

## Cluster approaches to random alloys: An appraisal

VIPIN SRIVASTAVA\*, MEENA CHATURVEDI and S K JOSHI

Department of Physics, University of Roorkee, Roorkee 247 672

\*Department of Physics, Heriot-Watt University, Edinburgh, UK

MS received 13 February 1978; revised 26 June 1978

**Abstract.** Some of the cluster extensions of the coherent potential approximation (CPA) based on the effective medium theory have been critically studied with respect to the decoupling schemes involved in them. Their computational tractability has been examined and it has been found that the *self-consistent* calculations in three-dimensional systems are immensely difficult to perform. A self-consistent calculation has been reported for simple cubic lattices with diagonal and off-diagonal disorder using a pair-CPA method. A significant finding of the paper is that it has been shown that *non-analyticities* are a general feature of extensions of CPA within multiple scattering framework. The non-analyticities were reported several times but a general proof of their existence was not noticed. It was also believed that the so-called molecular-CPA is analytic, this has been shown to be wrong here. The density of states results with off-diagonal randomness have been qualitatively understood to yield some information about the influence of off-diagonal randomness on Anderson localisation of an electron.

**Keywords.** Density of states; off-diagonal randomness; analyticity; Anderson-localisation.

### 1. Introduction

It is now known that the generalisation of the coherent potential approximation (CPA) (Soven 1967) to include the cluster effects in disordered alloys is non-unique, and presents a difficult problem when one tries to calculate the distribution of eigenvalues.

In this paper we present a self-consistent calculation of electronic density of states in a simple-cubic binary alloy using a pair-CPA. We discuss the numerous difficulties that one encounters with to perform a self-consistent calculation, and show how a series of approximations has to be made in order to make the numerical computation feasible. A comprehensive review of the attempts made to generalise CPA has been given by Elliott *et al* (1974a), more recent approaches have been discussed by Ehrenreich and Schwartz (1976) and Kumar and Joshi (1977), and most recent attempt, not included in these references, is by Bloom and Mattis (1977). The numerical results reported so far are mainly for one-dimensional systems. Except the self-consistent results of Moorjani *et al* (1974a), the rest are obtained either through non-self-consistent methods, employing iterative methods like average *t*-matrix approximation, or through the methods that deal with scattering from a single site and include in some approximate way the local environmental effects.

The development of cluster-CPA has taken two directions. One of them, to be termed as 'single-site framework', imbeds a pair of sites or triplet of sites, etc., in an effective medium and treats the scattering from it exactly. The other one, to be termed

as 'cluster framework', instead treats exactly the scattering from a cluster of nearest neighbours, and next nearest neighbours, etc. The two frameworks incorporate two different decoupling schemes, and yield different effective mediums after calculation. The latter can be reduced to the former after some approximations, but the former *cannot* be generalised to yield the self-consistent conditions of the cluster framework. We have discussed the subtleties involved in the two kinds of decoupling schemes.

A big problem with the cluster generalisations of CPA, which has been reported often but never investigated deeply, is that the Green's function becomes non-analytic for certain energies for certain sets of parameters. We have analysed this problem here and have found that the generalisations of CPA that involve an effective medium denoted by a self-energy matrix should inevitably suffer from this problem.

In §2 we categorise some of the effective medium approaches in two classes termed as single-site and cluster frameworks. We discuss the kinds of decouplings involved in them and assess the difficulties if computation is attempted, and keeping these difficulties in mind we develop a pair-CPA after a series of simplifications. Section 3 deals with the non-analyticity problem. Section 4 discusses the numerical results of density of states in presence of diagonal and off-diagonal randomness in the pair-CPA developed in §2.

## 2. Cluster generalisation of CPA

Following are the problems encountered in cluster generalisation of CPA.

- (a) Too many simultaneous equations have to be solved, making the numerical computation unmanageable.
- (b) In some cases the periodicity of the lattice for the configurationally averaged system breaks down.
- (c) The problem of non-analyticity in the solution of self-consistent equations appears to be inevitable.
- (d) The off-diagonal disorder should be taken into account and the perturbing atomic potentials should be chosen self-consistently to satisfy the Friedel sum rule. To date, only the model proposed by Stern and Zin (1974) is able to account for it correctly.

Taking these into consideration we briefly discuss in the following the *self-consistent* cluster generalisations of CPA with the purpose of understanding the subtleties involved in the decoupling schemes and see how they can be simplified to make the computation manageable. We restrict ourselves to the effective medium theories only.

The properties of the disordered system represented by a Hamiltonian  $H$  are determined by replacing it by a self-consistently chosen ordered *reference* system of Hamiltonian  $\tilde{H}$  and then doing a perturbation theory. The reference medium has a self-energy matrix  $\mathcal{E}(\mathbf{k}, z)$  whose elements are the site energies and the hopping integrals of the averaged system. The scattering in the system is governed by a scattering matrix,

$$T = V/[I - VG]; \quad G = (zI - H)^{-1}; \quad V = H - \tilde{H}. \quad (1)$$

Solution of the Dyson equation,

$$\langle G \rangle = \tilde{G} + \tilde{G} \Sigma \langle G \rangle, \quad (2)$$

yields  $\Sigma$ . Here  $\tilde{G} = (zI - \tilde{H})^{-1}$ , and the angular brackets denote configurational averaging. It is well known that (2) is solved self-consistently by putting  $\langle T \rangle = 0$  (Velicky *et al* 1968). In an infinite system it is impossible to solve  $\langle T \rangle = 0$ . So one needs to break it into components. We can do it in two ways. In 'single-site framework'  $T$  is written in terms of contributions from single sites,

$$T = \sum_n T_n, \quad (3)$$

and in 'cluster framework' contributions from clusters of a definite size are considered,

$$T = \sum_c T_c. \quad (4)$$

Equations (3) and (4) clearly need  $V$  to be written like,

$$V = \sum_n V_n \text{ and } V = \sum_c V_c \quad (5)$$

respectively.  $V_n$  and  $V_c$  are not necessarily site diagonal and cluster diagonal respectively, i.e. inter-site and inter-cluster elements exist.

We first consider the single-site framework and write  $\Sigma$  in momentum representation as (Nickel and Krumhansl 1971),

$$\begin{aligned} \Sigma_{\mathbf{k}} = & \Sigma^{(1)}(n) + \sum'_m \Sigma_m^{(2)}(nm) + \sum'_p \sum'_m \Sigma_{p,m}^{(3)}(nm) + \dots \\ & + \sum'_m \exp(i\mathbf{k} \cdot \mathbf{R}_{nm}) [\Sigma^{(2)}(nm) + \sum'_p \Sigma_p^{(3)}(um) + \dots]. \end{aligned} \quad (6)$$

Here  $\Sigma_m^{(2)}(nm)$  is the contribution from multiple scatterings between  $n$  and  $m$  sites such that the electron enters at  $n$  and leaves at  $n$ , whereas in  $\Sigma^{(2)}(nm)$  electron enters at  $n$  and leaves at  $m$ . The primes on the lattice sums indicate that no two indices are the same. In CPA  $\Sigma$  is taken to be cell localised so that in (6) all the contributions except  $\Sigma^{(1)}(n)$  are taken to be zero. To go beyond CPA other terms in (6) are to be included. Let us consider the simplest case of pairs. We will see in the following that generalisations to pair-CPA can be obtained in two different ways depending on how the pair under consideration can be decoupled from the rest of the system.

Expanding  $T_n$  in terms of single-site  $t$ -matrices (Velicky *et al* 1968) as,

$$T_n = t_n + t_n \tilde{G} \sum_{m \neq n} t_m + t_n \tilde{G} \sum_{m \neq n} t_m \tilde{G} \sum_{p \neq m, n} t_p + \dots \quad (7)$$

Cyrot-Lackmann and Ducastelle (1971) proposed the following self-consistency condition for determining  $\Sigma$ ,

$$\left\langle t_n + \sum_{m \neq n} (t_m \tilde{G} t_n + t_n \tilde{G} t_m \tilde{G} t_n + \dots) \right\rangle = 0, \quad (8)$$

i.e. the scattering from  $n$  and multiple scattering corrections due to *all* other sites in the system should go to zero on average. The nature of (8) clearly shows that it is capable of calculating  $N$  elements in (6), namely,  $\Sigma(n) = \Sigma^{(1)}(n) + \sum_{m \neq n} \Sigma_m^{(2)}(nn)$ , and the  $(N-1)$   $\Sigma^{(2)}(nm)$ 's (if the system has  $(N-1)$  pairs of different separations).

On the other hand, following different arguments, Aiyer *et al* (1969), Nickel and Krumhansl (1971), Ducastelle (1972a, b), Cyrot-Lackmann and Cyrot (1972) and Srivastava and Joshi (1973) obtained the following self-consistency condition,

$$\langle t_n + t_n \tilde{G} t_m + t_n \tilde{G} t_m \tilde{G} t_n + \dots \rangle = 0, \quad (9)$$

i.e. average scattering from  $n$  and multiple scatterings between  $n$  and  $m$  become zero. It is clear that if different pairs of  $n$  and  $m$  are considered separately, then (9) can evaluate  $(2N-1)$  elements in (6), namely,  $\Sigma^{(1)}(n)$ , the  $(N-1)$   $\Sigma_m^{(2)}(nm)$ 's and the  $(N-1)$   $\Sigma^{(2)}(nm)$ 's. Note that both (8) and (9) are incapable of including off-diagonal disorder because they are written in terms of single-site  $t$ -matrix which is site-diagonal.

Let us now try to extend the procedure to include the coherent scattering from a cluster of nearest neighbours (say). Suppose the central site is  $n$  and those on the nearest neighbour shell are denoted by  $(m)$ . Then,

$$T = T_n + \sum_{(m)} T_m + \sum_{p \neq n, (m)} T_p, \quad (10)$$

and 
$$\langle T \rangle = \left\langle T_n + \sum_{(m)} T_m \right\rangle + \sum_{p \neq n, (m)} \langle T_p \rangle. \quad (11)$$

Since the sites  $p$  lie in the effective medium,  $\langle T_p \rangle = 0$ , and the self-consistency requirement becomes,

$$\langle T_n + \sum_{(m)} T_m \rangle_{n,m} = 0. \quad (12)$$

Now further we have,

$$T_n = t_n + t_n \tilde{G} \sum_{(m) \neq n} T_m + t_n \tilde{G} \sum_{p \neq n, (m)} T_p, \quad (13)$$

and 
$$T_{m_1} = t_{m_1} + t_{m_1} \tilde{G} \sum_{q \neq m_1} T_q - t_{m_1} \tilde{G} \sum_{m_k \neq n, m_1} T_{m_k} - t_{m_1} \tilde{G} T_n$$

$$+ t_{m_1} \tilde{G} \sum_{m_k \neq n, m_1} T_{m_k} + t_{m_1} \tilde{G} T_n$$

$$= t_{m_1} + t_{m_1} \tilde{G} T_n + t_{m_1} \tilde{G} \sum_{m_k \neq m_1, n} T_{m_k} + t_{m_1} \tilde{G} \sum_{p \neq n, (m)} T_p. \quad (14)$$

Here  $m_1$  and  $m_k \in (m)$ . Substituting for  $T_n$  from (13) we have,

$$(1 - t_{m_1} \tilde{G} t_n \tilde{G}) T_{m_1} = (t_{m_1} + t_{m_1} \tilde{G} t_n) \times [1 + \tilde{G} (\sum_{m_k \neq n, m_1} T_{m_k} + \sum_{p \neq n, (m)} T_p)],$$

or  $T_{m_1} = t_n^{(2)}(m_1) [1 + \tilde{G} (\sum_{m_k \neq n, m_1} T_{m_k} + \sum_{p \neq n, (m)} T_p)],$  (15)

where  $t_n^{(2)}(m_1) = t_{m_1} + t_{m_1} \tilde{G} t_n + t_{m_1} \tilde{G} t_n \tilde{G} t_{m_1} + \dots$  (16)

Averaging over the configurations of the cluster and decoupling the cluster from rest of the medium we get,

$$\langle T_{m_1} \rangle = \left\langle t_n^{(2)}(m_1) [1 + \tilde{G} \sum_{m_k \neq n, m_1} T_{m_k}] \right\rangle_{n, (m)}.$$
 (17)

Similarly we have from other sites on the first shell

$$\langle T_{m_2} \rangle = \left\langle t_n^{(2)}(m_2) [1 + \tilde{G} \sum_{m_k \neq n, m_2} T_{m_k}] \right\rangle_{n, (m)}.$$
 (18)

It is clear from the nature of (17) and (18) that it is not possible to eliminate  $T_{m_k}$  from the right hand side, unless pairs of sites  $n - m_1$  and  $n - m_2$ , etc. are individually decoupled from  $m_k$ 's. Thus in the single-site framework a cluster cannot be successfully decoupled from the rest of the medium.

We now turn to the cluster framework and see if we can overcome the constraint in the single-site framework that off-diagonal randomness cannot be included. We represent  $T_c$  of eq. (4) by  $T_a^0$  for a cluster of nearest neighbour sites (0 is the central site and  $a$  is the shell of nearest neighbours). Then,

$$T_a^0 = \begin{pmatrix} T_{00} & T_{0a} \\ T_{a0} & T_{aa} \end{pmatrix} = \left( \begin{array}{c|cccc} \tau_{00} & \tau_{0n_1} & \tau_{0n_2} & \dots & \tau_{0n_z} \\ \tau_{n_1 0} & \tau_{n_1 n_1} & \tau_{n_1 n_2} & \dots & \tau_{n_1 n_z} \\ \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot \\ \tau_{n_z 0} & \tau_{n_z n_1} & \tau_{n_z n_2} & \dots & \tau_{n_z n_z} \end{array} \right),$$
 (19)

where  $n_1, n_2, \dots, n_z$  are the sites on the first shell, and the partitioning identifies  $T_{00}, T_{0a}$ , etc. If  $\langle T_a^0 \rangle$  be made zero after averaging over the configurations of 0 and  $a$ , it will be equivalent to putting  $\langle T \rangle = 0$  (see (4)). Hwang and Sher (1975) attempted to do this for a simple cubic lattice but found the computation unmanageable. They then resorted to first order perturbation theory (in the impurity concentration) for dilute alloys, and non-self-consistent ATA (Beeby 1964, Soven 1966) and iteration ATA (Chen 1973) for concentrated alloys with weak disorder ( $\delta = \epsilon_A - \epsilon_B = 0.8$ ).

The computation was enormously time taking even for 2 iterations of ATA. The features in their numerical results should be treated with caution because large number of iterations of ATA have to be done before it becomes equivalent to CPA (Chen 1973). It is not clear how the alloy bandwidths obtained by Hwang and Sher (1975) are greater than those of a virtual crystal.\*

It seems advisable to simplify (19) further but try to solve it self-consistently. Assume that  $\tau_{n_1 n_2}$ ,  $\tau_{n_2 n_3}$ , etc. due to second and higher neighbours are small enough to be ignored. So that (19) reduces to,

$$T_{\alpha}^0 = \begin{pmatrix} \tau_{00} & \tau_{0n_1} & \tau_{0n_2} & \cdots & \tau_{0n_z} \\ \tau_{n_1 n_1} & & & & \mathbf{O} \\ \cdot & \cdot & \cdot & \cdot & \cdot \\ \tau_{n_z 0} & \mathbf{O} & & & \tau_{n_z n_z} \end{pmatrix}. \quad (20)$$

Foo *et al* (1973) attempted to solve  $\langle T_{\alpha}^0 \rangle = 0$  but computation was too cumbersome to be manageable. An alternative way of writing (20) is,

$$T_{\alpha}^0 = \langle c | T | c \rangle = \frac{V_{cc}}{1 - \sum_{c'} V_{cc'} \tilde{G}_{c'c}}, \quad (21)$$

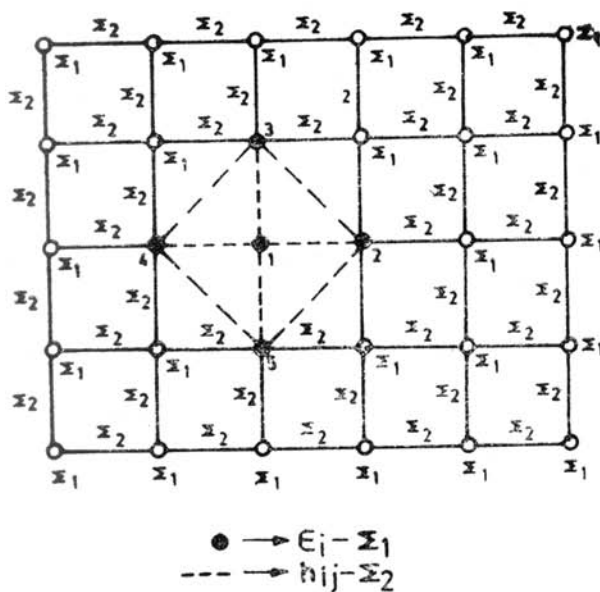
where  $c$  stands for the cluster that contains 0 and  $\alpha$ , and  $V_{cc} (\equiv V_c) = \langle c | V | c \rangle$ , etc. It is needed to discuss the nature of  $V_{cc}$  now. Figure 1 shows a nearest neighbour cluster in a square lattice.  $V_{cc}$  may be written as  $(v_{cc} - \Sigma_{cc})$  where  $v_{cc}$  and  $\Sigma_{cc}$  are  $2 \times 2$  matrices,

$$v_{cc} = \begin{pmatrix} \epsilon_i & h_{ii'} \\ h_{i'i} & \epsilon_{i'} \end{pmatrix}; \quad i, i' \in C \quad (22)$$

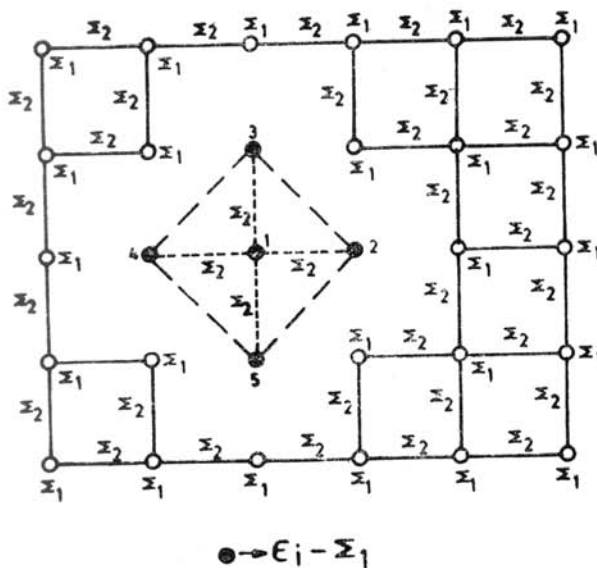
$$\Sigma_{cc} = \begin{pmatrix} \Sigma_1 & \Sigma_2 \\ \Sigma_2 & \Sigma_1 \end{pmatrix}, \quad (23)$$

where  $\epsilon_i$  is site energy at site  $i$  and  $h_{ii'}$  is the hopping integral between nearest neighbour sites  $i$  and  $i'$ . From figure 1 (a) it is clear that  $V_{cc'}$  will be zero, however  $\tilde{G}_{cc}$  in (21) will contain the information of full  $\Sigma$  matrix which makes the solution of  $\langle T_{\alpha}^0 \rangle = 0$  unmanageable. The problem can be resolved only if the cluster  $c$  is decoupled from the rest of the medium so that all the matrices in (21) become cluster diagonal. The picture is now as shown in figure 1(b). The system is partitioned into disjoint clusters of equal size, forming a super lattice. The translational invariance is broken. This method is called molecular CPA (MCPA), first given by Tsukada (1969, 1972) and later on developed by Ducastelle (1974) and Leath (1973).

\*It is well known that the virtual crystal bandwidth is equal to the union of  $2\omega_A$  and  $2\omega_B$  (Kirkpatrick *et al* 1970), where  $\omega_A$  and  $\omega_B$  are the half bandwidths of the constituents  $A$  and  $B$ . Eigenstates of  $H$  cannot lie outside this range.



(a)



(b)

Figure 1. Nearest neighbour cluster in a square lattice, (a) without, and (b) with cluster diagonality.

Zittartz (1974) has presented a cluster extension of CPA using a projection operator method. This is analogous to MCPA but does not suffer from the breakdown of translational invariance and follows the picture of figure 1 (a).

We come back to MCPA and write the self-consistency condition,

$$\langle T_a^0 \rangle = \left\langle \frac{V_{cc}}{1 - V_{cc} \tilde{G}_{cc}} \right\rangle = 0. \tag{24}$$

We tried computation with these  $(Z+1)$  simultaneous equations ( $Z$ =co-ordination number) but it was extremely time taking. So we had to reduce the problem to a pair of nearest neighbour states neglecting the effects of  $n_2 \dots n_z$  sites on the contribution from the pair  $0-n_1$ . The pictures in this case, corresponding to figures 1(a) and (b), are shown in figures 2(a) and (b). Using the picture of figure 2(b) and denoting the sites of the pair as 1 and 2, we have two simultaneous equations to be solved,

$$\langle T_{11} \rangle = \left\langle \frac{V_{11} + A}{B} \right\rangle = 0, \tag{25}$$

$$\langle T_{21} \rangle = \left\langle \frac{V_{21} + C}{D} \right\rangle = 0, \tag{26}$$

where  $A = V_{21}(V_{11}\tilde{G}_R + V_{12}\tilde{G}_0)/D,$  (27)

$$B = 1 - (V_{11}\tilde{G}_0 + V_{12}\tilde{G}_R) - (V_{11}\tilde{G}_R + V_{12}\tilde{G}_0)(V_{21}\tilde{G}_0 + V_{22}\tilde{G}_R)/D, \tag{28}$$

$$C = (V_{21}\tilde{G}_0 + V_{22}\tilde{G}_R)T_{11}, \tag{29}$$

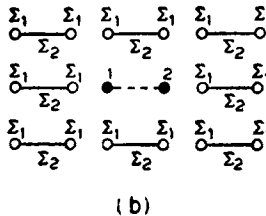
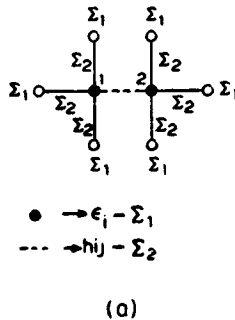


Figure 2. A pair of nearest neighbour sites imbedded in an effective medium, (a) without, and (b) with cluster diagonality.



$$D = 1 - (V_{21}\tilde{G}_R + V_{22}\tilde{G}_0), \quad (30)$$

$$V_{11} = \epsilon_1 - \Sigma_1, \quad (31)$$

$$V_{22} = \epsilon_2 - \Sigma_1, \quad (32)$$

$$V_{12} = V_{21} = h - \tilde{h}(1 - \Sigma_2), \quad (33)$$

$\epsilon_1$  and  $\epsilon_2$  take values  $\epsilon_A$  and  $\epsilon_B$  and  $h$  can be  $h_{AA}$ ,  $h_{BB}$ ,  $h_{AB}$  or  $h_{BA} = (h_{AA} + h_{BB})/2$  depending on the occupancy of the sites of the pair.  $\tilde{G}_0 = G_{11} = \tilde{G}_{22}$  and  $\tilde{G}_R = \tilde{G}_{12} = \tilde{G}_{21}$ . The particular form of  $h_{AB}$  is a simplification, not a requirement. Equations (25) and (26) yield two coupled equations in  $\Sigma_1$  and  $\Sigma_2$ .

$$\Sigma_1 = (\langle \epsilon_1/B \rangle + \langle A/B \rangle) / \langle 1/B \rangle, \quad (34)$$

$$\Sigma_2 = 1 - (\langle h/D \rangle + \langle C/D \rangle) / \tilde{h} \langle 1/D \rangle. \quad (35)$$

The averaging is done over the occupancy of the pair 1-2. Pairs *A-A*, *A-B*, *B-A* and *B-B* occur respectively with probabilities  $c^2$ ,  $c(1-c)$ ,  $(1-c)c$  and  $(1-c)^2$ , where  $c$  is the concentration of *A* atoms. The Green's function is obtained as follows. The diagonal part is,

$$\begin{aligned} \tilde{G}_0 &= \sum_{\mathbf{k}} \frac{1}{E - \Sigma_1(E) - \tilde{h} Z s(\mathbf{k}) [1 - \Sigma_2(E)]}, \\ &= \frac{1}{1 - \Sigma_2(E)} \sum_{\mathbf{k}} \frac{1}{\frac{E - \Sigma_1(E)}{1 - \Sigma_2(E)} - \tilde{\omega} s(\mathbf{k})}, \end{aligned} \quad (36)$$

where  $\tilde{\omega} = Z\tilde{h}$ ;  $s(\mathbf{k})$  is the structure factor. For convenience if we take  $\tilde{h} = h_{AA}$ , then (36) may be written as,

$$\tilde{G}_0 = \frac{1}{1 - \Sigma_2} \int \frac{\rho^A(E') dE'}{\frac{E - \Sigma_1(E)}{1 - \Sigma_2(E)} - E' + \epsilon_A} \quad (37)$$

$\rho^A(E')$  is the unperturbed density of states of pure *A* system. For deriving the off-diagonal part of Green's function, we proceed in the locator formulation (Leath 1973),

$$\tilde{G}_{11} = g_{11} + \frac{\sum}{2} g_{11} W_{12} \tilde{G}_{21}, \quad (38)$$

where  $W_{12} = \tilde{h}(1 - \Sigma_2)$ , and  $g_{11} = (E - \Sigma_1)^{-1}$  is the unperturbed locator and the Green's function of the system with no hopping. Here 2 denotes the nearest neighbours of 1. So we get,

$$\tilde{G}_R = \{ (E - \Sigma_1) \tilde{G}_0 - 1 \} / Z h_{AA} (1 - \Sigma_2). \quad (39)$$

Having obtained  $\Sigma_1$  and  $\Sigma_2$  from (34) and (35) the alloy density of states is given by,

$$\rho(E) = -\pi^{-1} \text{Im } \tilde{G}_0(E+io). \quad (40)$$

A brief account of partial (component) density of states  $\rho_{A(B)}(E)$  is given as follows. Conditionally averaged Green's functions are defined as (Velicky *et al* 1968, Brouers and Van der Rest 1972),

$$\begin{aligned} \tilde{G}_0^{(A)}(E) = & \langle 1 | [E - \tilde{H} - (\epsilon_A - \Sigma_1)]^{-1} | 1 \rangle \langle 1 | - \{h - h_{AA}(1 - \Sigma_2)\} \\ & \sum_{2 \neq 1} | 2 \rangle \langle 2 | ]^{-1} | 1 \rangle, \end{aligned} \quad (41)$$

and a similar expression for  $\tilde{G}_0^{(B)}(E)$ ;  $E \equiv E + io$ . After some transformations this can be written as,

$$\tilde{G}_0^{(A)}(E) = \tilde{G}_0(E) / [(E - \epsilon_A)\tilde{G}_0(E) - \{(E - \Sigma_1)\tilde{G}_0(E) - 1\} / (1 - \Sigma_2)], \quad (42)$$

$$\tilde{G}_0^{(B)}(E) = \tilde{G}_0(E) / [(E - \epsilon_B)\tilde{G}_0(E) - h_{BB}\{(E - \Sigma_1)\tilde{G}_0(E) - 1\} / h_{AA}(1 - \Sigma_2)]. \quad (43)$$

The partial densities of states are then given as,

$$\rho_{A(B)}(E) = -\pi^{-1} \text{Im } \tilde{G}_0^{(A)(B)}(E+io). \quad (44)$$

These quantities satisfy the natural identity,

$$\rho(E) = c\rho_A(E) + (1 - c)\rho_B(E). \quad (45)$$

### 3. The non-analyticity problem

The effective medium approaches for the cluster generalisations of CPA suffer from the problem of non-analyticity in the Green's function off the real energy axis. When this occurs, the local properties such as the density of states can no longer be uniquely defined and sum rules, such as the expressions for integrated density of states are not satisfied. The CPA has been proved to be analytic by Muller-Hartmann (1973). One should not *a priori* expect that an arbitrary extension of CPA will be analytic. Ducastelle (1974) has claimed to have proved the analyticity of MCPA. While performing the numerical computation using the MCPA in the form of a pair-CPA as developed in the preceding section, we came across the non-analyticity problem which led us to examine the proof given by Ducastelle, and we found it to be incomplete. The non-analyticity problem in MCPA in one dimension was earlier faced by Sen and Yndurain (1976) for large values of  $\delta (=16)$  contrary to the belief of Butler (1973). Other authors, like Moorjani *et al* (1974 b) and Nickel and Butler (1973) also came across the same problem in the course of their calculations. A detailed examination

has been used here to show the cluster-CPAs that involve an effective medium calculation in the sense of calculating a self-energy *matrix* shall inevitably suffer from the accidental occurrences of non-analyticity. Nickel and Butler (1973) had earlier made an intuitive conjecture to this effect.

The definitions of the medium propagator  $\tilde{G}(z) = (z - \tilde{H})^{-1}$  and the self energy  $\Sigma(z) [\tilde{H} = \sum_n \Sigma_1 |n\rangle \langle n| + \sum_m \Sigma_2 |n\rangle \langle m|]$  show that  $\tilde{G}$  and  $\Sigma$  are analytic in the half planes  $\text{Im } z \geq 0$ . They satisfy the reality condition,

$$\tilde{G}^*(z) = \tilde{G}(z^*); \Sigma^*(z) = \Sigma(z^*). \tag{46}$$

Further, since  $\text{Im } H$  is positive definite (i.e. eigenvalues of  $\text{Im } H$  are real and positive), it is simple to deduce that  $\text{Im } G$  is negative definite when  $\text{Im } z > 0$ . Now,

$$\text{Im } G = -GG^* \text{Im } z. \tag{47}$$

so that,  $\text{Im } \langle G \rangle = \text{Im } \tilde{G} = -\langle GG^* \rangle \text{Im } z.$  (48)

This shows that  $\text{Im } \tilde{G}$  is also negative definite. From the definition of  $\Sigma$  it follows that (48) can be written as

$$\text{Im } \tilde{G} = -\tilde{G}\tilde{G}^* \text{Im } (z - \Sigma), \tag{49}$$

which implies that  $\text{Im } (z - \Sigma)$  is positive definite or  $\text{Im } \Sigma$  is negative definite for  $\text{Im } z > 0$ . Using these facts Ducastelle (1974) has argued that the MCPA  $T_a^0$ -matrix given by (24) is analytic. Taking the denominator matrix as

$$D \equiv \tilde{G}_{cc}^{-1} - V_{cc},$$

he writes  $\text{Im } D = \text{Im } \tilde{G}_{cc}^{-1} + \text{Im } \sigma |c\rangle \langle c|$  [writing  $\Sigma_{cc} = \sigma |c\rangle \langle c|$ ],

$$\begin{aligned} &= -\frac{\text{Im } \tilde{G}_{cc}}{|\tilde{G}_{cc}|^2} + \text{Im } \sigma |c\rangle \langle c|, \\ &= -\frac{1}{|\tilde{G}_{cc}|^2} \langle c | \tilde{G}\tilde{G}^* | c \rangle \text{Im } (z - \sigma) |c\rangle \langle c| + \text{Im } \sigma |c\rangle \langle c| \\ &\hspace{15em} \text{[using (49)],} \\ &= \text{Im } z \tilde{G}_{cc}^{-1} \langle c | \tilde{G}\tilde{G}^* | c \rangle \tilde{G}_{cc}^{*-1} \\ &\hspace{10em} - \text{Im } \sigma |c\rangle \langle c| \sum_{c' \neq c} \tilde{G}_{cc}^{-1} \tilde{G}_{cc'} \tilde{G}_{c'c}^* \tilde{G}_{cc}^{*-1} > 0. \end{aligned} \tag{50}$$

because  $\text{Im } \sigma$  is negative definite,  $\text{Im } z > 0$ , and  $\langle c | \tilde{G}\tilde{G}^* | c \rangle = \Sigma_c' |\tilde{G}_{cc'}|^2 > 0$ . From this he concludes that,

$$\det D = \det [\tilde{G}_{cc}^{-1} - V_{cc} + \sigma | c \rangle \langle c |] \neq 0. \quad (51)$$

i.e.  $T_a^0 \neq \infty$ . But the conclusion (51) is not correct,  $\text{Im } D > 0$  implies  $\det [\text{Im } D] \neq 0$  and not  $\det D \neq 0$ . We take a simple example. Suppose  $D$  is a complex  $2 \times 2$  matrix,

$$\begin{aligned} D &= \begin{pmatrix} a_{11} + ib_{11} & a_{12} + ib_{12} \\ a_{21} + ib_{21} & a_{22} + ib_{22} \end{pmatrix} \\ &= \begin{pmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{pmatrix} + i \begin{pmatrix} b_{11} & 0 \\ 0 & B_{22} \end{pmatrix} \end{aligned} \quad (52)$$

Here  $\text{Im } D$  has been diagonalised. Since  $\text{Im } D$  is positive definite  $b_{11} > 0$  and  $B_{22} > 0$  and  $\det [\text{Im } D] = b_{11} B_{22} > 0$ . Determinant of  $D$  is,

$$\begin{aligned} |D| &= (a_{11} a_{22} - a_{12} a_{21}) + i (a_{11} b_{22} - b_{12} a_{21}) \\ &\quad + i (b_{11} a_{22} - a_{12} b_{21}) - (b_{11} b_{22} - b_{12} b_{21}) \\ &= (a_{11} a_{22} - a_{12} a_{21}) + i \{ (a_{11} b_{22} - b_{12} a_{21}) + (b_{11} a_{22} - a_{12} b_{21}) \} \\ &\quad - b_{11} B_{22}. \end{aligned} \quad (53)$$

That  $|D| = 0$ , is not out of the limit of the possibilities since nothing has been said about  $\text{Re } D$ . So the proof given by Ducastelle (1974) is not complete and under certain circumstances  $\det D$  may vanish giving rise to non-analyticity. It follows from the above that whenever  $\Sigma$  will be a matrix, one is bound to encounter with  $\det D$  in some form or the other in the formulations involving a scattering matrix, and as it has been just seen, vanishing of  $\det D$  cannot be ruled out, so non-analyticity may always occur accidentally at some sets of parameters. Whenever  $\Sigma$  will be scalar, proof by Muller-Hartmann (1973) will hold for analyticity. Krey (1976) has shown that his coherent exchange cluster approach for ferromagnetic Heisenberg spin alloys is analytic. His is a single parameter problem.

We now explicitly deal with the method used here for calculations. We derive the circumstances in which non-analyticity should occur and see how it is inevitable. For verification of the computer program we checked the reality condition (46) numerically. Also,  $\text{Im } \Sigma$  was found to be negative definite numerically. Here,  $\text{Im } \Sigma_1$  is always negative but  $\text{Im } \Sigma_2$  changes sign within the allowed energy range. From (25) and (26) it follows that the necessary and sufficient conditions for the non-analyticity of the pair- $t$ -matrix are,

$$V_{21} \tilde{G}_R + V_{22} \tilde{G}_0 = 1, \quad (54)$$

and 
$$V_{21} \tilde{G}_0 + V_{22} \tilde{G}_R = 0. \quad (55)$$

Using the relations (31)-(33), (37) and (39), (54) is written as,

$$\frac{\{h - \tilde{h}(1 - \Sigma_2)\} (z - \Sigma_1)}{1 - \Sigma_2} + (\epsilon_i - \Sigma_1) = \alpha \zeta \left( 1 + \frac{h - \tilde{h}(1 - \Sigma_2)}{1 - \Sigma_2} \right), \quad (56)$$

where  $\zeta = (z - \Sigma_1)/(1 - \Sigma_2)$ ,

and 
$$\alpha = \frac{1}{|F(\zeta)|^2} \int_{-\infty}^{\infty} \frac{d\epsilon \rho(\epsilon)}{|\zeta - \epsilon|^2}; \quad F(u) = \int_{-\infty}^{\infty} \frac{\rho(\epsilon) d\epsilon}{u - \epsilon} \geq 1, \quad (57)$$

is Schwartz's inequality. After laborious algebra, (56) can be written as

$$\frac{\text{Im } A[C \cdot D + (1 - \tilde{h})(\text{Im } \Sigma_2^2)] - \text{Im } \Sigma_2 \text{ Re } A(C - D + D\tilde{h}) - Ch \text{Im } B - h(1 - \tilde{h}) \text{Im } \Sigma_2 \text{ Re } B}{\text{Re } A[C \cdot D + (1 - \tilde{h})(\text{Im } \Sigma_2^2)] + \text{Im } \Sigma_2 \text{ Im } A(C - D + D\tilde{h}) - Ch \text{Re } B - h(1 - \tilde{h}) \text{Im } \Sigma_2 \text{ Im } B} = \frac{\text{Im } \zeta}{\text{Re } \zeta} = \alpha, \quad (58)$$

where  $A = \tilde{h}(z - \Sigma_1) - (\epsilon_i - \Sigma_1)$ ;  $B = z - \Sigma_1$ ;  $C = h + (1 - \tilde{h})(1 - \text{Re } \Sigma_2)$ ;  $D = 1 - \text{Re } \Sigma_2$ .

From (58) we have one of the conditions for non-analyticity in terms of  $\zeta$ :

$$\frac{\text{Im } \zeta}{\text{Re } \zeta} = \frac{(1 - \text{Re } \Sigma_2) \text{Im } (z - \Sigma_1) + \text{Im } \Sigma_2 \text{Re } (z - \Sigma_1)}{(1 - \text{Re } \Sigma_2) \text{Re } (z - \Sigma_1) - \text{Im } \Sigma_2 \text{Im } (z - \Sigma_1)} \geq 1, \quad (59)$$

or

$$\frac{1 - \text{Re } \Sigma_2}{\text{Im } \Sigma_2} \geq - \frac{\text{Re } (z - \Sigma_1) + \text{Im } (z - \Sigma_1)}{\text{Im } (z - \Sigma_1) - \text{Re } (z - \Sigma_1)}. \quad (60)$$

Now we explore the condition (55). If (55) is satisfied, it would imply that the real and imaginary parts vanish individually, i.e.

$$h - \tilde{h}(1 - \text{Re } \Sigma_2) + (1 - \alpha)[(\epsilon_i - \text{Re } \Sigma_1) \text{Re } \zeta + \text{Im } \Sigma_1 \text{Im } \zeta] = 0, \quad (61)$$

and

$$\tilde{h} \text{Im } \Sigma_2 + (1 - \alpha)[(\epsilon_i - \text{Re } \Sigma_1) \text{Im } \zeta - \text{Re } \zeta \text{Im } \Sigma_1] = 0. \quad (62)$$

Thus, for non-analyticity,

$$\frac{h - \tilde{h}(1 - \text{Re } \Sigma_2)}{(\epsilon_i - \text{Re } \Sigma_1) \text{Re } \zeta + \text{Im } \Sigma_1 \text{Im } \zeta} = \frac{\tilde{h} \text{Im } \Sigma_2}{(\epsilon_i - \text{Re } \Sigma_1) \text{Im } \zeta - \text{Re } \zeta \text{Im } \Sigma_1} = \alpha - 1. \quad (63)$$

This can be rewritten as,

$$\frac{\text{Im}\Sigma_2 [2\tilde{h}(1 - \text{Re}\Sigma_2) - h]}{(1 - \text{Re}\Sigma_2) [\tilde{h}(1 - \text{Re}\Sigma_2) - h] - \tilde{h}(\text{Im}\Sigma_2)^2} = \frac{\text{Im}\Sigma_1 \text{Re}(z - \Sigma_1) + (\epsilon_i - \text{Re}\Sigma_1) \text{Im}(z - \Sigma_1)}{\text{Im}\Sigma_1 \text{Im}(z - \Sigma_1) + (\epsilon_i - \text{Re}\Sigma_1) \text{Re}(z - \Sigma_1)} = \alpha - 1. \quad (64)$$

We can split it into two conditions,

$$\frac{\text{Im}\Sigma_2 [2\tilde{h}(1 - \text{Re}\Sigma_2) - h]}{(1 - \text{Re}\Sigma_2) [\tilde{h}(1 - \text{Re}\Sigma_2) - h] - \tilde{h}(\text{Im}\Sigma_2)^2} \geq 0, \quad [\text{because } \alpha \geq 1], \quad (65)$$

and

$$\frac{\text{Im}\Sigma_1}{\epsilon_i - \text{Re}\Sigma_1} > - \frac{\text{Re}(z - \Sigma_1) + \text{Im}(z - \Sigma_1)}{\text{Im}(z - \Sigma_1) - \text{Re}(z - \Sigma_1)} \quad \text{if } \alpha > 1$$

$$\frac{\text{Im}\Sigma_1}{\epsilon_i - \text{Re}\Sigma_1} = \frac{\text{Im}(z - \Sigma_1)}{\text{Re}(z - \Sigma_1)} \quad \text{if } \alpha = 1. \quad (66)$$

If the conditions (60), (65) and (66) are satisfied for a set of parameters, non-analyticity will occur. The only definite restriction is that  $\text{Im}(z - \Sigma_1) > 0$ . Therefore, that the above conditions may be satisfied in the allowed energy regions, is not at all improbable. Hence the non-analyticity is inevitable in the present case.

#### 4. Numerical results

There are several results of self-consistent cluster-CPA calculations in the relatively simple case of one-dimensional systems (Butler 1973; Horiguchi *et al* 1973a, b; Foo *et al* 1971). As mentioned in §1, there is only one self-consistent calculation for three-dimensional b.c.c. lattices, by Moorjani *et al* (1974). In this section we report the calculations using the self-consistent method developed in §2.

The coupled equations (25) and (26) have been solved iteratively. Having obtained  $\Sigma_1$  and  $\Sigma_2$  from (34) and (35), component densities of states are obtained from (44) and total density of states from (45). For weak disorder (small  $\delta$ ) we employed simple iteration method, whereas, for larger  $\delta$  we had to use Newton-Raphson's method. The amount of computation per iteration is very large in the latter as compared to the former, but the latter method yields convergence at places where the former fails. In the impurity band region the convergence becomes very tough, 45 to 50 iteration are required even at very close intervals of energy. The calculation is thus very time taking even on the IBM 360/44 computer. We did the calculations for the following parameters:  $\delta = 0.4$ ,  $C_A$  (concentration of A atoms) = 0.6, and  $\delta = 1.0$ ,  $C_A = 0.1$  and 0.2, taking  $h_{AA} = h_{BB}$ . For studying the effects of off-diagonal randomness we chose  $h_{AA} = 2h_{BB}/3$  and  $h_{AA} = 3h_{BB}/2$ , with the earlier sets of  $\delta$  and  $C_A$ .

## 4.1. Diagonal randomness

Figure 3 shows the density of states for  $\delta=0.4$ ,  $C_A=0.6$ . Comparison has been made with the result of Blackmann *et al* (1971) (hereafter referred as BEB). Very little and trivial difference has been observed between the pair calculation and the CPA result (BEB method reduces to CPA for no off-diagonal disorder case). Figure 4 quantified the difference in terms of  $\Sigma_2$ .  $\Sigma_2$  which is zero for CPA is only about 7% of  $\Sigma_1$  (if the maximum values are compared). Figures 5 and 6 show two examples in the strong scattering regime:  $\delta = 1.0$  and  $C_A = 0.1$  and  $0.2$ . Plots of self-energy for  $\delta = 1.0$  and  $C_A = 0.1$  are shown in figure 7, CPA self energy has been plotted for comparison. In this regime  $\Sigma_2$  becomes very significant.  $\Sigma_1$  and  $\Sigma_2$  have comparable magnitudes, also  $\Sigma_1$  reduces by a large magnitude as compared to its CPA value. The effect of large magnitude of  $\Sigma_2$  is seen in the density of states—CPA gives an isolated impurity band, whereas in the present calculations gap between the host and the impurity band is eroded. Also, the impurity band shows some structure and some tailing at the edges, as compared to CPA, where sharp cut is found.

The non-analyticity appears in the strong scattering regime. In both the examples, namely,  $\delta=1$ ,  $C_A=0.1$  and  $0.2$ , the problem is encountered in the region where the impurity band starts to build up. Density of states shows a steady fall up to  $E=0.38$  when a sudden jump to a higher value occurs at  $E=0.39$ , from there onwards, a continuous variation is obtained. Convergence in the region of  $E=0.38$  to  $0.39$  could not be obtained even though the energy step length was reduced up to  $0.0005$ . We tried the calculation from the top of the impurity band coming down on the energy axis. In this case the impurity band was retraced and from  $E=0.39$  downwards different values for density of states were obtained which finally joined the main band at  $E=0.32$ . The region between  $E=0.32$  and  $0.39$  is controversial, the two sets of values obtained by taking  $E$  in ascending order and in descending order are shown by broken lines.  $\Sigma_1$  and  $\Sigma_2$  are not holomorphic functions (analytic+single valued) in this region. Between  $E=0.32$  and  $0.38$  they are analytic but many valued, whereas, between  $E=0.38$  and  $0.39$  they are non-analytic.

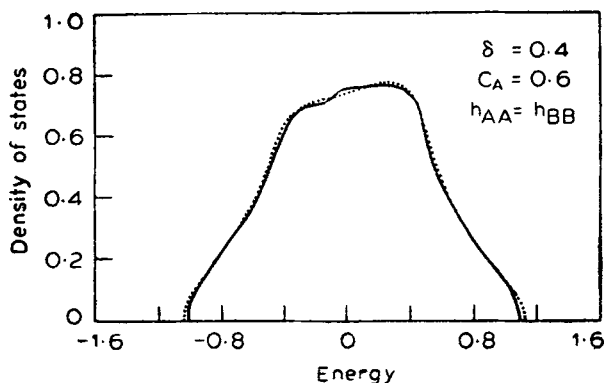


Figure 3. Plot of density of states versus energy for  $\delta=0.4$ ,  $C_A=0.6$  and  $h_{AA} = h_{BB}$ . The results of BEB calculations are shown by broken line.

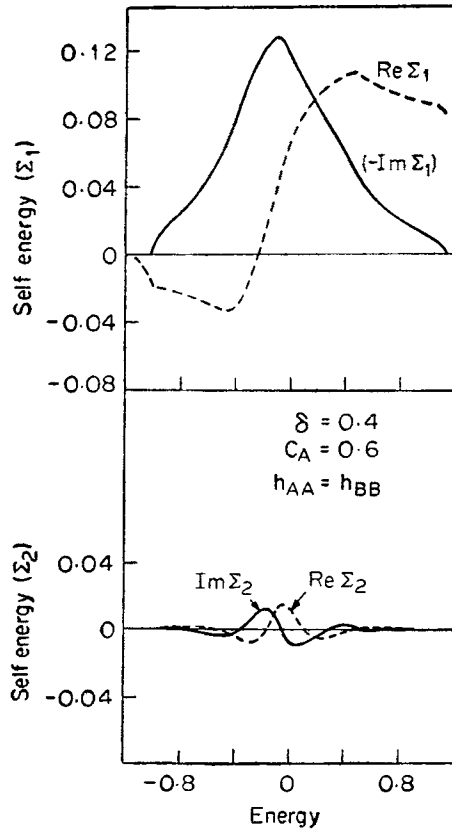


Figure 4. Plots of self energies versus energy for  $\delta=0.4$ ,  $C_A=0.6$  and  $h_{AA}=h_{BB}$ .

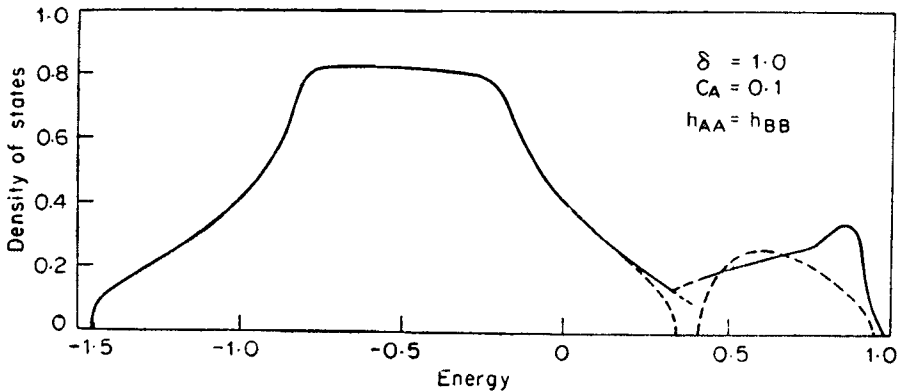


Figure 5. Plot of density of states versus energy for  $\delta=1$ ,  $C_A=0.1$  and  $h_{AA}=h_{BB}$ . The big dash-line shows the CPA result, and the small dashes show the controversial region discussed in the text.



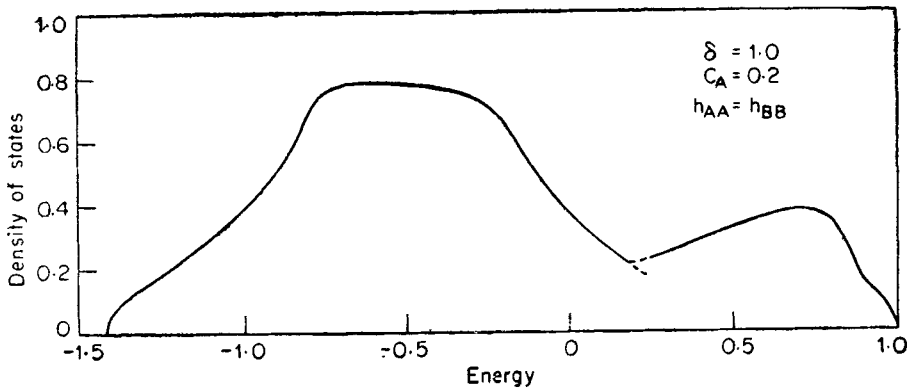


Figure 6. Plot of density of states versus energy for  $\delta=1$ ,  $C_A=0.2$  and  $h_{AA}=h_{BB}$ . The small dashes show the controversial region of non-analyticity discussed in the text.

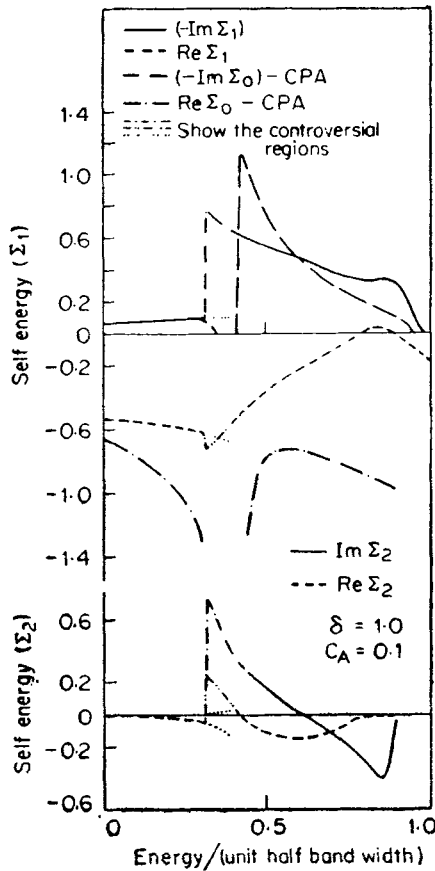


Figure 7. Plots of self energies versus energy for  $\delta=1$ ,  $C_A=0.1$  and  $h_{AA}=h_{BB}$ .

It is interesting that the shape of the impurity band as found by us looks almost like that obtained in continued fraction methods (Cyrot-Lackmann 1974; Gaspard and Cyrot-Lackmann 1977). It is important to mention that the feature of  $\text{Im } \Sigma_2$ , that it changes sign in the impurity band region as seen in figure 7, was also seen by Moorjani *et al* (1974) and was discussed to be compatible with the dispersion relations and with the interpretation of associating the side bands as originating from bonding and antibonding states of a molecule.

#### 4.2. Off-diagonal randomness

Figures 8 and 9 show the total and component densities of states when,  $\delta=0.4$ ,  $C_A=0.6$ , and  $h_{AA}=3h_{BB}/2$  and  $h_{AA}=2h_{BB}/3$  respectively, i.e. the bandwidth of  $A$  component is  $3/2$  and  $2/3$  times the bandwidth of  $B$  component in the two cases. The figures also show the corresponding results obtained by BEB. The  $\Sigma_1$  and  $\Sigma_2$  for these cases are plotted in figures 10 and 11.

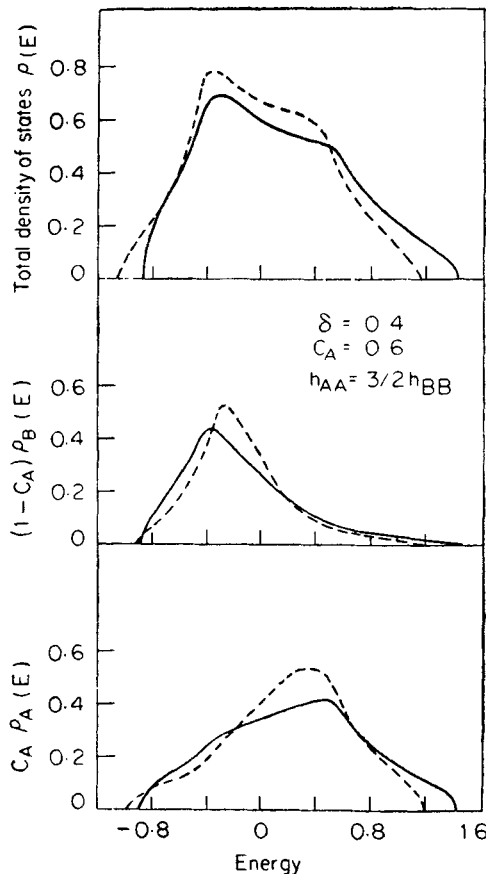
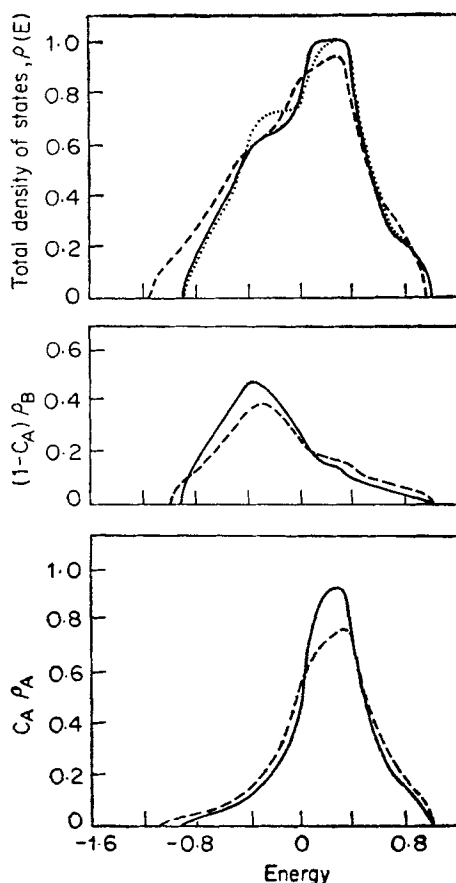


Figure 8. Plots of total and component densities of states versus energy for  $\delta=0.4$ ,  $C_A=0.6$  and  $h_{AA}=3h_{BB}/2$ . Broken lines show the results of BEB calculation.



**Figure 9.** Plots of total and component densities of states versus energy for  $\delta=0.4$ ,  $C_A=0.6$  and  $h_{AA}=2h_{BB}/3$ . Broken line shows the results of BEB calculation, and the dash-dot line is the total density of states calculated from eq. (40).

The effect of narrower solute ( $B$ ) band (figure 8) shows up in the negative energy portion of total and partial densities of states ( $\rho$ ,  $\rho_A$  and  $\rho_B$ ).  $\rho$  and  $\rho_B$  have distinct peaks at almost the same energy and  $\rho_A$  has a shoulder in the same region. The results of BEB are almost like ours except that in our case the bandwidth is larger than the BEB results which indicates that the BEB-theory underestimates the larger bandwidth of host ( $A$ ) band.

The case of narrower host ( $A$ ) band is shown in figure 9 with the corresponding self energies shown in figure 11.  $\Sigma_2$  is now much larger than  $\Sigma_1$ , and  $\text{Im } \Sigma_1$  and  $\text{Im } \Sigma_2$  are peaked over a narrower energy range compared with the earlier case. The imaginary parts of self energies indicate the width caused by disorder in the dispersion curves, hence they are expected to be larger in the region where the contributions to  $\rho$  from  $A$  and  $B$  are comparable. This region is narrower in the case of figure 9 than that shown in figure 8.

Figures 12 and 13 show the effects of off-diagonal randomness for stronger disorder ( $\delta=1$ ) with  $C_A=0.1$  and  $0.2$  and  $h_{AA}=3h_{BB}/2$ . The features of the impurity bands

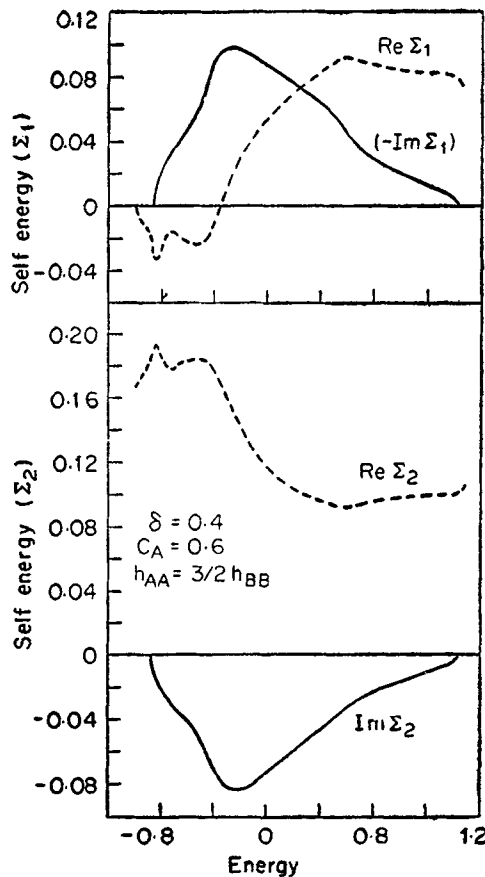


Figure 10. Plots of self energies versus energy for  $\delta=0.4$ ,  $C_A=0.6$  and  $h_{AA}=3h_{BB}/2$ .

as found in figures 5 and 6 are retained except that the impurity bands are stretched considerably to the high energy side forming tails. We guess that this stretching could be qualitatively related with the Anderson localisation (Anderson 1958), in that the situations in figures 12 and 13 are more favourable for localisation of electron than the situations in figures 5 and 6. Here  $h_{AA}$  being larger than  $h_{BB}$  would cause the electron to preferably hop to a neighbouring  $A$  site, if there is any, than to a  $B$  site, i.e. the electron will have relatively stronger tendency to stick to the  $A$  atom clusters. The  $C_A$  is much less than the percolation threshold (Shante and Kirkpatrick 1971, and Srivastava and Weaire (1978)) which means that the  $A$  atoms will be distributed throughout the system in the form of small clusters. However, disorder ( $\delta=1$ ) is not strong enough to stop the quantum mechanical tunnelling of the electron and also the method used here uses an averaged effective medium, both of these tend to destroy the localisation which is the local property of the  $A$  atom clusters. Yet it appears that the off-diagonal randomness under consideration cancels the above two effects to some extent and tends to restore the localisation. This tendency to restore the cluster property in the effective medium theory should pull some states out of the band edges to form tails.

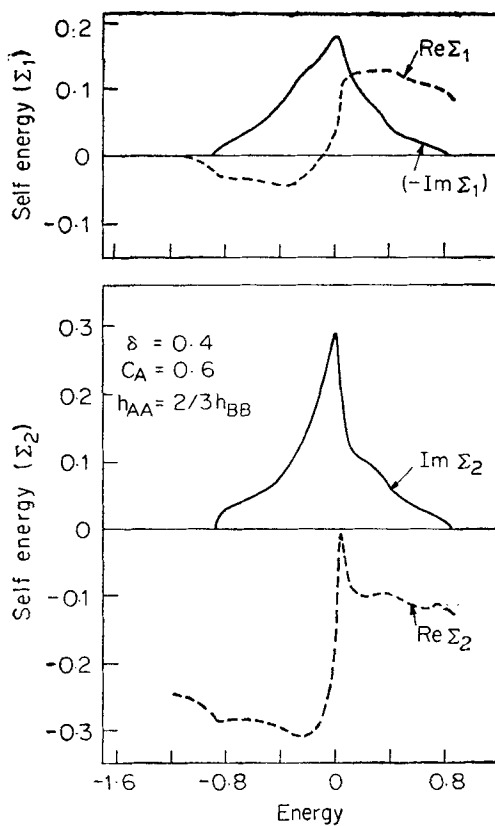


Figure 11. Plots of self energies versus energy for  $\delta=0.4$ ,  $C_A=0.6$  and  $h_{AA}=2h_{BB}/3$ .

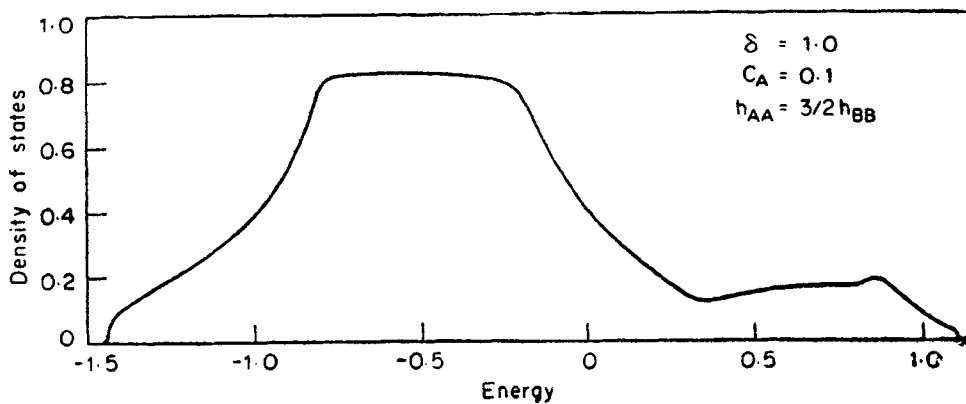


Figure 12. Plot of density of states versus energy for  $\delta=1$ ,  $C_A=0.1$  and  $h_{AA}=3h_{BB}/2$ .

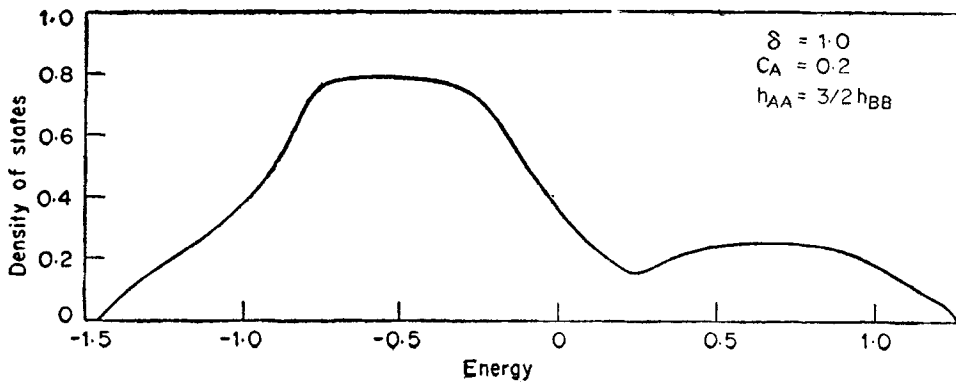


Figure 13. Plot of density of states versus energy for  $\delta=1$ ,  $C_A=0.2$  and  $h_{AA}=3/2 h_{BB}$ .

Non-analyticity does not occur in the particular examples shown in figures 12 and 13. It should not be concluded that inclusion of off-diagonal randomness removes the non-analyticity problem. It simply means that the particular choice of parameters in these cases was not the unfortunate one. The possibility remains open that there will be other sets of parameters where the non-analyticity conditions of §3 will be satisfied.

## 5. Conclusions

The two-site MCPA calculation presented here gives a fair idea about the effects of disorder in diagonal and off-diagonal parts of the Hamiltonian of a disordered binary alloy on the distribution of the electronic eigen-values. Our proof of the general result, that the effective medium theories that involve a self energy *matrix* should be non-analytic for certain sets of parameters, might help in the further development of the subject.

## Acknowledgements

Thanks are due to Dr D Kumar for fruitful discussions. Financial support from CSIR (India) is gratefully acknowledged. One of us (VS) would like to thank Science Research Council (UK) for financial aid during the course of this work.

## References

- Aiyer R N, Elliot R J, Krumbansl J A and Leath P L 1969 *Phys. Rev.* **181** 1006
- Anderson P W 1958 *Phys. Rev.* **109** 1492
- Beeby J L 1964 *Phys. Rev.* **135** A130
- Bloom P and Mattis D C 1977 *Phys. Rev.* **B15** 3633
- Blackmann J A, Esterling I M and Berk N F 1971 *Phys. Rev.* **B4** 2412
- Brouers F and Van der Rest J 1972 *J. Phys.* **F2** 1070
- Butler W H 1973 *Phys. Rev.* **B8** 4499

- Chen A B 1973 *Phys. Rev.* **B7** 2230  
Cyrot-Lackmann F and Ducastelle F 1971 *Phys. Rev. Lett.* **27** 429  
Cyrot-Lackmann F and Cyrot M 1972 *J. Phys.* **C5** L209  
Cyrot-Lackmann F 1974 *J. de Phys.* **35** C4-109  
Ducastelle F 1972a *J. de Phys.* **33** C3-269  
Ducastelle F 1972b *J. Phys.* **F2** 468  
Ducastelle F 1974 *J. Phys.* **C7** 1795  
Ehrenreich H and Schwartz L M 1976 *Solid State Physics* eds H Ehrenreich, F Seitz and D Turnbull (New York and London: Academic Press) **31** 149  
Elliott R J, Krumhansl J A and Leath P L 1974 *Rev. Mod. Phys.* **46** 465  
Foo E-Ni, Bose S M and Ausloos M 1973 *Phys. Rev.* **B7** 3454  
Foo E-Ni, Amar H and Ausloos M 1971 *Phys. Rev.* **B4** 3350  
Gaspard J P and Cyrot-Lackmann F 1977 *J. Phys.* **C6** 3077  
Horiguchi T, Chen C C and Morita T 1973a *Solid State Commun.* **12** 1243  
Horiguchi T, Chen C C and Morita T 1973b *Solid State Commun.* **13** 957  
Hwang H C and Sher A 1975 *Phys. Rev.* **B12** 5514  
Kirkpatrick S, Velicky B and Ehrenreich H 1970 *Phys. Rev.* **B1** 3250  
Krey U 1976 *Solid State Commun.* **18** 1047  
Kumar V and Joshi S K 1977 *Indian J. Phys. and Proc. of Indian Association for Cultivation of Science*, Commemoration vol. Part II  
Leath P L 1973 *J. Phys.* **C6** 1559  
Moorjani K, Tanaka T, Sokolski M M and Bose S M 1974a *J. Phys.* **C7** 1098  
Moorjani K, Tanaka T, Sokolski M M and Bose S M 1974b *J. de Phys.* **35** C4-153  
Muller-Hartmann E 1973 *Solid State Commun.* **12** 1269  
Nickel B G and Krumhansl J A 1971 *Phys. Rev.* **B4** 4354  
Nickel B G and Butler W H 1973 *Phys. Rev. Lett.* **30** 373  
Sen P N and Yndurain F 1976 *Phys. Rev.* **B13** 4387  
Shante V K S and Kirkpatrick S 1971 *Adv. Phys.* **20** 325  
Soven P 1966 *Phys. Rev.* **151** 539  
Soven P 1967 *Phys. Rev.* **156** 809  
Srivastava V and Joshi S K 1973 *J. Phys.* **F 3** L179  
Srivastava V and Weaire D L 1978 *Phys. Rev.* (in press)  
Stern E A and Zin A 1974 *Phys. Rev.* **B9** 1170  
Tsukada M 1961 *J. Phys. Soc. Jpn.* **26** 684  
Tsukada M 1972 *J. Phys. Soc. Jpn.* **32** 1475  
Velicky B, Kirkpatrick S and Ehrenreich H 1968 *Phys. Rev.* **175** 747  
Zittartz J 1974 *Solid State Commun.* **14** 51