are N muffin-tin spheres in the system. A basis in this space is denoted by the *cardinality sequence* $\{C\} = \{R_1, R_2, \dots, R_C\}$ [1] which gives us the positions where we have a $|\downarrow\rangle$ configuration. The configuration $\{\emptyset\}$ refers to that with a null cardinality sequence, i.e. one in which we have $|\uparrow\rangle$ at *all* sites.

Using equations (1), (2) and (4) we may rewrite the expression for the configuration average as

$$\langle k, L \otimes \{\emptyset\} | \tilde{\mathcal{D}} (\tilde{\mathcal{A}} + \tilde{\mathcal{B}} + \tilde{\mathcal{F}} - \tilde{\mathcal{S}})^{-1} \tilde{\mathcal{D}} | k, L \otimes \{\emptyset\} \rangle \tag{5}$$

where

$$\begin{aligned} \tilde{\mathcal{A}} &= \sum_L A[(E - \hat{C}_L)/\Delta_L] \{ \mathcal{I} \otimes \mathcal{P}_L \otimes \mathcal{I} \} \\ \tilde{\mathcal{B}} &= \sum_{RL} B[(E - \hat{C}_L)/\Delta_L] \{ \mathcal{P}_R \otimes \mathcal{P}_L \otimes \mathcal{P}_\downarrow^R \} \\ \tilde{\mathcal{F}} &= \sum_{RL} C[(E - \hat{C}_L)/\Delta_L] \{ \mathcal{P}_R \otimes \mathcal{P}_L \otimes \{ \mathcal{T}_{\downarrow\downarrow}^R + \mathcal{T}_{\downarrow\uparrow}^R \} \} \\ \tilde{\mathcal{S}} &= \sum_{RL} \sum_{R'L' \neq RL} S_{RL,R'L'} \{ \mathcal{T}_{RR'} \otimes \mathcal{T}_{LL'} \otimes \mathcal{I} \} \\ \tilde{\mathcal{D}} &= \sum_L A(\Delta_L^{1/2}) \{ \mathcal{I} \otimes \mathcal{P}_L \otimes \mathcal{I} \} + \sum_{RL} B(\Delta_L^{1/2}) \{ \mathcal{P}_R \otimes \mathcal{P}_L \otimes \mathcal{P}_\downarrow^R \} \\ &\quad + \sum_{RL} C(\Delta_L^{1/2}) \{ \mathcal{P}_R \otimes \mathcal{P}_L \otimes \{ \mathcal{T}_{\downarrow\downarrow}^R + \mathcal{T}_{\downarrow\uparrow}^R \} \} \end{aligned}$$

and $A(V) = xV_A + yV_B$, i.e. the average of V , $B(V) = (y - x)(V_A - V_B)$ and $C(V) = \sqrt{xy}(V_A - V_B)$.

We now note that since

$$|k, L\rangle = (1/\sqrt{N}) \sum_R \exp(-ik \cdot R) |R, L\rangle$$

in general such a basis in the augmented k -space has the form

$$(1/\sqrt{N}) \sum_R \exp(-ik \cdot R) |R, L \otimes \{C\}\rangle$$

where $\{C\}$ is the cardinality sequence $\{R_1, R_2, \dots, R_C\}$. We can write this in short-hand notation as $||\{C\}\rangle$ where $||$ stands for $(1/\sqrt{N}) \sum_R \exp(-ik \cdot R) |R, L \otimes \{C\}\rangle$. We have

$$\tilde{\mathcal{D}} ||\{\emptyset\}\rangle = A(\Delta_L^{1/2}) ||\{\emptyset\}\rangle + C(\Delta_L^{1/2}) ||\{R\}\rangle = |1\rangle.$$

The ket $|1\rangle$ is not normalized. We first write the above in terms of a normalized ket $|1\rangle = A(1/\Delta)^{-1/2} |1\rangle$. We may now rewrite (5) as

$$\langle 1 | (E - \tilde{\mathcal{A}}' + \tilde{\mathcal{B}}' + \tilde{\mathcal{F}}' - \tilde{\mathcal{S}}')^{-1} | 1 \rangle \tag{6}$$

where

$$\begin{aligned} \tilde{A}' &= \{A(\hat{C}_L/\Delta_L)/A(1/\Delta_L)\} \tilde{\mathcal{I}} \\ \tilde{B}' &= \{B[(E - \hat{C}_L)/\Delta_L]/A(1/\Delta_L)\} \sum_{RL} \mathcal{P}_R \otimes \mathcal{P}_L \otimes \mathcal{P}_\downarrow^R \\ \tilde{F}' &= \{C[(E - \hat{C}_L)/\Delta_L]/A(1/\Delta_L)\} \sum_{RL} \mathcal{P}_R \otimes \mathcal{P}_L \otimes \{T_{\downarrow}^R + T_{\uparrow}^R\} \\ \tilde{S}' &= \sum_{RL} \sum_{R'L' \neq RL} \{A(1/\Delta_L)^{-1/2}\} S_{RL,R'L'} \{A(1/\Delta_L)^{-1/2}\} T_{RR'} \otimes T_{LL'} \otimes \mathcal{I}. \end{aligned}$$

This equation is now exactly in the form in which the recursion method may be applied. At this point we note that the above expression for the averaged $G(k,E)_{LL}$ is *exact*. The recursion transforms the basis through a three-term recurrence:

$$|\phi_1\rangle = |1\rangle \quad b_{n+1}|\phi_{n+1}\rangle = \tilde{H}|\phi_n\rangle - a_n|\phi_n\rangle - b_n|\phi_{n-1}\rangle. \tag{7}$$

The averaged Green function can then be written as a continued fraction:

$$\frac{b_1^2}{E - a_1 - \frac{b_2^2}{E - a_2 - \frac{b_3^2}{\ddots}}}$$

Since this can also be written in the form $1/(E - E(k) - \Sigma(E, k))$, the self-energy $\Sigma(E, k)$ may also be obtained from the continued fraction. The approximation involved has to do with the termination of this continued fraction. The coefficients are calculated exactly up to a finite number of steps and the asymptotic part is replaced by a terminator. Haydock and co-workers [6] have carried out extensive studies of the errors involved and precise estimates are available in the literature. Haydock [7] has shown that if we carry out recursion exactly up to n steps, the resulting continued fraction maintains the first $2n$ moments of the exact result. Several terminators are available and we have chosen to use that of Lucini and Nex [8].

Before we go on to actual calculations, it is instructive to check several known results. For example, let us take a single s-band nearest-neighbour model, with disorder only in the diagonal terms. It has a simple Hamiltonian

$$\mathcal{H} = \sum_R \varepsilon_R \mathcal{P}_R + \sum_R \sum_{\chi} V T_{R,R+\chi}$$

where χ are the nearest-neighbour vectors on the underlying lattice, ε has a binary distribution and V is not random. It is known that within the CPA the self-energy is k independent. For this simple model, the recursion results can be explicitly written out:

$$\begin{aligned} a_1 &= V_S(k) + Ab_2^2 = W^2 \\ a_2 &= A'b_3^2 = ZV^2 \\ a_3 &= Ab_4^2 = (Z - 1)V^2 + W^2 \\ a_4 &= \frac{Z(Z - 1)V^2A + W^2(V_S(k) - ZA')}{Z(Z - 1)V^2 + ZW^2}. \end{aligned}$$

Here

$$\begin{aligned}
 A &= x\varepsilon_A + y\varepsilon_B & A' &= y\varepsilon_A + x\varepsilon_B \\
 s(\mathbf{k}) &= \sum_{\chi} \exp(-i\mathbf{k} \cdot \chi) & W &= \sqrt{xy}(\varepsilon_A - \varepsilon_B)
 \end{aligned}$$

where Z is the number of nearest neighbours. We note that $\{a_n, b_n\}$ up to $n = 3$ are the same as that of the CPA. There is no \mathbf{k} dependence in these continued fraction coefficients. a_4 onwards begins to differ from the CPA results and the \mathbf{k} dependence begins at this stage. In an earlier work [9] the relation between moments and continued fraction coefficients was discussed in great detail using the idea of self-avoiding walks proposed by Haydock [7]. It was shown that the first closed self-avoiding walk in augmented space whose contribution to the averaged Green function is ignored in the CPA is of length eight. This leads to errors in moments higher than eight and its contribution begins at the fourth level of the continued fraction. Thus our results are consistent with the fact that the CPA self-energy is \mathbf{k} independent, its first eight moments are correct and consequently any k -dependence in more accurate estimates of the self-energy should begin at moments higher than eight, i.e. at levels equal to or lower than the fourth in the continued fraction. Note also that in all lattices where symmetry implies that if χ is a nearest-neighbour vector so is $-\chi$, $s(\mathbf{k})$ and hence all continued fraction coefficients are real.

It is important to note that the operators \tilde{A}' , \tilde{B}' , \tilde{F}' are all projection operators in real space (i.e. unit operators in k -space) and act on an augmented-space basis only to change the configuration part (i.e. the cardinality sequence $\{C\}$):

$$\begin{aligned}
 \tilde{A}'||\{C\} &= A_1||\{C\} \\
 \tilde{B}'||\{C\} &= A_2||\{C\} & \text{if } R \in \{C\}, 0 \text{ otherwise} \\
 \tilde{F}'||\{C\} &= A_3||\{C \pm R\}.
 \end{aligned}$$

The coefficients A_1 – A_3 can be obtained from the form of the operators given above. The remaining operator \tilde{S}' is diagonal in k -space and acts on an augmented space only to change the configuration part:

$$\tilde{S}'||\{C\} = \sum_{\chi} \exp(-i\mathbf{k} \cdot \chi)||\{C - \chi\}. \tag{8}$$

Here, the χ are the nearest-neighbour vectors. The operation of the effective Hamiltonian is thus entirely in the configuration space and the calculation does not involve the space Φ at all. This is an enormous simplification over the standard augmented-space recursion described earlier [1], where the entire reduced real-space part as well as the configuration part was involved in the recursion process. Earlier we had to resort to symmetry reduction of this enormous space in order to make the recursion tractable. Here the rank of only the configuration space is much smaller and we may further reduce it by using the local symmetries of the configuration space, as described in our earlier letter [1]. However, this advantage is offset by the fact that the effective Hamiltonian $\tilde{A}' - \tilde{B}' - \tilde{F}' + \tilde{S}'$ has an energy dependence in the second and third terms. This means that to obtain the averaged $[G(\mathbf{k}, E)]$ we have to carry out the recursion for each energy point. This was not a problem, as recursion at each energy point took a fraction of a second on a desktop 486 PC.

Finally, in figure 1 we present the results for the spectral functions for $\text{Ag}_{80}\text{Pd}_{20}$ alloy along the Γ -X direction. The reason for this choice is that both TB-LMTO-CPA [10]

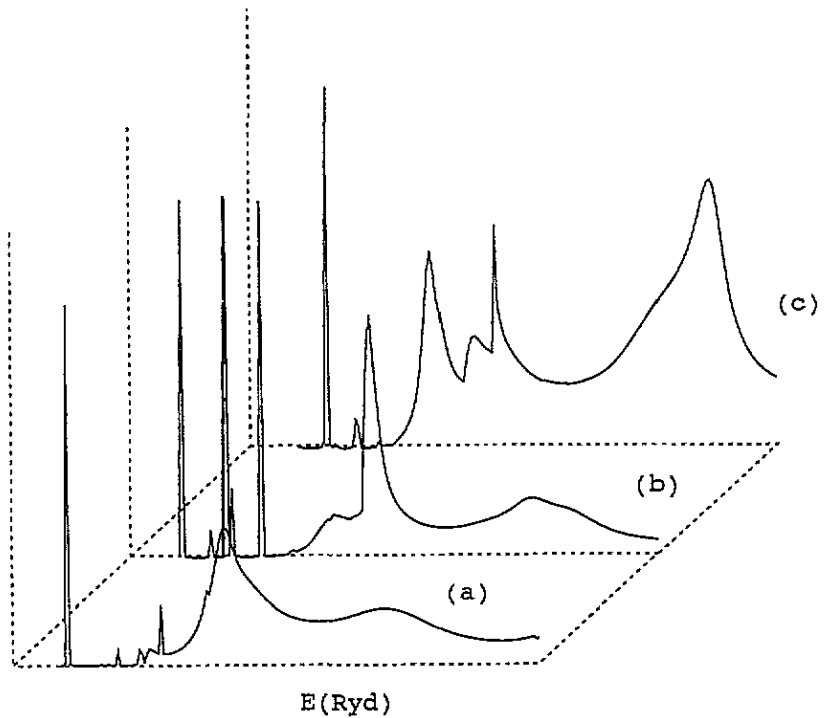


Figure 1. The spectral densities for $\text{Ag}_{80}\text{Pd}_{20}$ alloy in the Γ -X direction for (a) $\frac{2\pi}{a}$ (000), (b) $\frac{2\pi}{a}$ ($\frac{1}{2}$ 00) and (c) $\frac{2\pi}{a}$ (100).

(for the 75–25 alloy) and KKR-CPA [11] (for the 80–20 alloy) results are available. Our results are in good agreement with those for the KKR-CPA. The TB-LMTO-CPA seems to have more width with less sharp peaks in the spectral functions and consequently more width in the complex bands. This is particularly noticeable in the s-like peak at the Γ point. We cannot explain this difference, other than the fact that the TB-LMTO-CPA uses a methodology which starts from a complex energy value and then takes the limiting case onto the real energy axis. If the limit is not reached properly, an artificial imaginary part to the energy could give rise to an extra width.

This brings us to the last point in our communication. We propose that the method is also eminently suitable for application to the screened KKR as well. The relevant KKR Green function over which we have to configuration average is

$$G_{LL}(E) = \sum_L T_{LL'}(E) \left(\delta_{LL'} \frac{d\tau_L^{-1}(E)}{dE} - \frac{dS_{LL'}(E)}{dE} \right)$$

i.e.

$$G = TN \tag{9}$$

$$T_{LL'}(E) = [\tau_L^{-1}(E) - S_{LL'}(E)]^{-1}. \tag{10}$$

This equation is very similar to equation (5); $S(E)$ is the structure matrix in the screened KKR representation. It is sparse and non-random, but energy dependent. $\tau(E)$ is the single-site scattering operator, which is random in a binary alloy. The augmented-space theorem will then give

$$[G]_{av} = \langle \phi | (\bar{\epsilon} - \bar{S})^{-1} \bar{N} | \phi \rangle = A(\mathcal{N}) \langle \phi | (\bar{\epsilon} - \bar{S})^{-1} | \phi \rangle + C(\mathcal{N}) \langle \phi | (\bar{\epsilon} - \bar{S})^{-1} | \{R\} \rangle. \quad (11)$$

The two terms on the right-hand side of the equation can be obtained by two recursions, one starting from $|1\rangle = |\phi\rangle + |\{R\}\rangle$ and another from $|1\rangle = |\phi\rangle - |\{R\}\rangle$. The form of the effective Hamiltonian is almost identical to the TB-LMTO and the effective Hamiltonian is energy dependent. Thus, once the KKR potential parameter and the screened structure matrix are obtained, the augmented-space recursion is no more complicated than the TB-LMTO discussed earlier.

The aim of future work is to carry out the augmented-space recursion within both the TB-LMTO and screened KKR for an extensive comparison. Note that, as introduced earlier, both short-ranged order [2] and local lattice distortion effects [12] can be introduced without difficulty within the formalism.

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