

## Cluster densities of states of nonrandom substitutionally disordered alloys

A. Gonis

*Department of Physics and Astronomy and Materials Research Center, Northwestern University, Evanston, Illinois 60201*

A. J. Freeman

*Department of Physics and Astronomy and Materials Research Center, Northwestern University, Evanston, Illinois 60201 and Center for Materials Science, Los Alamos National Laboratory, Los Alamos, New Mexico 87445*

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The embedded-cluster method is used to calculate the density of states (DOS) of nonrandom substitutionally disordered alloys. This method is based on the calculation of the Green's function for a cluster of atoms embedded in an effective medium. The effect of increasing cluster size as well as of different choices of the effective medium is investigated numerically in terms of one-dimensional alloys with various scattering strengths and degrees of short-range-order (SRO). A method for the self-consistent treatment of SRO in terms of the pair distribution function is proposed and in many cases is found to lead to results in much better agreement with exact DOS's than those obtained when SRO is not treated self-consistently.

## I. INTRODUCTION

The introduction and application of the coherent-potential approximation<sup>1,2</sup> (CPA) has increased greatly our understanding of disordered systems, particularly of random, substitutionally disordered alloys. In these alloys, atoms of various species are randomly distributed over the  $N$  sites of a regular lattice. The CPA provides the most satisfactory prescription for the calculation of the site-diagonal element of the Green's-function operator, and hence for the calculation of the one-particle properties of these systems within a single-site approximation. In the CPA, one considers that the real, disordered material is replaced by a self-consistently determined effective medium which is characterized by an energy-dependent site-diagonal self-energy, and which preserves all symmetries of the lattice. The CPA yields unique and analytic results, i.e., densities of states (DOS's) and momentum spectral weight functions that are non-negative and satisfy fundamental sum rules. There exist several reviews of the CPA (Refs. 3–5) both for systems describable by tight-binding<sup>3</sup> (TB) and muffin-tin<sup>4,5</sup> (MT) Hamiltonians.

In spite of its many desirable properties, however, the CPA possesses several limitations. The most important among these are the following: (i) the CPA is applicable only to random substitutionally disordered alloys and cannot account for the effects of short-range order (SRO) which is known to be present in many disordered systems, and (ii) the CPA cannot treat the effects of many-site statistical fluctuations. By SRO, we mean the tendency of atoms of a given kind to surround atoms of the same kind (clustering) or of a different kind (ordering). In principle, both of these limitations can be removed in a multisite, or cluster extension of the CPA, and several such extensions have been proposed<sup>6–31</sup> in the literature. In this paper we propose new methods and cluster techniques for the calculation of the DOS of nonrandom, substitutionally disordered alloys.

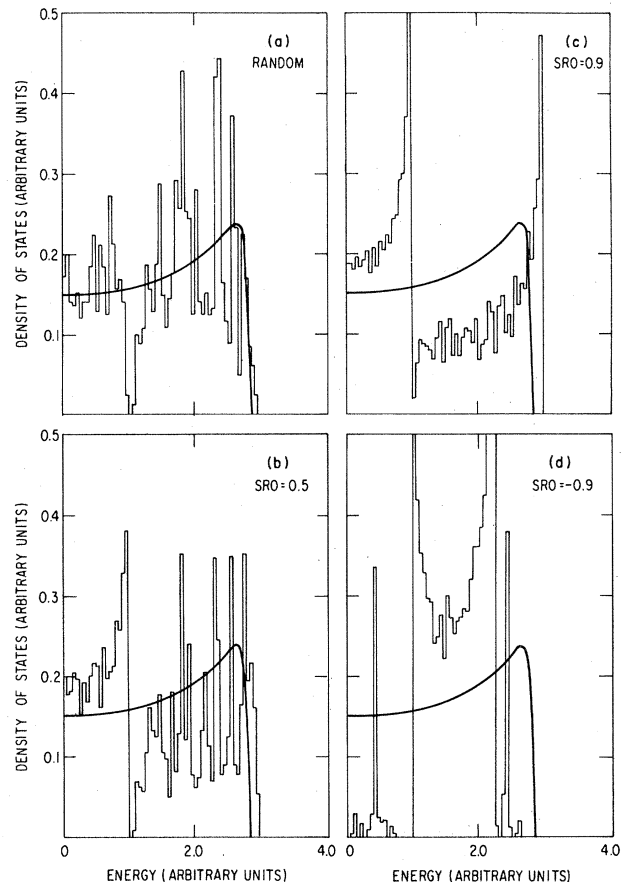


FIG. 1. Exact DOS's (histograms) for one-dimensional weak-scattering alloys with  $\epsilon_A = -\epsilon_B = 1.0$ ,  $W = 1.0$  ( $\delta = 1.0$ ),  $c = 0.5$ , and various degrees of SRO designated in the manner defined in the text. The CPA DOS's (solid curve) for a random alloy is also shown for comparative purposes.

A satisfactory cluster theory of disordered systems must satisfy a rather stringent set of criteria, the most important of which are listed below. Among other properties, the theory should include the following:

(1) It should yield analytic, physically meaningful results, i.e., non-negative DOS and momentum spectral weight functions. Analyticity is necessary for the satisfaction of causality and of fundamental sum rules on the DOS.

(2) It should be unique in the sense that it can be derived within various formalisms and from various points of view. For example, the CPA can be derived<sup>3</sup> within the locator, propagator, variational, diagrammatic, and functional<sup>6</sup> formalisms. There is strong indication that uniqueness is necessary for the analyticity of a cluster theory as exemplified by the analyticity of the molecular CPA (MCPA),<sup>7</sup> and the nonanalytic behavior of nonunique theories, some of which are discussed below.

(3) It should preserve the symmetries of the underlying lattice. Such preservation is essential to the calculation of meaningful momentum spectral weight functions.

(4) It should become exact in the weak scattering and dilute-alloy limits.

(5) It should be applicable to multicomponent alloys

describable by either TB or MT Hamiltonians.

(6) It should incorporate various kinds of disorder, such as disorder in the diagonal as well as the off-diagonal elements of the alloy Hamiltonian in a TB description.

(7) It should yield DOS's which become exact as the cluster size increases.

(8) It should allow the calculation of one- and two-particle properties in essentially the same formalism.

(9) It should allow the incorporation of multisite correlation effects for random as well as nonrandom alloys. Thus, it should describe correctly the structure of the DOS's inside the band as well as yield the proper tailing of the DOS's at the edges of the band.

(10) It should give correctly as many moments of the DOS's as possible, since the moments of the DOS's can be used<sup>8</sup> to obtain physical information such as interatomic interactions in the disordered material.

(11) It should be computationally feasible.

(12) It should be applicable to certain TB disordered systems that obey the Goldstone theorem, such as disordered Heisenberg ferromagnets and alloys characterized by both mass and force-constant disorder.<sup>9</sup>

Even though some success had been achieved<sup>9</sup> in limiting cases, no theory, single-site or multisite, has been developed that allows the treatment of Goldstone systems in general, in spite of attempts<sup>10-12</sup> in that direction. The

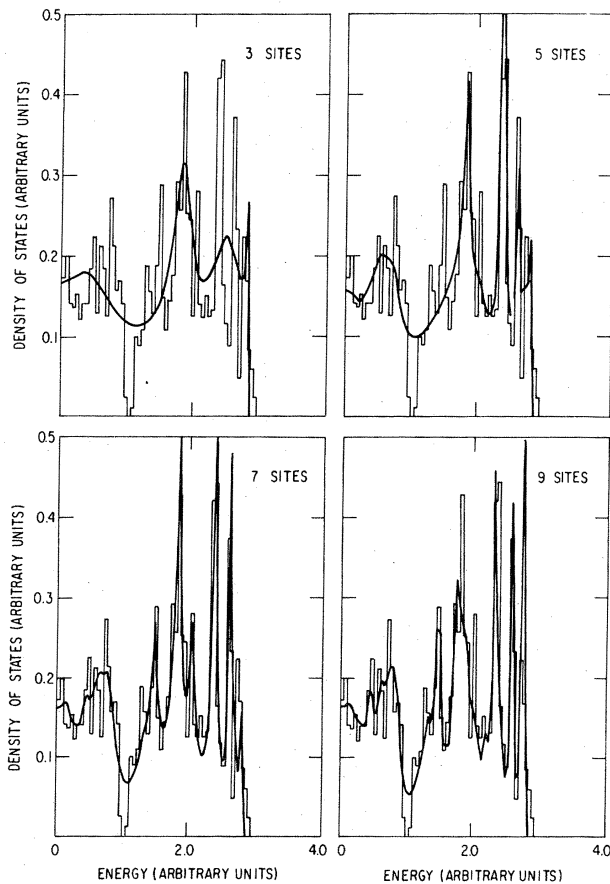


FIG. 2. Cluster DOS's associated with the centers of clusters of three, five, seven, and nine sites (solid curves) embedded in a CPA medium for a random alloy with  $\epsilon_A = -\epsilon_B = 1.0$ ,  $W = 1.0$ , and  $c = 0.5$ , compared with exact DOS histograms. Compare also with Fig. 1(a).

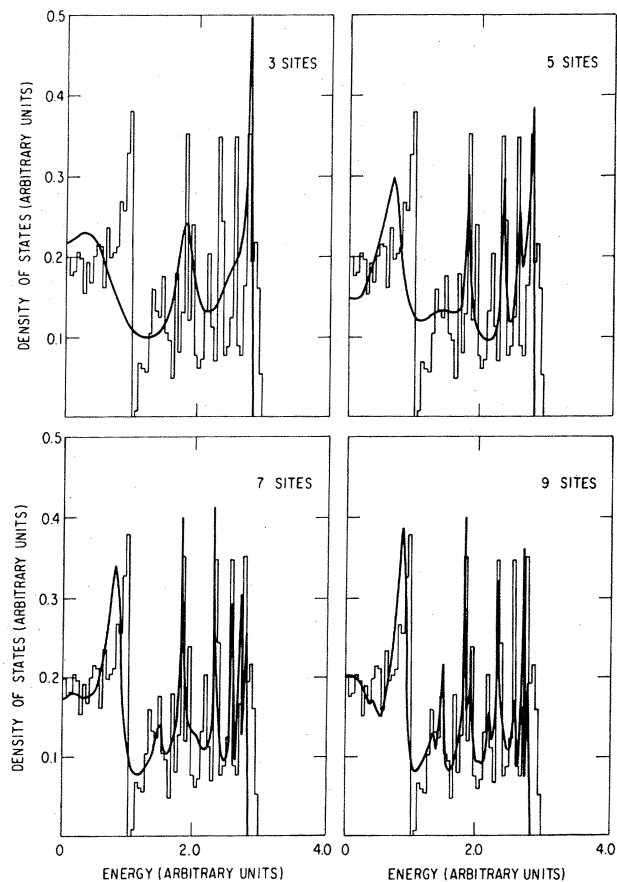


FIG. 3. Results analogous to those depicted in Fig. 2 and for the same energy parameters but for a nonrandom, weakly clustering alloy with  $SRO = 0.5$ . Compare also with Fig. 1(b).

other criteria are satisfied to various degrees by cluster theories<sup>13-31</sup> applied to electronic systems; many of these theories have been discussed in previous publications.<sup>13,14</sup> A discussion of some recent attempts at the construction of theories that could incorporate the effects of SRO and local environment fluctuations is given below.

It is convenient to classify cluster theories in terms of the medium in which the cluster is embedded. On that basis, one can distinguish at least three types of cluster theories: (1) self-consistent cluster theories in which statistical fluctuations within a cluster of atoms are incorporated into the theory in a self-consistent way; (2) non-self-consistent cluster theories in which the cluster is embedded in a medium determined in a non-self-consistent way; and (3) cluster theories in which a cluster is embedded in a medium that is determined in some self-consistent way and which includes the fluctuations of a cluster (usually a single-site) smaller than the embedded cluster.

The forerunner of the completely self-consistent cluster theories is the MCPA.<sup>7</sup> In the MCPA the disordered material is considered to be a collection of clusters (or molecules) chosen so that the entire lattice can be generated by the translation of the points in a cluster through a set of translation vectors. The cluster Green's function now becomes a matrix and the scalar CPA self-consistency con-

dition is generalized to a matrix self-consistency condition. The MCPA satisfies many of the criteria enumerated above, e.g., criteria 1, 2, 4-7, and the number of moments given correctly by the theory increases with increasing cluster size. However, the MCPA yields an effective medium that possesses cluster periodicity (superstructure) rather than point periodicity and thus violates the symmetry of the underlying lattice. In addition, the MCPA is very difficult to implement computationally, becoming impractical even for nearest-neighbor clusters in three-dimensional systems.

The self-consistent central site approximation<sup>7,15,16</sup> (SCCSA) was introduced in an attempt to overcome the difficulties of the MCPA mentioned above. In the SCCSA one retains only one of the MCPA self-consistency conditions. The effective medium is determined by requiring that the cluster-averaged Green's function associated with the central site of the cluster be equal to the site-diagonal element of the effective-medium Green's function. Thus the SCCSA preserves the translational periodicity of the lattice while being computationally much simpler than the MCPA. However, the SCCSA has been shown to yield<sup>17</sup> nonanalytic results, such as two-valued DOS's, and therefore is not a satisfactory theory of disordered system.

The self-consistent boundary site approximation<sup>18</sup>

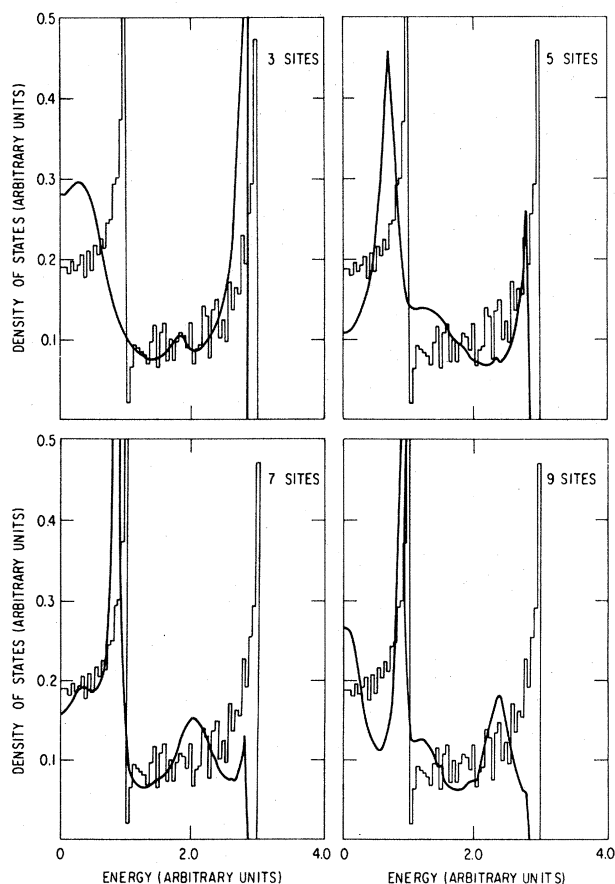


FIG. 4. Results analogous to those shown in Figs. 2 and 3 but for a strongly clustering alloy with  $SRO=0.9$ . Compare also with Fig. 1(c).

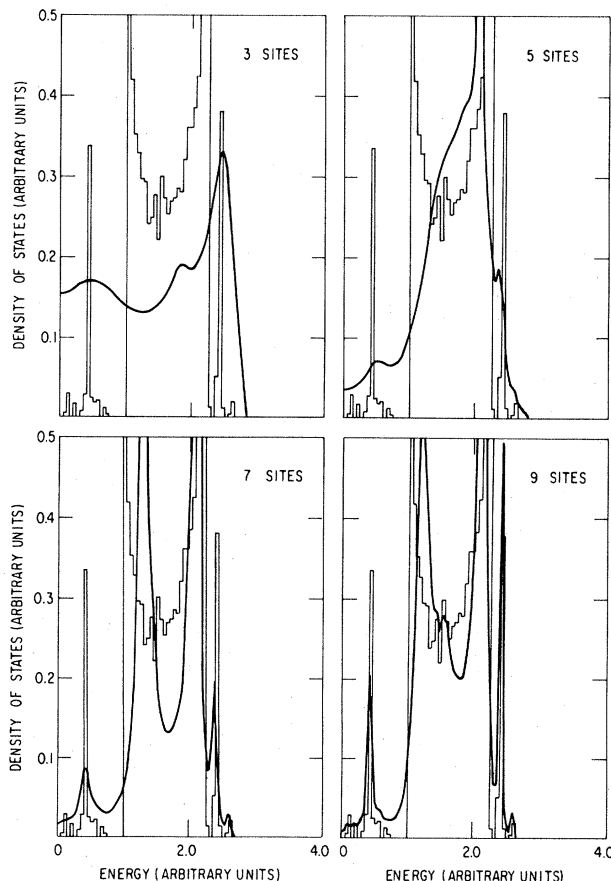


FIG. 5. Results analogous to those shown in Figs. 2-4 but for a strongly ordering alloy with  $SRO=-0.9$ . Compare also with Fig. 1(d).

(SCBSA) resembles the SCCSA in that it also involves a single self-consistency condition for the effective medium, but differs from the SCCSA by using a boundary site rather than the central site in that condition. It has been shown<sup>18</sup> that for a one-dimensional TB disordered system with nearest-neighbor hopping, the SCBSA yields DOS's that are identical to those obtained in the MCPA. Thus, in the case of such systems the SCBSA yields results with the correct analytic properties. Even though no general proof of analyticity of the SCBSA exists, published calculations,<sup>19</sup> as well as unpublished work,<sup>20</sup> indicate that the SCBSA may be analytic in general. One unsatisfactory aspect of the SCBSA is that the boundary of a given cluster is not uniquely defined for all clusters.

The augmented-space formalism<sup>21</sup> has been used in attempts<sup>11,12</sup> to incorporate the effects of SRO in a self-consistent theory. These methods yield analytic results but the results do not reflect the rich structure in the DOS of one-dimensional systems as accurately as those obtained in the SCBSA (or MCPA). The augmented-space formalism has also been criticized<sup>22</sup> for its inability to account for the fluctuations in compact clusters of atoms. Finally, the traveling-cluster approximation<sup>23</sup> (TCA) yields results that are in overall good agreement with

those obtained in computer simulations for three-dimensional random alloys. However, the TCA is an exceedingly difficult theory to apply computationally and apparently can not be used in connection with systems with SRO.

In a non-self-consistent cluster theory,<sup>24</sup> one calculates the Green's function for a cluster of atoms embedded in an effective medium that is chosen so as to satisfy several fundamental requirements. This approach has the advantage of being computationally very simple and yields results that are in good agreement with the computer-simulated DOS's of disordered systems. However, this method suffers from various drawbacks. Since the self-energy of the effective medium is not very strongly dependent on the alloy under investigation, the resulting DOS's may possess the incorrect structure especially near the edges of the band and extend into mathematically forbidden regions, i.e., where the DOS of the alloy is mathematically shown to vanish. As a result, fundamental sum rules on the DOS may be violated. Finally, non-self-consistent cluster theories yield nonunique results that depend on the choice of the effective medium.

In contrast to the methods just described, the embedded-cluster method<sup>13,25</sup> (ECM), representing the

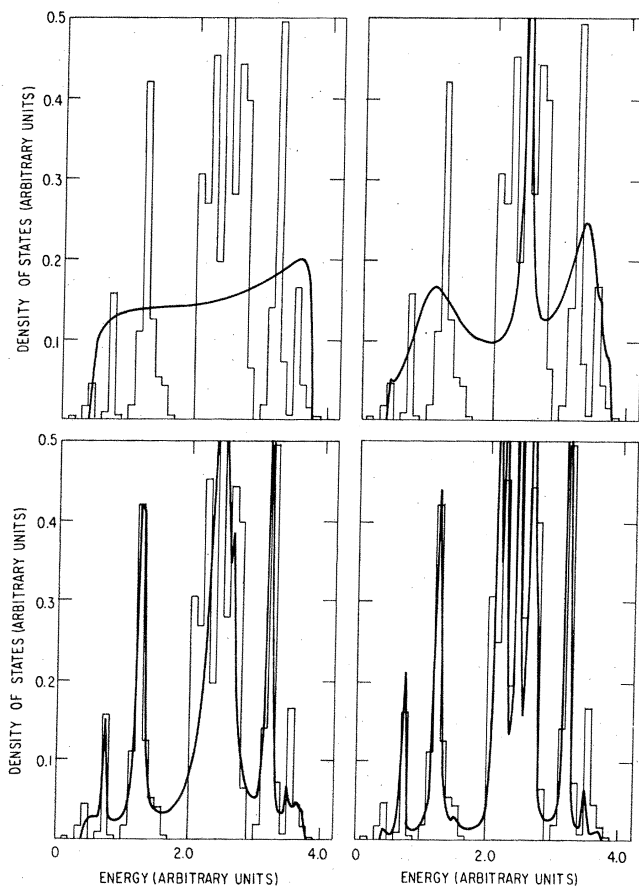


FIG. 6. Cluster DOS's in the CPA and associated with the centers of three-, five-, and seven-site clusters embedded in a CPA medium for a one-dimensional, random strong-scattering alloy with  $\epsilon_A = -\epsilon_B = 2.0$ ,  $W = 1.0$ , and  $c = 0.5$ , compared with exact DOS histograms.

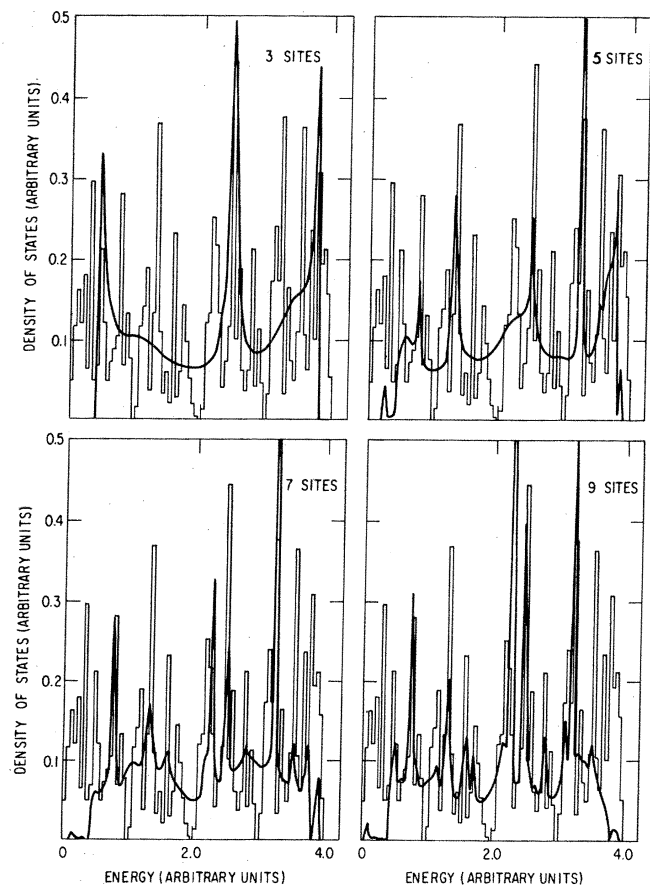


FIG. 7. Cluster DOS's associated with the centers of clusters of three, five, seven, and nine sites embedded in a CPA medium for an alloy with the same energy parameters as in Fig. 6 but with  $SRO = 0.5$ .

third class of cluster theories mentioned above, strikes a balance between analytic requirements and computational simplicity. Of all cluster theories proposed, it comes closest to possessing the desirable characteristics of an alloy theory. In the ECM, one calculates the Green's function for a cluster of atoms embedded in a self-consistently determined effective medium. The medium is chosen in some optimal way, and is usually<sup>13,25,26</sup> that determined in the single-site CPA. When the method is used in its full generality,<sup>13,25-27</sup> the structure of the medium surrounding the cluster is properly treated. In simplified versions,<sup>28</sup> the true lattice is replaced by a Bethe lattice (or Cayley-tree lattice) with the concomitant<sup>13</sup> possible loss of structure in the DOS, or the introduction of the wrong structure. Such a replacement is usually not necessary since for most systems the complete version of the theory is quite simple computationally, particularly with the use of modern day supercomputers.

The ECM has been shown<sup>13,25</sup> to yield analytic results and DOS's that are in excellent agreement with exact DOS obtained by eigenvalue counting methods<sup>29</sup> for a large variety of substitutionally disordered random alloys. As we show in the following sections, the ECM can also be used to obtain accurate DOS's for alloys with various degrees of SRO. Furthermore, it can be used in conjunction with a two-site generalization of the CPA that allows the self-consistent treatment of the two-particle distribu-

tion function. Some previous theories that have been proposed<sup>30,31</sup> for the treatment of SRO are based on the augmented-space formalism,<sup>30</sup> and thus suffer from the shortcomings of that approach. In a recent attempt,<sup>31</sup> SRO is treated in a fashion that requires an educated guess of the effective medium associated with a fully ordered structure, and the results are nonunique, depending on the choice of that medium. In the approach taken here, arbitrary SRO can be taken into account without prior knowledge of the nature of the ordered medium. This is an advantage, since most often it is not clear what that medium ought to be. Also, it will be shown that SRO can be incorporated into the theory in a self-consistent manner with only a slight increase in computational effort. In fact, our numerical investigations reveal that the effective medium plays a vital role in determining the DOS of disordered alloys, and in many cases the self-consistent incorporation of SRO is necessary for obtaining accurate results.

In the following sections we develop methods for calculating the cluster average of the site-diagonal element of the Green's function at the central site of the cluster, denoted by 0, and are given by the expression

$$n^J(\epsilon) = -\frac{1}{\pi} \text{Im} G_{00}^J(\epsilon), \quad (1.1)$$

where  $\epsilon$  is an energy parameter, and  $J$  denotes a cluster configuration. The total DOS's are obtained as an average over all cluster configurations of the partial DOS given by Eq. (1.1),

$$n(\epsilon) = \sum_J P_J n^J(\epsilon), \quad (1.2)$$

where  $P_J$  is the probability of the occurrence of configuration  $J$ . Clearly, any degree of SRO can be included in the average through the quantities  $P_J$ .

The remainder of the paper takes the following form. In Sec. II we derive briefly the equation determining the Green's function of a cluster embedded in an effective medium. In Secs. III and IV we discuss various methods for determining the effective medium in general as well as in some limiting cases. Numerical results obtained using the formalism of Secs. II-IV are presented in Sec. V. Sec. VI contains a discussion of our results and several conclusions that can be drawn from them.

## II. THE EMBEDDED CLUSTER METHOD

The formalism for calculating the Green's function for a cluster of atoms embedded in an effective medium has been presented in detail in previous publications, both for TB (Refs. 12, 14, and 25) and for MT (Refs. 26 and 27) Hamiltonians. For the sake of completeness, a brief outline of the method is given in this section for systems describable by TB Hamiltonians.

In a TB formalism, the Hamiltonian describing a substitutionally disordered alloy can be written in the form

$$H = \sum_i \epsilon_i a_i^\dagger a_i + \sum_{i,j} W_{ij} a_i^\dagger a_j, \quad (2.1)$$

where the  $a_i^\dagger$  ( $a_i$ ) create (destroy) an electron on site  $i$ . In

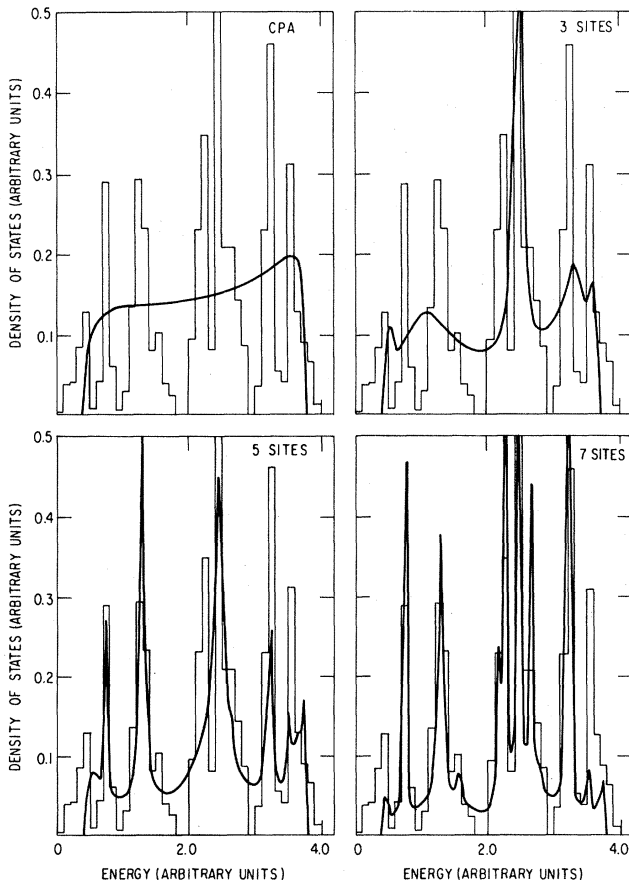


FIG. 8. Results analogous to those depicted in Fig. 6 but for weakly ordering alloys with  $SRO = -0.5$ .

a binary alloy,  $A_cB_{1-c}$ , atoms of species  $A$  and  $B$  are distributed with concentrations  $c$  and  $1-c$ , respectively, over the  $N$  sites of a lattice. The quantities  $\epsilon_i$  can in general depend on the chemical occupation as well as on the environment of sites  $i$ , but only the dependence on the atom on site  $i$  is usually considered. Thus, the  $\epsilon_i$  can assume the values  $\epsilon_A$  and  $\epsilon_B$ , with probabilities  $c$  and  $1-c$ , respectively. The variation of the  $\epsilon_i$  from site to site is known as diagonal disorder. The transfer terms  $W_{ij}$  describe electron hopping from site  $i$  to site  $j$ , and can depend on the chemical occupation as well as the environment of site  $i$  and  $j$ . Any dependence of the  $W_{ij}$  on the chemical configuration of an alloy is known as off-diagonal disorder (ODD). Even though the dependence of  $W_{ij}$  on the chemical occupation of sites  $i$  and  $j$  can be incorporated into the single-site CPA (Refs. 6 and 32) as well as into the ECM,<sup>14</sup> we will assume for simplicity that the  $W_{ij}$  depend only on the distance between sites  $i$  and  $j$ , and are independent of the chemical occupation of these sites. ODD can easily be incorporated into the formalism that follows through a generalization to matrices of the appropriate scalar quantities.

From the definition

$$G(z) = (z - H)^{-1} \quad (2.2)$$

for the Green's-function operator at (complex) energy  $z$ , it

follows that in a site or Wannier representation the matrix elements  $G_{ij}$  satisfy the equation of motion

$$G_{ij} = g_i \left[ \delta_{ij} + \sum_k W_{ik} G_{kj} \right]. \quad (2.3)$$

Here,  $g_i$  is the "bare" locator for site  $i$  and is defined by the expression

$$g_i = (z - \epsilon_i)^{-1}. \quad (2.4)$$

If the material is considered as a collection of nonoverlapping clusters  $C$ , the equation of motion, Eq. (2.3), can be cast into the form

$$G_{CC'} = g_C \left[ \delta_{CC'} + \sum_{C''} W_{CC''} G_{C''C'} \right]. \quad (2.5)$$

Here, the various cluster quantities are defined through their site matrix elements. We have

$$(G_{CC'})_{ij} = G_{ij}, \quad i \in C, \quad j \in C', \quad (2.6a)$$

$$(g_C^{-1})_{ij} = \begin{cases} z - \epsilon_i, & i = j \\ W_{ij}, & i \neq j \end{cases} \quad (2.6b)$$

and

$$(W_{CC'})_{ij} = W_{ij}, \quad i \in C, \quad j \in C'. \quad (2.6c)$$

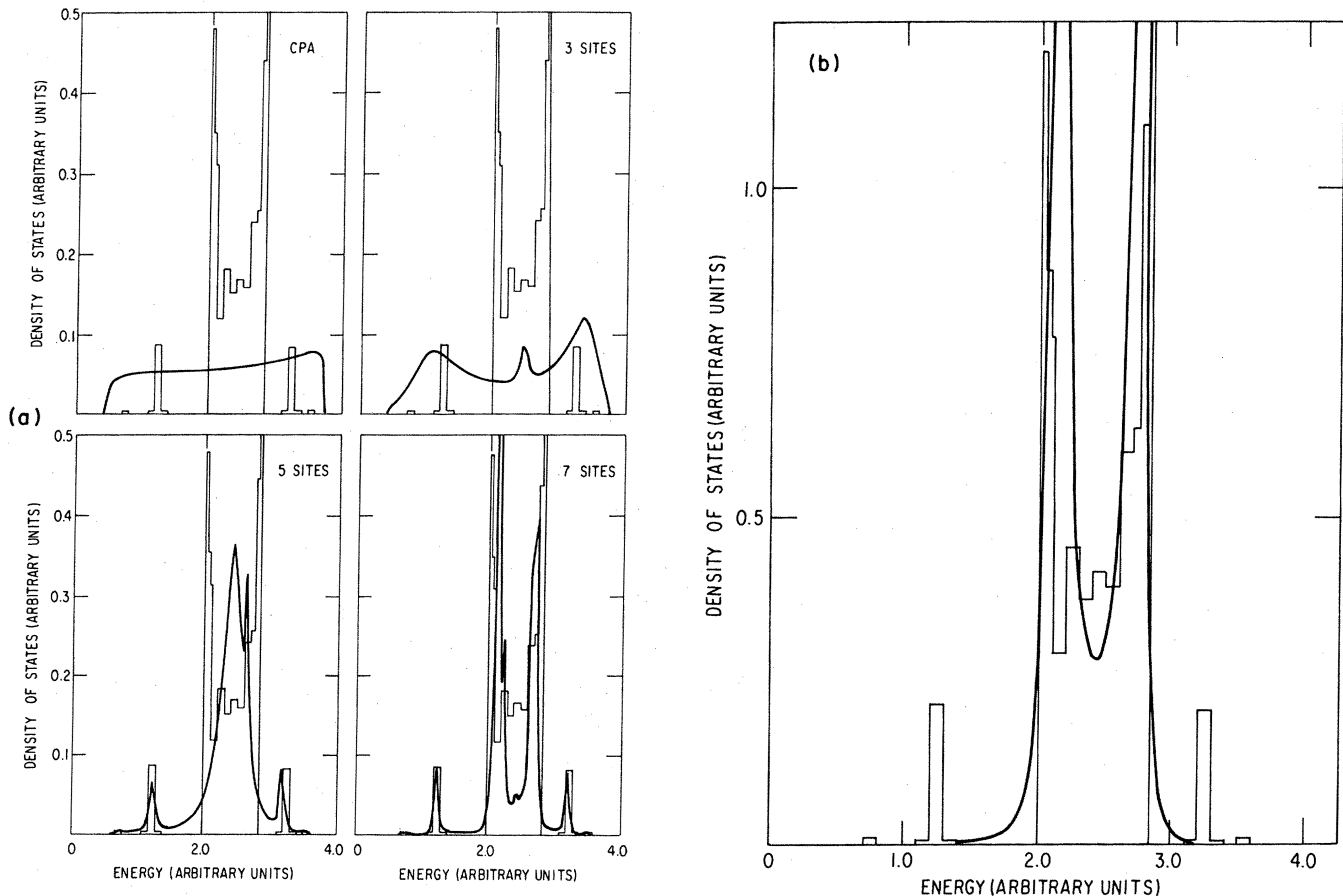


FIG. 9 (a) Results analogous to those depicted in Fig. 7 but for strongly ordering alloys with  $SRO = -0.9$ . (b) Cluster DOS's associated with the center of a single nine-site ordered cluster for the same energy parameter as those in Figs. 6-8 and for  $SRO = -0.9$ .

The cluster equation of motion, Eq. (2.5), can be iterated<sup>13</sup> with the second term on the right-hand side being treated formally as a perturbation. One then obtains the expression

$$G_{CC} = (z - H_C - \Delta_C)^{-1} \quad (2.7)$$

for the cluster-diagonal part of the Green's function. In this equation,  $z$  stands for  $zI$ , where  $I$  is the unit matrix in cluster space, and  $H_C$  is the intracluster Hamiltonian with matrix elements

$$(H_C)_{ij} = \begin{cases} \epsilon_i, & i=j \\ W_{ij}, & i \neq j \end{cases} \quad (2.8)$$

The cluster-renormalized interactor  $\Delta_C$  has site matrix elements given by the expression

$$(\Delta_C)_{ij} = \sum_{k \neq C} W_{ik} g_k W_{ij} + \sum_{\substack{k \neq C \\ l \neq C}} W_{ik} g_k W_{kl} g_l W_{lj} + \dots \quad (2.9)$$

It is clear from this expression that  $(\Delta_C)_{ij}$  represents the sum of all paths that start at site  $i$  and end at site  $j$  of the cluster  $C$  but avoid all sites in  $C$  at intermediate steps.

For substitutionally disordered alloys describable by the Hamiltonian (2.1),  $\Delta_C$  depends on the material surrounding the cluster  $C$  but is independent of the chemical configuration of the cluster. Let us then assume that the cluster is surrounded by an effective medium characterized by a self-energy  $\Sigma$  with matrix elements,

$$\Sigma_{ij} = \sigma \delta_{ij} + \bar{W}_{ij} (1 - \delta_{ij}) \quad (2.10)$$

For simplicity, we will assume<sup>13</sup> that  $\bar{W}_{ij} = W_{ij}$ . Then, the expression for the cluster-diagonal elements of the Green's-function operator corresponding to a cluster embedded in that medium can be written in the form

$$G_{CC} = (z - H_C - \bar{\Delta}_C)^{-1}, \quad (2.11)$$

where  $\bar{\Delta}_C$  is given by an expression analogous to Eq. (2.9) but with every  $g_i$  replaced by the effective-medium locator,

$$\bar{g} = (z - \sigma)^{-1} \quad (2.12)$$

The cluster-renormalized interactors  $\bar{\Delta}_C$  can now be obtained in terms of the self-energy  $\sigma$ . If every  $\epsilon_i$  in  $H_C$  is replaced with  $\sigma$ , Eq. (2.11) yields an expression for the cluster-diagonal part of the effective-medium Green's function,

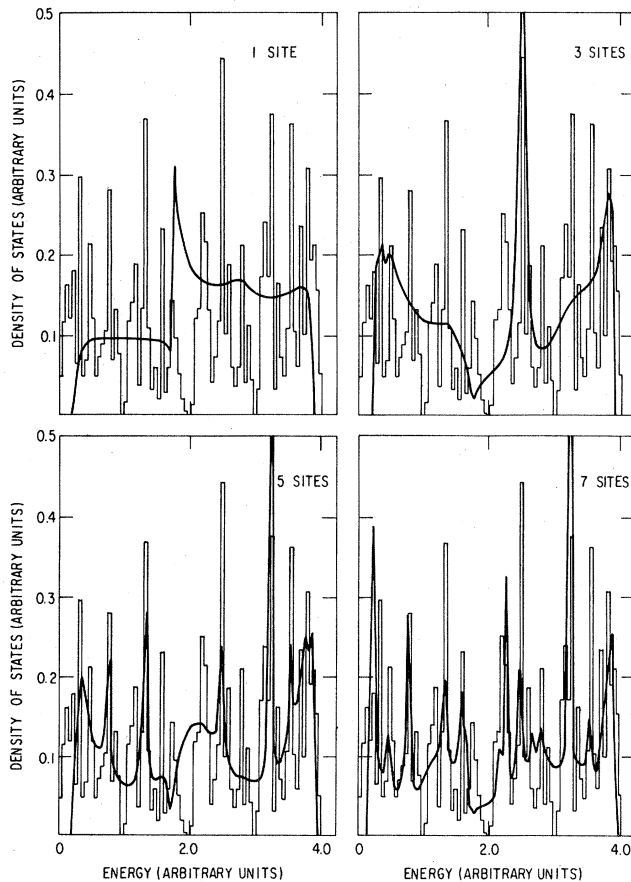


FIG. 10. Cluster DOS's associated with the centers of clusters of one, three, five, and seven sites embedded in a two-site SCBSA medium that incorporates SRO self-consistently. Here,  $\epsilon_A = -\epsilon_B = 2.0$ ,  $W = 1.0$ ,  $c = 0.5$ , and  $\text{SRO} = 0.5$ .

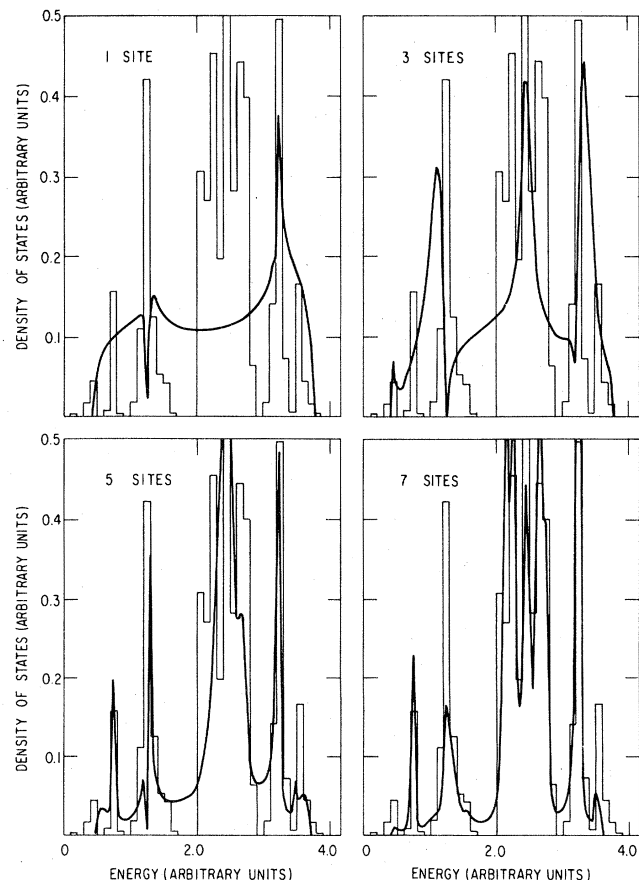


FIG. 11. Results analogous to those shown in Fig. 10 but with  $\text{SRO} = -0.5$ .

$$\bar{G}_{CC} = (z - \bar{H}_C - \bar{\Delta}_C)^{-1}, \quad (2.13)$$

with an obvious definition of  $\bar{H}_C$ . The effective-medium Green's function  $(\bar{G}_{CC})_{ij}$  can also be evaluated by Fourier transforming its equation of motion, e.g., Eq. (2.3) with every  $\epsilon_i$  replaced by  $\sigma$ . The matrix elements of  $\bar{G}_{CC}$  are then given by the expressions

$$\begin{aligned} (\bar{G}_{CC})_{ij} &= \bar{G}_{ij} \\ &= \frac{1}{\Omega_{BZ}} \int_{BZ} e^{i\vec{k} \cdot (\vec{R}_i - \vec{R}_j)} [z - \sigma - W(\vec{k})]^{-1} d\vec{k}, \end{aligned} \quad (2.14)$$

where the integration extends over the Brillouin zone (BZ) of the lattice,  $\Omega_{BZ}$  denotes the volume of the zone, and  $\vec{R}_i$  denotes the position of site  $i$  with respect to a fixed origin. The Fourier transformation of the transfer terms entering Eq. (2.14) is defined by the expression

$$W(\vec{k}) = N^{-1} \sum_{\{\vec{R}_i - \vec{R}_j\}} W_{ij} e^{i\vec{k} \cdot (\vec{R}_i - \vec{R}_j)}. \quad (2.15)$$

Equation (2.13) can now be used to obtain an expression for the renormalized interactor of the effective medium

$$\bar{\Delta}_C = z - \bar{H}_C - \bar{G}_{CC}^{-1}. \quad (2.16)$$

With the elements of  $\bar{G}_{CC}$  determined as in Eq. (2.14), one can evaluate  $G_{CC}$ , the Green's function for a cluster embedded in an effective medium.

A convenient choice for the effective medium is that which is determined in the single-site CPA. The self-consistency condition determining the CPA effective medium can be stated in terms of the Green's function in the form

$$\langle G_{00} \rangle = \bar{G}_{00}. \quad (2.17)$$

Here,  $G_{00}$  is the site-diagonal element of the Green's function corresponding to a single site embedded in an effective medium, and  $\bar{G}_{00}$  is the corresponding quantity for that medium.

In the original applications<sup>13,25</sup> of the ECM, the effective medium was chosen to be that determined in the CPA. This choice was also made in much of the numerical work presented in Sec. V. However, for certain non-random alloys it was found that the CPA did not provide an adequate embedding medium and a different choice of the medium had to be made. A method which yields an effective medium that incorporates the pair correlation function, and thus the effects of SRO, in a self-consistent way is discussed in the following section.

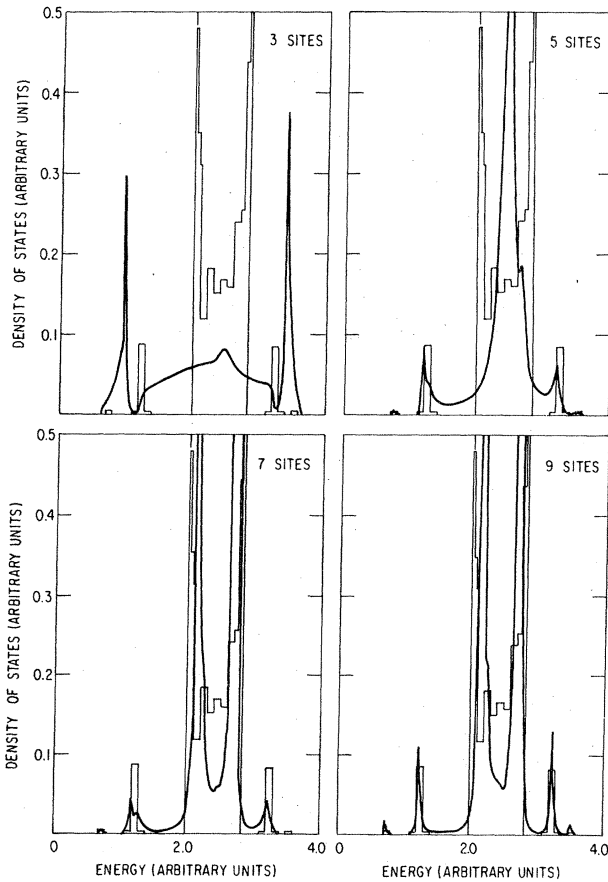


FIG. 12. Cluster DOS's associated with the centers of clusters of three, five, seven, and nine sites embedded in a two-site SCBSA medium for an alloy with the same energy parameters as those in Figs. 10 and 11, and with  $SRO = -0.9$ .

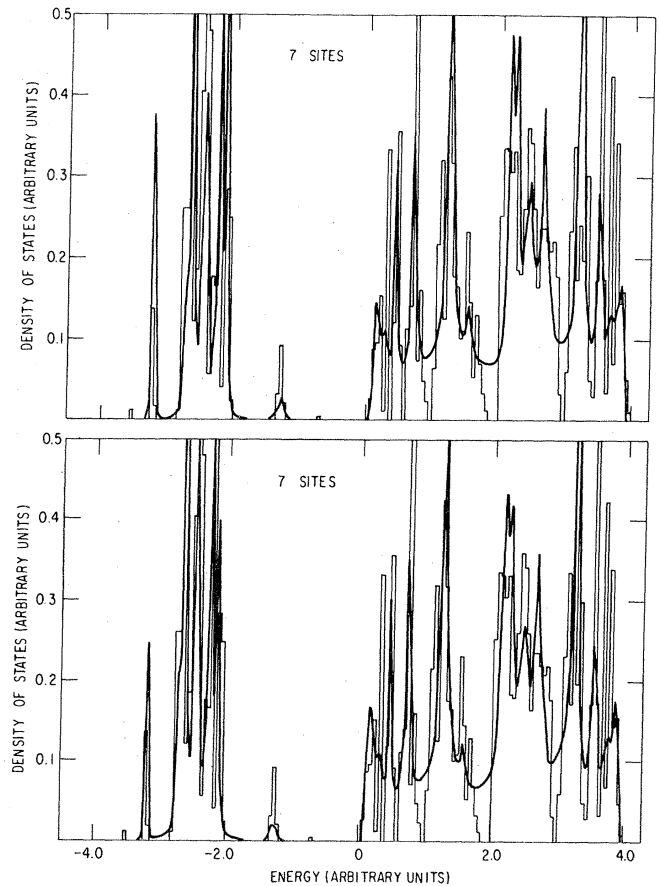


FIG. 13. Cluster DOS's associated with the centers of seven-site clusters embedded in a CPA medium (top part) and in a two-site SCBSA medium (bottom part) for an alloy with  $\epsilon_A = -\epsilon_B = 2.0$ ,  $W = 1.0$ ,  $c = 0.7$ , and  $SRO = -0.4$ .



### III. TWO-SITE GENERALIZATION OF THE CPA

As was mentioned in the last paragraph, it is often necessary to consider the cluster as embedded in a medium that includes any possible SRO in a self-consistent way. Clearly, any theory that accomplishes this task can also be used for random alloys, although for such alloys the CPA usually provides a satisfactory embedding medium. A comparison between the cluster DOS's for random alloys obtained with a CPA embedding medium and with a medium analogous to that proposed below has been given elsewhere.<sup>14</sup>

The pair correlation function can be incorporated self-consistently into the SCBSA applied to a two-atom cluster. The self-consistency condition determining the effective medium takes the form

$$\langle (G_C)_{00} \rangle_C = \bar{G}_{00}, \quad (3.1)$$

where  $G_{00}$  is the site-diagonal element of the Green's function for one of the two sites in the cluster, and  $\langle \dots \rangle_C$  denotes an average over all cluster configurations. Note that Eq. (3.1) represents a very different condition from the CPA condition (2.17). Explicitly  $G_C$  is given as the  $2 \times 2$  matrix [see Eq. (2.11)]

$$G_C = \left[ \begin{array}{cc} z - \epsilon_0 & -W \\ -W & z - \epsilon_1 \end{array} \right] - \left[ \begin{array}{cc} \bar{\Delta}_{00} & \bar{\Delta}_{01} \\ \bar{\Delta}_{10} & \bar{\Delta}_{11} \end{array} \right]^{-1}, \quad (3.2)$$

where by symmetry  $\bar{\Delta}_{00} = \bar{\Delta}_{11}$  and  $\bar{\Delta}_{01} = \bar{\Delta}_{10}$ . The quantities  $\Delta_{ij}$  appearing in Eq. (3.2) are given by Eq. (2.16) and the self-energy  $\sigma$  is determined through the single self-consistency condition, Eq. (3.1). Thus, a two-site SCBSA yields an effective medium which preserves the translational invariance of the lattice.

### IV. TWO-SUBLATTICE MODEL

Although not true in general, some disordered systems with strong ordering tendencies can be viewed as disordered states of a nearly ordered system. As a concrete example, consider a one-dimensional binary alloy,  $A_{0.5}B_{0.5}$ , in which atoms of type  $A$  have a strong preference to being surrounded by atoms of type  $B$ , and vice versa. Such a system may then be considered to result upon slightly disordering a perfectly ordered system of the type  $ABABAB \dots$ . Thus, one may describe the disordered system as consisting of two interpenetrating sublattices, each characterized by individual  $A$  and  $B$  atom concentrations. Since an  $A$  atom in sublattice 1, say, is nearly always surrounded by atoms of type  $B$  one could approximate  $C_1^A$ , the  $A$  atom concentration in sublattice 1, by  $P_{AB}$  the probability of finding an  $A$  atom next to a  $B$  atom in the disordered material. Then, the concentration of  $B$  atoms in sublattice 1,  $C_1^B$ , is given by the relation  $C_1^B = 1 - C_1^A$ . Similar considerations hold for sublattice  $B$  with the roles of  $A$  and  $B$  interchanged.

In the two-sublattice model, the disordered material is considered as an alloy in which the concentration varies periodically through the material in some particular direction. Thus, in the limiting case of very strong SRO, a disordered material may be treated as a compositionally modulated alloy (CMA). The extension of the CPA to CMA (MODCPA) has been described fully elsewhere,<sup>33</sup> where it was shown that the MODCPA, essentially a single-site theory, gives an accurate representation of the DOS's of strongly modulated alloys. In fact, the accuracy of the MODCPA increases with increasing modulation strength and in the limit of an ordered system the MODCPA becomes exact. The formalism for extending the CPA to a two-sublattice model is practically identical

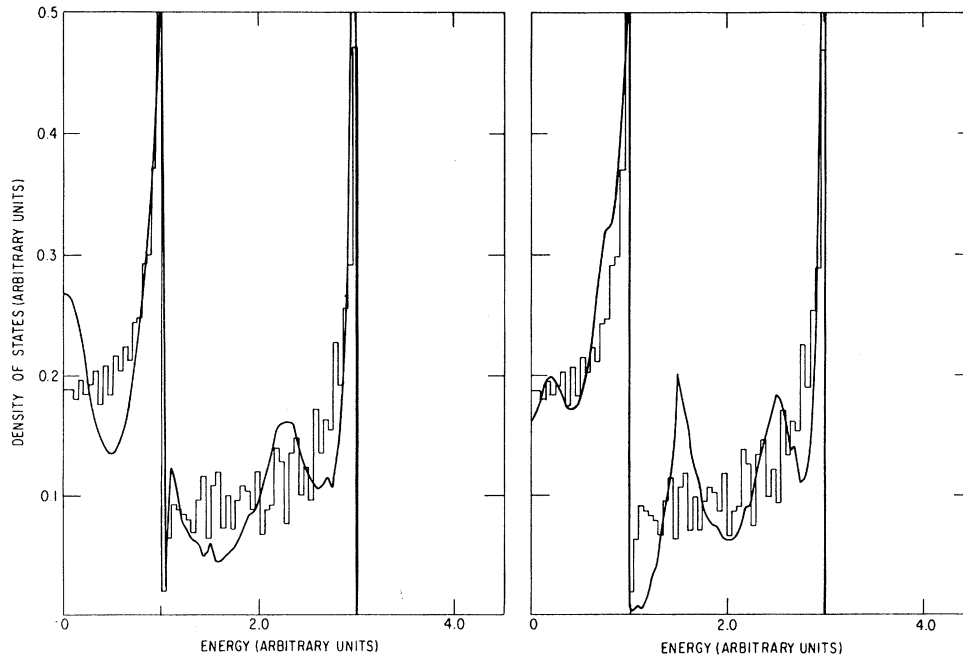


FIG. 14. Cluster DOS's associated with the centers of clusters of nine and eleven sites embedded in a two-site SCBSA medium for an alloy with  $\epsilon_A = -\epsilon_B = 1.0$ ,  $W = 1.0$ ,  $c = 0.5$ , and  $SRO = 0.9$ . Compare with Fig. 4.

to that of the MODCPA (Ref. 33) and will not be presented here.

The advantage of using the MODCPA lies in the fact that it may be possible to obtain a fairly accurate representation of the DOS's of strongly ordering systems by means of a single-site theory. Numerical results, presented in the following section, confirm this conjecture. Clearly, it is always possible to calculate the DOS's for clusters embedded in a MODCPA medium and this approach has been shown<sup>33</sup> to improve on the MODCPA and to yield quite accurate results for weakly to moderately strongly modulated alloys. For strongly modulated alloys, on the other hand, not much improvement of the MODCPA results upon the use of a cluster theory. Thus, by appropriately choosing the effective medium, one can indeed reduce the size of the cluster that is necessary for a faithful representation of the DOS's of nonrandom substitutionally disordered alloys.

## V. NUMERICAL RESULTS

We have carried out extensive numerical calculations based on the formal considerations presented in Secs. II–IV. Our aim is to investigate the following three questions with respect to calculating DOS's for nonrandom substitutionally disordered alloys: (i) Is the ECM able to reproduce the DOS's of nonrandom alloys? (ii) How large a cluster is needed for an accurate representation? (iii)

How important is the effective medium in which the clusters are embedded in determining accurate DOS's for nonrandom alloys?

Our calculations were carried out for a one-dimensional single-band model substitutional alloy describable by a TB Hamiltonian of the type displayed in Eq. (2.1). Alloys of two different scattering strengths, and of various degrees of SRO, were investigated. The scattering strength  $\delta$  is defined by the expression

$$\delta = |\epsilon_A - \epsilon_B| / w, \quad (5.1)$$

where  $\epsilon_A$  and  $\epsilon_B$  are the site energies of the  $A$  and  $B$  atoms, respectively, and  $w$  is  $\frac{1}{2}$  the bandwidth of either species, taken as equal to 2 in all cases. For  $\epsilon_A = -\epsilon_B = 1.0$ ,  $\delta = 1.0$ , corresponding to an intermediate scattering strength, non-split-band case, and for  $\epsilon_A = -\epsilon_B = 2.0$ ,  $\delta = 2.0$ , corresponding to a strong scattering, split-band regime. Short-range order (clustering or ordering) was incorporated into the theory by means of the pair distribution functions  $P_{\mu\nu}$ , where  $\mu, \nu$  designate any of the species  $A$  or  $B$ . In particular, we chose the model

$$P_{\mu\mu} = C_\mu + \alpha(1 - C_\mu), \quad \text{with } \mu = A \text{ or } B. \quad (5.2)$$

Clearly,  $\alpha > 0$  ( $\alpha < 0$ ) indicates clustering (ordering), and  $\alpha = 0$  denotes a random alloy. In the following figures, the values displayed for the SRO parameters are the values of  $\alpha$  in Eq. (5.2).

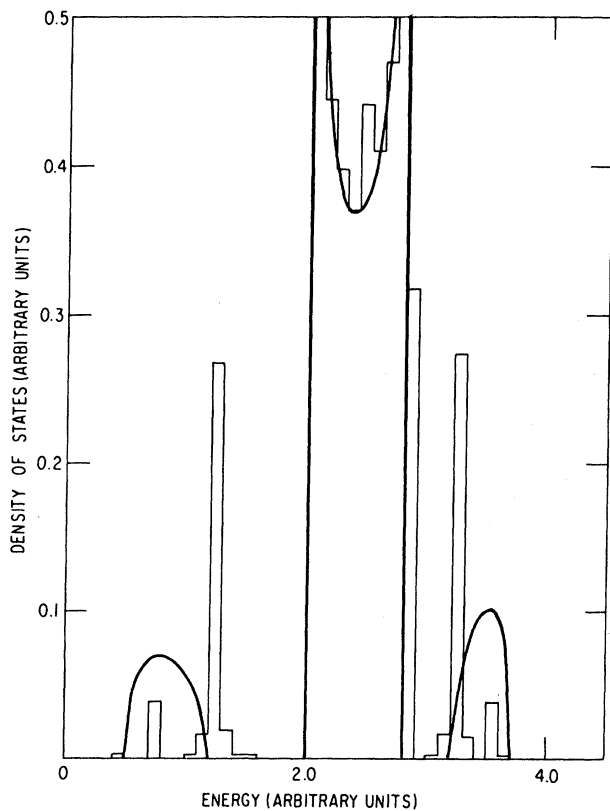


FIG. 15. Single-site DOS's (solid curve) calculated in the two-sublattice model described in the text for an alloy with  $\epsilon_A = -\epsilon_B = 2.0$ ,  $W = 1.0$ ,  $c = 0.5$ , and  $\text{SRO} = 0.85$ , compared with an exact DOS histogram.

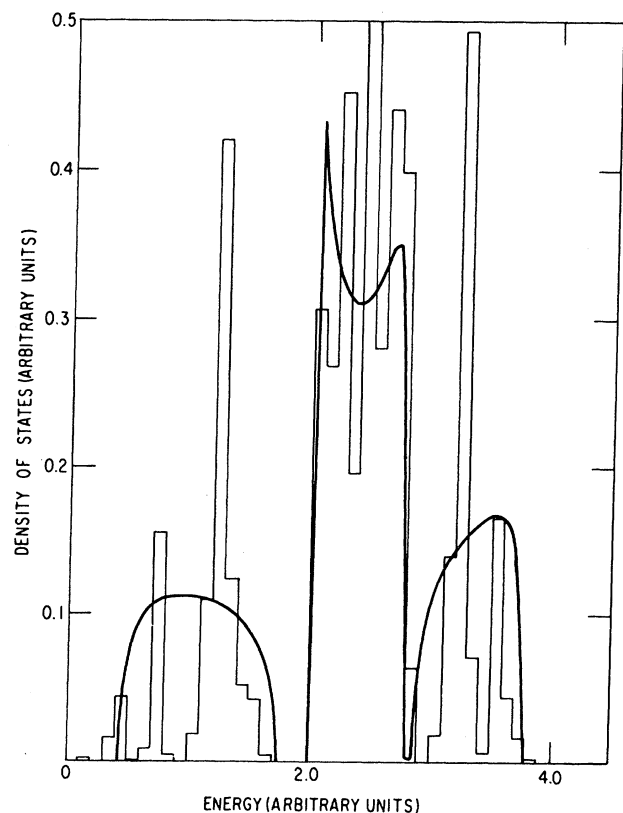


FIG. 16. Results analogous to those shown in Fig. 15 but for a weakly ordering alloy with  $\text{SRO} = -0.5$ .

In order to follow the discussion in the text, we divide our presentation of the numerical results of the ECM according to the medium chosen to embed the cluster. Thus, Figs. 1–9 depict results obtained with clusters embedded in a medium determined in the CPA. Figures 10–14 show DOS's obtained with clusters embedded in a two-site SCBSA medium, and compare some of these results with corresponding results obtained with a single-site CPA medium. Densities of states obtained in a two-sublattice model are presented in Figs. 15–17. Figures 18 and 19 show comparisons between exact moments of the DOS's for various nonrandom alloys with the moments obtained in the embedded-cluster method. Unless otherwise stated, the DOS's associated with the center of a cluster were used averaged over all cluster configurations.

#### A. Clusters embedded in a CPA medium

Figure 1 shows exact DOS histograms for alloys with energy parameters  $\epsilon_A = -\epsilon_B = 1.0$ ,  $W = 1.0$  ( $\delta = 1.0$ ), concentration  $c = 0.5$ , and with various degrees of SRO. The CPA DOS's for the random alloy are also shown. It is clear from these figures that clustering [parts 1(b) and 1(c)] and ordering [part 1(d)] tendencies can strongly affect the DOS. It is to be kept in mind that in all figures corresponding to alloys with  $c = 0.5$ , the bands are symmetric about  $\epsilon = 0.0$ . We see then that increasing clustering causes the weight of the DOS's to shift toward the edges of the subbands associated with the alloy constituents. This effect can be understood intuitively as follows. In strongly clustering alloys, the greatest contribution to the DOS's arises from large clusters of atoms of a given

kind and thus resembles the DOS's of the corresponding pure materials. Similar arguments yield an insight into the shape of the DOS's of strongly ordering alloys. Thus, for strongly clustering alloys the DOS is very nearly equal to the average of the DOS of the two pure systems *A* and *B*. On the other hand, ordering causes the DOS to concentrate near the centers of the subbands and produces a split-band effect. It is also clear from these figures that the CPA expectedly gives an increasingly poorer representation of the DOS with increasing clustering or ordering. Note in particular that the width of the CPA DOS is about equal to that of the exact DOS for the case of a random alloy, but it is narrower than the exact results for clustering alloys and wider for ordering alloys.

Figure 2 shows cluster DOS's for the case of a random alloy associated with the centers of three-, five-, seven-, and nine-site clusters embedded in a CPA medium. These figures show the increased accuracy that is obtained with increasing cluster size. The DOS's obtained with a seven- and a nine-site cluster represent the exact DOS's quite faithfully, resolving all major peaks and even some minor ones. As has been pointed out in previous publications,<sup>13,25</sup> the structure in the DOS is associated with specific configurations of compact clusters of atoms. This point is discussed further below.

Figure 3 shows results analogous to those of Fig. 2, but for alloys of intermediate clustering strength. It is again seen that cluster DOS's represent the exact numerical results quite accurately within the band. However, the edges of the band are represented somewhat less accurately. This is because the CPA effective medium produces a band which is much narrower than that of a clustering alloy, and the cluster DOS's vanish in the region in which

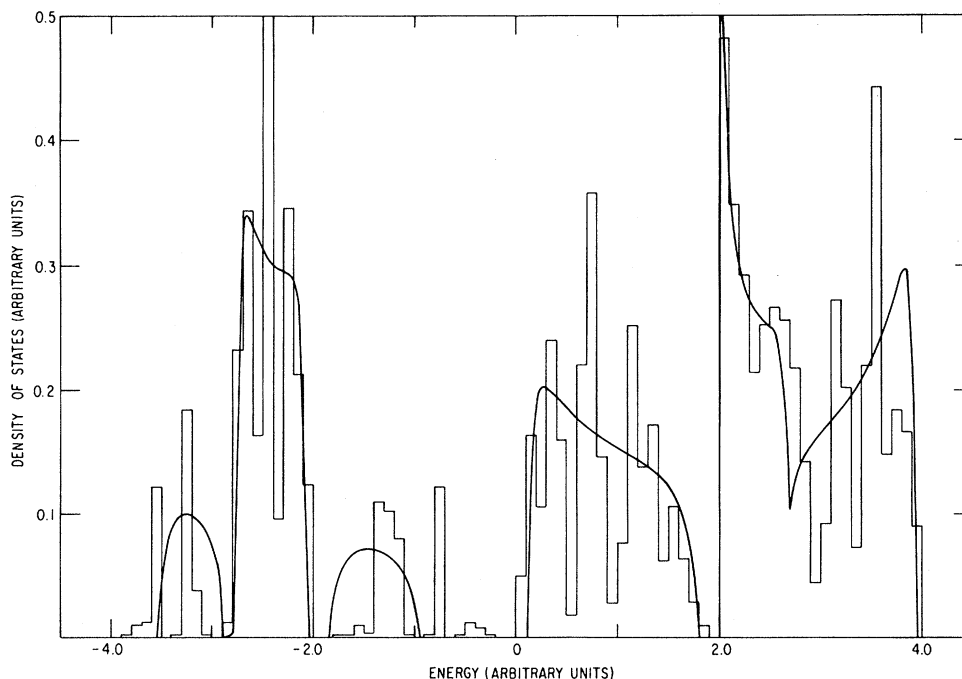


FIG. 17. Single-site DOS's calculated in the MODCPA for a modulated alloy with  $\epsilon_A = -\epsilon_B = 2.0$ ,  $W = 1.0$ ,  $C_{A1} = 0.9$ , and  $C_{A2} = 0.5$ , compared with an exact DOS histogram.

the CPA DOS's vanish. This effect is seen more dramatically in Fig. 4, which depicts the results for a strongly clustering alloy. The cluster DOS's give an adequate representation of the exact DOS inside the band, but a very poor representation near the edges especially with increasing cluster size. Note that the cluster DOS's would correctly tend to move toward the edges of the subbands with increasing cluster size, but in the outermost of these regions the CPA DOS's vanish. We will see later that this deficiency is remedied with the introduction of a two-site self-consistent cluster theory.

Densities of states for strongly ordering alloys are shown in Fig. 5. This figure shows results analogous to those in Figs. 2–4, and it is seen that a nine-site cluster gives an excellent representation of the main part of the DOS's and even resolves the minor peaks on the sides of the central peak. Recall from Fig. 1(d) that the CPA bandwidth is larger than that of the ordered alloy and thus the CPA effective medium can support the structure induced by intracluster fluctuations.

Figures 6–9 depict exact and cluster DOS's for strong-scattering split-band alloys,  $\delta=2.0$ , with concentration  $c=0.5$  and various degrees of SRO. Figure 6 shows DOS's for a random alloy. It is seen that the seven- and nine-site cluster DOS's agree quite well with the exact results inside the band, with the greatest differences between exact and calculated results occurring near the edges of the band. Analogous results are obtained for clustering alloys in Fig. 7. As was the case for clustering, weak-scattering ( $\delta=1$ ) alloys, the edges of the bands are represented poorly by cluster DOS's, especially for large clusters.

Figure 8 represents results analogous to those of Fig. 6, but for ordering alloys. In this case, the CPA provides an adequate medium in which a cluster can be embedded, and cluster DOS's give a very accurate representation of the exact DOS. This is also found to be the case for strongly ordering alloys, Fig. 9(a). Note in particular that the main contribution to the DOS's arises from the single-ordered configuration,  $ABABAB\dots$ , as is shown in Fig. 9(b). Here, the solid curve represents the DOS at the center of a nine-site cluster in the ordered configuration.

#### B. Clusters embedded in a two-site SCBSA medium

Figure 10 depicts cluster DOS's for clustering alloys associated with clusters embedded in a two-site SCBSA medium as described in Sec. III. Short-range order is incorporated into the theory in a self-consistent way through the use of the appropriate two-site distribution functions,  $P_{AA}$ ,  $P_{BB}$ , and  $P_{AB}$ , in the cluster average in Eq. (3.1). It is seen in this figure that the cluster DOS's especially those for the seven-site cluster, give a faithful representation of the exact DOS's inside the band, and even represent the structure near the edges of the band quite accurately. Thus, the self-consistent treatment of SRO yields a more appropriate embedding medium than that obtained with the CPA. Note in particular that the DOS's for a single site embedded in a SCBSA medium are almost as wide as the exact results. The gains resulting from a self-consistent treatment of SRO are evident upon comparison of the cluster DOS's for five- and seven-site clus-

ters shown here with the corresponding clusters embedded in the CPA medium (Fig. 7).

Results analogous to those shown in Fig. 10 (but for ordering alloys) are shown in Fig. 11. Comparing them with Fig. 8, which shows analogous results for clusters embedded in a CPA medium, we observe that (i) small size cluster, one and three sites, embedded in a two-site SCBSA medium for relatively weakly ordering alloys, yield a somewhat more accurate representation of the DOS's than corresponding clusters embedded in a CPA medium for random alloys, and (ii) for larger clusters, five and seven sites, the cluster DOS's for clusters embedded in an SCBSA medium are quite similar to those obtained in a CPA embedding medium. Thus, the embedding medium becomes less and less important with increasing cluster size, provided that it is an appropriate medium, i.e., its bandwidth is sufficiently large to support the structure in the DOS's produced by local environment fluctuations. Equivalently, the more appropriate the embedding medium the smaller may be the size of the cluster required to produce an adequate representation of the DOS's. Results analogous to those in Fig. 11 (but for strongly ordering alloys) are depicted in Fig. 12, which should be compared with Fig. 9(a).

It should be noted that the DOS's associated with a single-site or a three-site cluster embedded in a two-site SCBSA medium (Fig. 11) can possess very sharp structure. This structure is not an indication of nonanalytic behavior since the SCBSA for one-dimensional TB alloys with nearest-neighbor hopping yields DOS's identical to those of the MCPA which is known to yield analytic results. Figure 11 shows that clusters larger than a single site are indeed necessary for an accurate representation of the DOS's.

The discussion just given is further illustrated by the results shown in Fig. 13. Here, the energy parameters of the alloy are the same as those in Figs. 6–12, but with concentration  $c=0.7$  and  $\alpha=0.4$  (weak ordering). For this case both the CPA and the SCBSA provide appropriate effective media. Thus, the cluster DOS's for a seven-site cluster embedded in a CPA medium (top part) are very similar to those obtained with an SCBSA medium (bottom part).

Further comparison between the results obtained with CPA and SCBSA embedding media is afforded by Fig. 14. Here, the curves represent cluster DOS's for 9- and 11-site clusters, left- and right-hand side panels, respectively, embedded in a 2-site SCBSA medium for the same alloy parameters as those in Fig. 4. Comparing the results for the nine-site clusters we see that the DOS's in the interior of the band are similar in the two methods, but that the clusters embedded in an SCBSA medium are in excellent agreement with the exact DOS's near the band edges in contrast to the results obtained with a CPA medium. Thus, we see once again that for band regions that are within the span of the effective medium either a CPA or a two-site SCBSA medium can be used in conjunction with the embedded-cluster method. However, the SCBSA provides an embedding medium that is appropriate for a wider range of alloy parameters than that obtained in the CPA.

### C. Two-sublattice model calculations

Figure 15 shows DOS's for an alloy with the same energy parameters as those in Figs. 6–12, with concentration  $c=0.5$  and  $\alpha=-0.85$  (strong clustering). The curve is calculated in the two-sublattice model introduced in Sec. IV. It is seen that even a single-site theory can produce an adequate representation of the DOS's for an appropriately chosen effective medium. Comparison with the very similar case shown in Figs. 9 and 12 shows that the single-site results provide a better representation of the DOS's in the interior of the band than the ECM, but represent the minority peaks less accurately. Thus, as was mentioned in the previous subsection, with an appropriate embedding medium a small cluster, even as small as a single site, may yield DOS's in satisfactory agreement with exact results. Figure 16 shows results analogous to those of Fig. 15 but for a somewhat smaller ordering parameter.

Finally, Fig. 17 shows the DOS's for a two-site modulated alloy. Here,  $C_{A1}=0.9$  and  $C_{A2}=0.5$  are the  $A$ -atom concentrations in the two sublattices and  $C_{BI}=1-C_{AI}$ ,  $I=1,2$ . The results obtained in the MODCPA (Ref. 33) (solid curve) for a two-site modulated alloy are in good overall agreement with the exact results.

### D. Moments of the DOS's

The  $n$ th moment  $\mu_n$  of the DOS's with respect to some energy origin  $\epsilon_0$  is defined by the expression

$$\mu_n = \int (\epsilon - \epsilon_0)^n g(\epsilon) d\epsilon. \quad (5.3)$$

Clearly, the zeroth moment equals the charge and the first moment yields the band energy of a system. More generally, moments can be used<sup>8</sup> to obtain information about the interatomic potentials in substitutionally disordered alloys. Also, comparisons between exact and calculated moments may be used as a gauge of the accuracy of various approximations for calculating the DOS's in disordered systems. Thus, it has been shown<sup>34</sup> that the CPA gives correctly the first eight moments of the DOS's of random substitutionally disordered alloys.

Figure 18 shows moments of cluster DOS's for various size clusters and various SRO parameters compared with numerically computed moments. Here, the decimal numbers denote the value of the SRO parameter  $\alpha$  in Eq. (5.2), and the numbers in parentheses indicate the numbers of sites in the clusters used in the calculations. The CPA moments fit the first eight exact moments of the DOS's for a random alloy as expected. Although not shown in the figure, more moments of a random alloy can be fit by using DOS's associated with clusters embedded in a CPA medium. For ordering alloys (cf. the two lower curves in Fig. 18), a large number of moments can be fit, up to 20 for strong-ordering alloys, by using DOS's for clusters embedded in a CPA medium. For clustering alloys (cf. the upper two curves), it was necessary to use a two-site SCBSA embedding medium with SRO self-consistently taken into account to obtain the fits shown. This is in accord with our discussion of the cluster DOS's for clustering alloys given above. Figure 19 shows the gradual ap-

proach of the calculated to the exact moments with increasing cluster size for the case of strongly ordering alloys.

## VI. DISCUSSION AND CONCLUSIONS

Our aim in this paper was to investigate the applicability of the embedded-cluster method to calculate the single-particle Green's function, in particular the DOS's, of nonrandom disordered alloys. Our numerical results allow us to reach several conclusions.

(1) The ECM provides a reliable and efficient method for calculating the DOS's in nonrandom as well as random alloys.

(2) The accuracy of the CM increases with increasing cluster size provided that an appropriate embedding medium is used in the calculation. Such a medium becomes less important as the size of the cluster increases.

(3) The embedding medium can play a vital role in the accuracy of the calculated results. For a well-chosen embedding medium a small cluster, even a single-site cluster, can yield an adequate representation of the DOS's of a substitutionally disordered alloy, as is indicated by the results obtained in the two-sublattice model and in the MODCPA.

(4) In many cases, such as for one-dimensional alloys

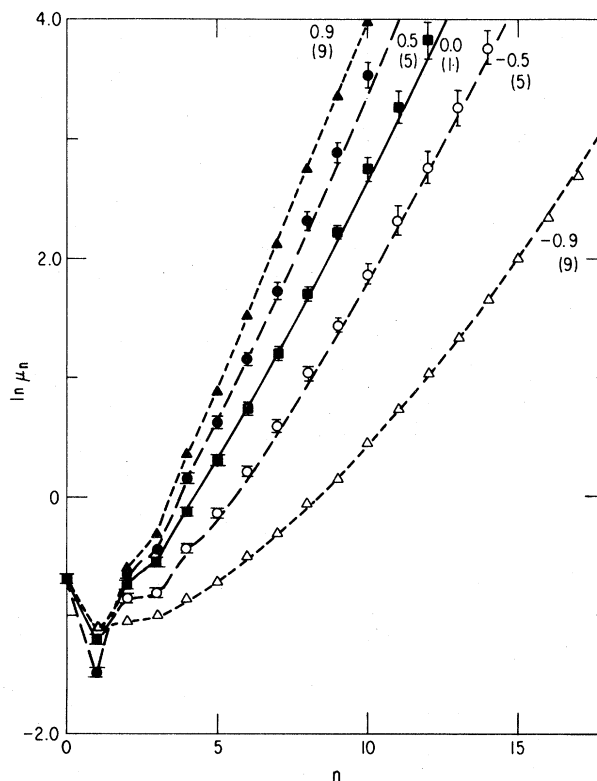


FIG. 18. Logarithms of the moments of the cluster DOS's about  $\epsilon_0=1.0$  for alloys with  $\epsilon_A=-\epsilon_B=1.0$ ,  $W=1.0$ ,  $c=0.5$ , and various degrees of SRO indicated by the decimal numbers next to each curve, compared with numerical (exact) results. The numbers in parentheses indicate the number of sites in the cluster used to calculate the DOS's. The two top curves (clustering alloys) were calculated with a two-site SCBSA effective medium.

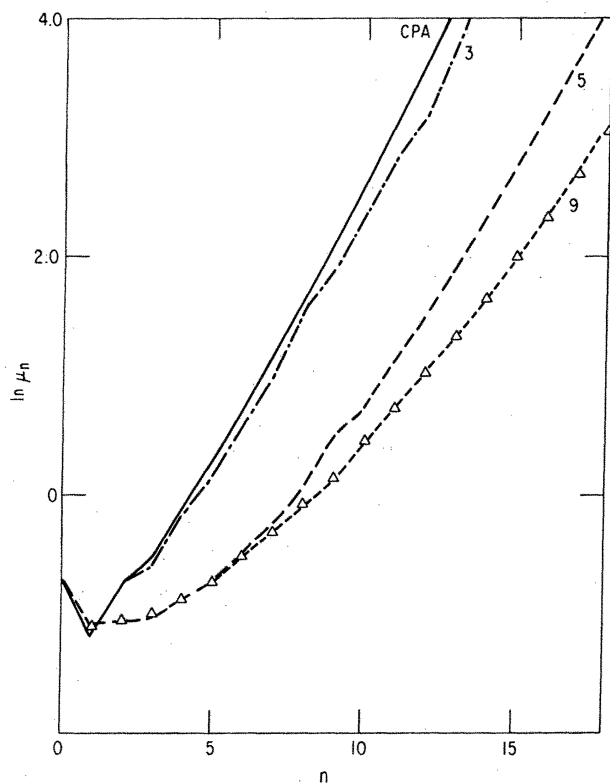


FIG. 19. Logarithms of the moments of the cluster DOS's about  $\epsilon_0=1.0$  for various size clusters for an alloy with  $\epsilon_A=-\epsilon_B=1.0$ ,  $W=1.0$ , and  $c=0.5$ , and  $SRO=-0.9$  compared with the exact results. The size of the clusters used are shown next to the corresponding curves.

with clustering tendencies, it may be necessary to incorporate the SRO self-consistently into the calculation in order to obtain an appropriate embedding medium.

The self-consistent treatment of the SRO necessitated

the generalization of the single-site CPA to a two-site self-consistent cluster theory. For one-dimensional TB alloys with nearest-neighbor hopping, the DOS's obtained in the SCBSA are identical to those obtained<sup>18</sup> in the MCPA and thus the two-site SCBSA used in this paper yields analytic results. Indeed, no analytic difficulties were encountered during the performance of the numerical calculations. For higher-dimensional systems, no proof of analyticity of the SCBSA exists. However, given the results of the various SCBSA calculations,<sup>19,20</sup> it is to be expected that the two-site SCBSA will yield analytic, well-defined physical results in all cases. Note also that in the two-site SCBSA the boundary of the cluster is always well defined. As a further indication of analyticity, in all our calculations the DOS's were found to satisfy the fundamental sum rules.

The methods presented here are applicable to disordered systems of any dimensionality describable by either TB or MT Hamiltonians. In most realistic alloys, clustering or ordering tendencies are not very strong and a CPA embedding medium can be used in conjunction with the ECM. In some cases, however, where strong clustering or ordering tendencies may exist, the self-consistent treatment of SRO may be necessary in order to obtain accurate results.

#### ACKNOWLEDGMENTS

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