PHYSICAL REVIEW B VOLUME 44, NUMBER 7 15 AUGUST 1991-I

Coherent-potential approximation with the continued-fraction formalism

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(Received 16 July 1990; revised manuscript received 26 March 1991)

We present a general approach to perform coherent-potential electronic-structure calculations of semiconductor alloys within the coherent-potential approximation, using continued fractions for the representation of the relevant Green's-function matrix elements. Starting from a tight-binding representation of the constituent-semiconductor Hamiltonian, it is shown how to evaluate self-consistently a large number of continued-fraction coefficients by means of the construction of an appropriate biorthonormal basis set. A simplified procedure for situations in which groups of energy bands can be treated independently is also proposed. With respect to other approaches in the literature, our procedure presents some special formal and technical advantages that should allow much more manageable treatment of semiconductor alloys.

I. INTRODUCTION

The subject of this paper is the application of the continued-fraction apparatus to determine the electronic spectra of substitutional semiconductor alloys within the coherent-potential approximation (CPA). The conventional calculation procedures presented in the literature are very laborious indeed, as they require appropriate summations over the Brillouin zone at each iteration to self-consistency and for each energy E. The investigation of alternative procedures and the development of techniques with reduced computational complexity to perform CPA calculations is also important for possible perspectives opened beyond the CPA itself.

It is well known that the CPA basic strategy[1,2] is to mimic all the configurations accessible to the alloy by means of an effective self-consistent energy-dependent potential to be added to the physical Hamiltonian. The CPA has been widely used in literature, especially in connection with the Korringa-Kohn-Rostoker method[3] (KKR-CPA formalism), with the tight-binding linear-muffin-tin-orbital method[4] (LMTP-CPA) and with the tight-binding approach[5,6] (TB-CPA). In this latter case the conventional approach is to start from a tight-binding description[7] of the constituent semiconductors, then the virtual-crystal alloy Hamiltonian is constructed, and its Green's-function matrix elements are evaluated by direct diagonalization in **k** space and appropriate summations in the Brillouin zone, and finally an energy-dependent self-energy for each orbital per unit cell is calculated and the procedure is iterated until self-consistency is achieved.

In this paper we systematically analyze the possible advantages of implementing the coherent-potential approximation with the recursion method and the continued-fraction formalism,[8-10] which has been proved so valuable in the calculation of the electronic spectra of solids.[8-12] To achieve this purpose, several problems, both formal and technical, have been encountered. First of all, the continued-fraction procedure and the recursion method are to be considered in their generalized form because the effective Hamiltonian is non-Hermitian; the solution of this difficulty requires the two-sided recursion method procedure.[9] Second, the self-consistent conditions of the CPA are also expressed using continued fractions; an elegant operative solution is provided within the general concepts of the augmented-space formalism.[13,14] In this paper the augmented-space formalism is adopted in an appropriate form to the CPA, but we also notice that more sophisticated analytic theories, such as the traveling cluster approximation,[14] could benefit from continued fractions and renormalization procedures. Finally, a sufficiently large number of steps in the continued fractions has to be obtained; for this we use recent symmetry-based results that have produced high accuracy in the Green's-function calculation[15,16] for perfect crystals.

In Sec. II we provide the general formulation of the CPA continued-fraction procedure. Our formulation uses a biorthonormal basis set and some concepts of the augmented-space formalism. In Sec. III we consider a simplified version of the method and discuss the case in which groups of conduction or valence bands can be treated independently. This way each group of bands can be mapped on a one-dimensional system perfectly equivalent to the three-dimensional original one for the evaluation of the CPA Green's-function matrix elements. Section IV contains the conclusions.

II. THEORY OF THE COHERENT-POTENTIAL APPROXIMATION IN THE FRAMEWORK OF THE CONTINUED FRACTIONS

A. General considerations

The system under consideration is a homogeneously disordered substitutional alloy; the geometrical periodicity is preserved, but the sites of the lattice (or of a sublattice) may be occupied by two or more different types of atoms which are labeled as A or B in the case of a binary alloy. The one-electron Hamiltonian of the crystal in the localized basis approximation can be written in the form

$$H=\sum_{m\mu}|\phi_{m\mu}\rangle e_{\mu(A,B)}\langle\phi_{m\mu}| + \sum_{\substack{m\mu,n\nu \\ \mu\neq\nu \text{ if } m=n}} |\phi_{m\mu}\rangle T_{m\mu,n\nu}\langle\phi_{n\nu}| \ . \tag{1}$$

In Eq. (1), $|\phi_{m\mu}\rangle$ are orthonormal independent localized orbitals in the positions $\mathbf{d}_\mu$ within the cell τ_m. The orbital energies $e_{\mu(A,B)}$ depend on the type of atom occupying the lattice site; the off-diagonal matrix elements $T_{m\mu,n\nu}$ between atomic orbitals on different sites are assumed to be unaffected by the disorder. The diagonal energy $e_{\mu(A,B)}$ has the following probability distribution:

$$P(e_\mu)=c\delta(e_\mu-e_{\mu A})+(1-c)\delta(e_\mu-e_{\mu B}) \ , \tag{2}$$

where c and $(1-c)$ are the concentrations of the atomic species A and B, respectively. Our treatment is also applicable to the more general distribution

$$P(e_\mu)=\sum_{s=1}^{N} W_s\delta(e_\mu-e_{\mu s}) \tag{3}$$

with $\sum_{s=1}^{N}W_s=1$, or also to the case of a continuous distribution $P(e_\mu)$. Moreover, it includes the possibility that some orbitals in the unit cell do not fluctuate, as may occur in III-V compounds when only the anion or cation sublattice fluctuates.

Instead of considering the Hamiltonian (1) for all possible alloy configurations, in agreement with the CPA concepts we consider a translationally invariant Hamiltonian, the diagonal part of which includes appropriate orbital-dependent self-energies $\sigma_\mu(E)$:

$$H=\sum_{m\mu}|\phi_{m\mu}\rangle \sigma_\mu(E)\langle\phi_{m\mu}| + \sum_{\substack{m\mu,n\nu \\ \mu\neq\nu \text{ if } m=n}} |\phi_{m\mu}\rangle T_{m\mu,n\nu}\langle\phi_{n\nu}| \ . \tag{4}$$

At the very first step of the method, $\sigma_\mu(E)$ is simply the average orbital energy

$$\sigma_\mu(E)=\bar{e}_\mu=\int P(e_\mu)e_\mu de_\mu \tag{5}$$

and the Hamiltonian (4) corresponds to the virtual-crystal approximation (VCA).

We now consider how to obtain the orbital-dependent self-energies $\sigma_\mu(E)$ by an iterative procedure. Let us indicate with $|\phi_\mu\rangle$ the orbitals within the reference unit cell and with $G_{\mu\mu}(E)$ the site diagonal Green's-function matrix elements:

$$G_{\mu\mu}(E)=\left\langle\phi_\mu\left|\frac{1}{E-H}\right|\phi_\mu\right\rangle \ . \tag{6}$$

At this stage we exploit the continued-fraction procedure to evaluate $G_{\mu\mu}(E)$, avoiding both the explicit diagonalization of the Hamiltonian (4) and the time-consuming integrations over the Brillouin zone.

The presence of the complex self-energy $\sigma_\mu(E)$ makes the Hamiltonian (4) non-Hermitian, so we have to use the general biorthonormal recurrence relations:[9]

$$\begin{aligned} &|f_0\rangle=|\phi_\mu\rangle, \quad \langle\tilde{f}_0|\equiv\langle\phi_\mu| \ , \\ &|f_{n+1}\rangle=(1-P_{n-1})(1-P_n)H|f_n\rangle \ , \\ &\langle\tilde{f}_{n+1}|=\langle\tilde{f}_n|H(1-P_{n-1})(1-P_n) \ , \\ &P_n=\frac{|f_n\rangle\langle\tilde{f}_n|}{\langle\tilde{f}_n|f_n\rangle}, \quad P_{-1}\equiv0 \ , \\ &a_n(E)=\frac{\langle\tilde{f}_n|H|f_n\rangle}{\langle\tilde{f}_n|f_n\rangle}, \quad b_{n+1}^2(E)=\frac{\langle\tilde{f}_{n+1}|f_{n+1}\rangle}{\langle\tilde{f}_n|f_n\rangle} \ . \end{aligned} \tag{7}$$

We explicitly note that the coefficients a_n and b_n are energy dependent due to the quantities $\sigma_\mu(E)$. The two-sided recursion method, summarized by Eqs. (7), leads to the following continued-fraction representation of the Green's function $[a_0(E)\equiv\sigma_\mu(E)]$:

$$G_{\mu\mu}(E)=\cfrac{1}{E-\sigma_\mu(E)-\cfrac{b_1^2(E)}{E-a_1(E)-\cfrac{b_2^2(E)}{E-a_2(E)-\ddots}}} \ . \tag{8}$$

It is convenient to write Eq. (8) in the form

$$G_{\mu\mu}(E)\equiv\frac{1}{E-\sigma_\mu(E)-M_{\mu\mu}(E;\{\sigma_\nu(E)\})} \ . \tag{9}$$

This defines the memory function $M_{\mu\mu}(E;\{\sigma_\nu(E)\})$ which, of course, depends parametrically on the whole set $\{\sigma_\nu(E)\}$ of the self-energies of the independent orbitals; notice that the self-energies $\sigma_\nu(E)$, as we shall see, satisfy, by construction, the Herglotz properties and, namely, are analytic in the upper complex energy plane.

B. Augmented-space formalism for averaging continued fractions

The standard CPA formalism requires that the self-energies $\sigma_\mu(E)$ for each orbital are such that the weighted mean of the Green's function on the orbital μ satisfies the system of coupled equations:

$$\sum_{s=1}^{N} W_s\frac{1}{E-e_{\mu s}-M_{\mu\mu}(E;\{\sigma_\nu(E)\})} =\frac{1}{E-\sigma_\mu(E)-M_{\mu\mu}(E;\{\sigma_\nu(E)\})} \ . \tag{10}$$

This complicated system of coupled self-consistent equations can be solved iteratively even in the case of a continuous distribution with the help of the augmented-space formalism.

The basic idea of the augmented-space formalism[13] is to replace a probability distribution function with a perfectly deterministic effective operator in an extended space. In the case of a binary alloy where the site energy can assume the values e_A and e_B with probability c and $(1-c)$, it is well known[13] that the disorder space is two dimensional and the operator describing the site fluctuating energy is represented by the 2×2 matrix:

$$A=\begin{bmatrix}\alpha_0 & \beta_1\\ \beta_1 & \alpha_1\end{bmatrix}, \tag{11a}$$

where

$$\begin{aligned}\alpha_0&=ce_A+(1-c)e_B=\bar{e}\ ,\\ \alpha_1&=ce_B+(1-c)e_A\ ,\\ \beta_1&=|e_A-e_B|\sqrt{c(1-c)}\ .\end{aligned}\tag{11b}$$

We can extend this procedure to the case in which the diagonal energies may assume N possible values e_i with probabilities W_i $(i=1,2,\ldots,N)$. The first step is the formal definition of the operator Γ:

$$\Gamma=\sum_{i=1}^{N}|u_i\rangle e_i\langle u_i|\ , \tag{12}$$

whose eigenvalues are the possible site energies e_i. Then we consider the initial state

$$|f_0\rangle=\sum_{i=1}^{N}\sqrt{W_i}\,|u_i\rangle\ . \tag{13}$$

It is evident that

$$-\frac{1}{\pi}\lim_{\varepsilon\to0}\mathrm{Im}\left\langle f_0\left|\frac{1}{E+i\varepsilon-\Gamma}\right|f_0\right\rangle$$

gives the distribution probability $P(e_i)$. By applying the standard recursion relations with initial state (13) and Hamiltonian (12), we arrive at the tridiagonal representation of the given distribution function of the type

$$A=\begin{bmatrix}\alpha_0 & \beta_1 & 0 & 0\\ \beta_1 & \alpha_1 & \beta_2 & 0\\ 0 & \beta_2 & \alpha_2 & \ddots\\ 0 & 0 & \ddots & \ddots\end{bmatrix}. \tag{14}$$

In the case of a continuous distribution $P(e)$, the matrix A can be of infinite rank.

Let us consider now the chain representation of $G_{\mu\mu}(E;\{\sigma_\nu(E)\})$ with the augmented-space formalism to treat the energy fluctuation of the state $|f_0\rangle$. The diagrammatic representation of the operators of interest in the direct product space is schematically indicated in Fig. 1. Because of the structure of the interactions among the chains, we can easily eliminate by renormalization all the chains but the first one, on the first site of which we evaluate the Green's function. For a multivalued distribution of the energy, we thus obtain, for the self-energy of the orbital μ at step $i+1$ of the iterative procedure

$$\sigma_\mu^{(i+1)}(E)=\alpha_0+\cfrac{\beta_1^2}{E-\alpha_1-M_{\mu\mu}(E;\{\sigma_\nu^{(i)}(E)\})-\cfrac{\beta_2^2}{E-\alpha_2-M_{\mu\mu}(E;\{\sigma_\nu^{(i)}(E)\})-\ddots}}\ . \tag{15}$$

The continued-fraction expression $\sigma_\mu^{(i+1)}$ derived by us constitutes a convenient operative solution of the CPA set of equations (10). In fact, the $\{\sigma_\mu^{(i+1)}\}$ obtained by Eqs. (15) can be inserted into Eq. (4) and a new iteration is then started until self-consistency is achieved. A further bonus of Eq. (15) is to explicitly show the Herglotz properties of the self-energies at any stage of the iterative process and thus the definite positiveness of the generated density of state in the coherent-potential approximation.

III. SIMPLIFIED VERSION OF THE GENERAL CPA CONTINUED-FRACTION EQUATIONS

The general equations (4), (7), and (15) in Sec. II allow us to perform the CPA calculation using a continued-fraction representation both for the Green's function and the self-energy. Such a general procedure, in a number of physical situations, can be further simplified.

Consider the case of a binary alloy; Eq. (15), with the use of Eq. (9), then becomes

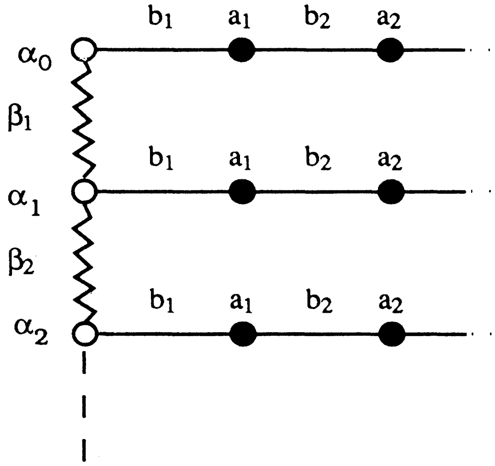

FIG. 1. Graphical representation of the tridiagonal operator corresponding to the Green's function $G_{\mu\mu}(E)$ (first horizontal chain), of the disorder operator (vertical chain), and of the direct-product augmented space.

$$\sigma_\mu^{(i+1)}(E)=\alpha_0+\cfrac{\beta_1^2}{-\alpha_1+\sigma_\mu^{(i)}(E)+\cfrac{1}{G_{\mu\mu}(E;\{\sigma_\nu^{(i)}(E)\})}}\ . \tag{16}$$

The self-consistent solution of Eqs. (4), (7), and (16) is still a complicated problem. A remarkable simplification occurs if we consider only one fluctuating orbital for each site so that $G_{\mu\mu}(E;\{\sigma_\mu(E)\})$ is simply $G_{\mu\mu}[E-\sigma_\mu(E)]$ and the Green's function has to be evaluated only once. At the self-consistency

$$\sigma_\mu^{(i+1)}(E)=\sigma_\mu^{(i)}(E)=\sigma_\mu(E)\ ,$$

using Eq. (11b), we can rearrange Eq. (16) in the familiar form[9]

$$\bar{e}-\sigma_\mu(E)=[e_A-\sigma_\mu(E)][e_B-\sigma_\mu(E)]\times G_{\mu\mu}[E-\sigma_\mu(E)]\ . \tag{17}$$

Since, in this case, the Green's function must be calculated only once, the continued-fraction expansion entails a very simple procedure indeed.

To evaluate the Green's function with high accuracy, it has been recently proposed and discussed how to perform recursions in reciprocal space,[16] and how to separately treat different parts of the Brillouin zone.[15] We briefly reconsider this point in connection with CPA calculations.

Relations (7) are written in a very general way; to be more precise, one can work equally well in real or in reciprocal space. We can write the crystal Hamiltonian in the reciprocal space by introducing the Bloch functions $|\Phi_{k\mu}\rangle$ defined by

$$|\Phi_{k\mu}\rangle=\frac{1}{\sqrt{N}}\sum_{\tau_m}e^{i\mathbf{k}\cdot\tau_m}|\phi_{m\mu}\rangle\ , \tag{18}$$

where N is the total number of unit cells of the crystal. The crystal Hamiltonian in Eq. (4) can be written as

$$H=\sum_{\mathbf{k},\mu}\sigma_\mu(E)|\Phi_{\mathbf{k}\mu}\rangle\langle\Phi_{\mathbf{k}\mu}| + \sum_{\mathbf{k},\mu,\nu}T_{\mu\nu}(\mathbf{k})|\Phi_{\mathbf{k}\mu}\rangle\langle\Phi_{\mathbf{k}\nu}|\ , \tag{19}$$

$T_{\mu\nu}(\mathbf{k})$ being the Fourier transform of $T_{m\mu,n\nu}$.

An initial state $|\phi_\mu\rangle$, localized in real space, is extended in **k** space and it then takes the expression

$$|\phi_\mu\rangle=\frac{1}{\sqrt{N}}\sum_{\mathbf{k}}|\Phi_{\mathbf{k}\mu}\rangle\ . \tag{20}$$

It is convenient to start the iterative procedure with the initial state (20) and the Hamiltonian (19). It is now possible[15] to exploit the separability in **k** space and perform recurrences successively in separated small subzones of the Brillouin zone. This technique allows us to overcome limitations due to the finite size of computer storage and to obtain a large number (100 or more) of continued-fraction coefficients whenever needed. This high number of continued-fraction coefficients, obtained by the recursion method in **k** space, and the possibility to merge in the asymptotic region are of great utility for an accurate control and termination of the continued fractions.

The continued-fraction expansion also appears to be very useful for a description of separated groups of bands (for instance, valence bands or conduction bands). We have, in fact, generalized the above procedure as follows. We start with the virtual crystal Hamiltonian in the Bloch sums representation, and diagonalize it at the various **k** vectors to have the energy bands. Among them we can isolate, for instance, the block of valence bands. We then tridiagonalize the valence part of the total Hamiltonian in order to put it in a suitable form for an iterative chain scheme. The continued-fraction coefficients relative to this new Hamiltonian will exhibit damped oscillating behavior if the valence bands are connected; usually the asymptotic region can soon be reached in 30–50 iterations, and then the single-band terminator can be applied. In other situations double- or multiple-band terminators can be used in the presence of energy gaps.

For several systems of physical relevance and, in particular, for group-IV elemental and III-V compound and other semiconductors, one can separately treat the fluctuations in each set of valence and conduction bands following the basic simplification introduced by Chen and Sher.[5] In the Chen-Sher model, the use of continued fractions becomes particularly rewarding; it can be carried out along the following steps.

(i) The first to be constructed is the virtual-crystal Hamiltonian from the tight-binding representation of the constituent semiconductors. Conduction and valence electronic energy bands of the VCA crystal are separated into groups of connected bands and tridiagonalized independently with the recursion method. This way each group of bands is mapped on a one-dimensional solid-state chain, perfectly equivalent to the three-dimensional original system as far as CPA calculations are concerned.

(ii) The CPA calculations are now easily performed on the one-dimensional models so obtained in the framework of the augmented-space formalism. It is worthwhile to emphasize that the recursion procedure for the determination of the continued-fraction coefficients is done only once. CPA calculations now become trivial due to the peculiar way in which energy appears in the continued fractions. On the contrary, in the traditional treatments provided in the literature, where tridiagonalization is not performed, the self-consistent CPA procedure can only be achieved with laborious summations throughout the Brillouin zone for every trial energy.

The simplifications of our procedure are thus evident. In the traditional approach to CPA calculations, the most laborious part is the sum throughout selected **k** vectors in the Brillouin zone of appropriate functions with poles at the Hamiltonian eigenvalues; this time-consuming procedure has to be repeated at every energy several times in order to achieve self-consistency. Typically one needs about 100 energy values to span the whole energy spectrum and 5–10 steps to achieve self-consistency. Instead, in our present continued-fraction procedure, we have to evaluate the continued-fraction coefficients only once (the amount of computational labor required for this is comparable with the one required to perform only once the sum on the selected **k** vectors in the Brillouin zone); from the knowledge of the continued-fraction coefficients, the Green's function is immediately available for any energy. Thus, the effective reduction of the computational effort between the continued-fraction procedure and the traditional one amounts to almost two orders of magnitude.

To test our procedure for the treatment of alloy disorder and verify its manageability in realistic CPA calculations, we have studied the $GaAs_{0.5}P_{0.5}$ and $GaSb_{0.5}P_{0.5}$ semiconductor alloys described within the Chen-Sher model. In this model the disorder scattering strength is measured by the differences between the energy mean values of groups of connected bands (in general, the valence and the conduction bands). For these cases, alternative CPA calculations already exist in literature and the results we have obtained definitively show the convenience and flexibility of our treatment based on the continued-fraction approach. In each case we verified that the mapping into a one-dimensional chain with about 100 steps was more than sufficient for accurate numerical results. In the case of $GaAs_{0.5}P_{0.5}$, we are in the weak scattering regime due to the small difference in the energies of s and p anion orbitals used in the adopted parametrization of Vogl, Hjalmarson, and Dow.[17] Very few differences exist between VCA and CPA densities of states thus confirming the minor role of disorder in the alloying, in agreement with the work of Chen and Myles:[5] in particular, the valence bands remain practically unchanged, while the conduction bands, shown in Fig. 2, present minor differences within the two approximations.

As a second example we have considered the $GaSb_{0.5}P_{0.5}$ alloy. In this case there is a significant difference between the diagonal orbital energies of antimony in GaSb and phosphorus in GaP. We expect noticeable differences between VCA and CPA approximations, as confirmed in Fig. 3. This fact[17–19] is not a particular feature of the model of Vogl, Hjalmarson, and Dow but is also common to other kinds of Hamiltonians.

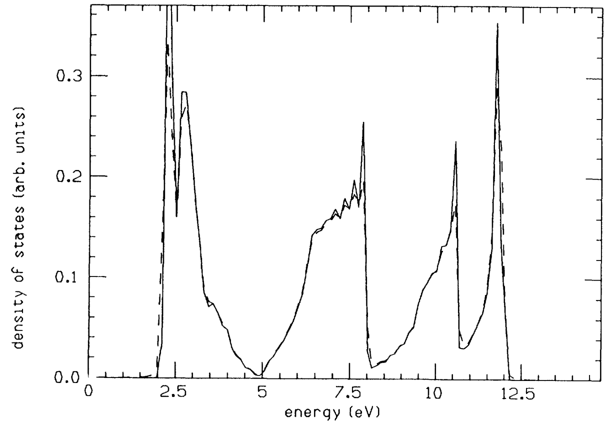

FIG. 2. CPA (dashed line) and VCA (solid line) total density of states for the conduction band of the alloy $GaAs_{0.5}P_{0.5}$.

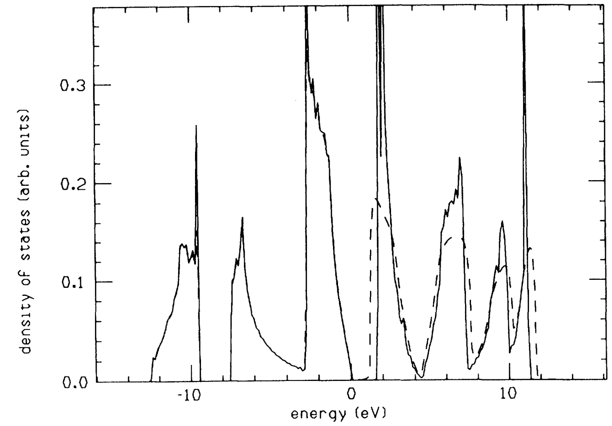

FIG. 3. CPA (dashed line) and VCA (solid line) total density of states for the alloy $GaSb_{0.5}P_{0.5}$.

As a final comment we wish to stress that the proposed continued-fraction procedure to perform CPA calculations goes in the direction of a significant reduction of numerical labor, without introducing additional approximations. We think this line is of value not only to reduce the heavy calculations in the general CPA treatments, involving different self-energies or different orbitals, but also in the numerous attempts and extensions beyond the CPA itself.

IV. CONCLUSIONS

In this paper we have presented a general theory that adopts the continued-fraction formalism for both the calculation of the Green's function and for the description of the one-site energy fluctuations within the coherent-potential approximation. We have also provided a simplified version, which allows us to exactly map groups of bands on a one-dimensional model separately. The method presented here allows less laborious calculations within the CPA theory and should also be much help for attempts beyond it, mainly in the context of analytic theories of disorder and particularly in the traveling cluster approximation. Further investigations are also in progress in this direction.

ACKNOWLEDGMENTS

This work has been partially supported by the Commissione delle Comunitá Europee through Contract No. ST2J-0254-2-I.

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