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# Densities of electronic states for substitutionally disordered alloys

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**Abstract.** A formal treatment of the theory of the electronic density of states for substitutional alloys is considered and the results of applications to a simple case are presented. The method is self-consistent, simple in computation and readily extended to ternary and more complex alloys. Numerical examples are given for the tight-binding limit.

## 1. Introduction

Calculations of the density of electronic states in disordered systems have been an important topic for many years. Most progress has been made in the case of substitutional alloys, for which the Coherent Potential Approximation (CPA), first introduced by Soven [1] and Taylor [2], has been widely used. However, the CPA has a number of disadvantages, including concerns about multiple solutions to the self-consistent equations and difficulties with generalization. The nature of the CPA is not one which lends itself to a systematic extension and the only expansion parameter in this type of problem is the inverse of the number of near neighbours, which does not usually appear naturally in the formulation.

The approach used in this paper is based upon a particular procedure for carrying out the statistical averaging associated with site occupations in a random alloy. The underlying physical approximation is the muffin-tin approximation for the potential, for which an expansion of the total scattering can be undertaken in terms of the  $t$ -matrices associated with each site. The terms of the expansion represent all possible paths through the alloy involving a sequence of scatterings from sites. The difficulties of the approach are related to the need to deal with multiple returns to the same site and the fact that the interest is in the divergences of the series, which are dominated by higher, more complex terms.

There have been many papers presenting approaches which go some way towards solving this problem [1–6]. It is well known that a self-consistent approach is required to produce reasonable approximations to the density of states [7–9]. In determining the self-consistent procedure, it is necessary to evaluate averages of the terms in the series in a defined manner, which is usually aided by the use of diagrammatic techniques. This paper follows that standard approach using a formulation for evaluating averages which was presented earlier by one of us [10]. From this follows a self-consistent procedure based on defining effective scattering from each site which can be used with the free particle propagator to determine the density of states. This leads to densities of states which are very similar to those of the CPA but with the

essential difference of ease of computation. It is believed that this is a better starting point for calculations for alloys with short range order.

The primary step in this analysis is to consider the averaging process for scattering paths through the system which return repeatedly to a particular site. The method proposed for dealing with this averaging problem is explained in the next section. Section 3 describes how this leads to the definition of self-consistent scattering which can lead directly to the density of states. The essential difference between this method and the CPA is highlighted. Section 4 considers the nature of the approximation and the steps in using it as the first in a series of approximations. Numerical results, based on a simple iterative solution of the self-consistent equations, are presented in section 5. The results suggest that this first approximation is a very reasonable one and that there is no need to go beyond this step except in special circumstances, such as when there is local order in the alloy. A brief discussion completes the paper.

## 2. The scattering matrix approach

Some of the electronic properties of solids can be determined from the Green function or propagator and the electronic density of states is one such property. Many theories based on this approach use the simplification that the potential is assumed to have a muffin-tin form, which is to say that it is only non-zero outside non-overlapping spheres. As a result the spectral function  $\rho(\mathbf{k}, E)$  can be written exactly as an infinite series in the scattering matrices  $\mathbf{t}_i$  associated with the sphere of potential around  $\mathbf{R}_i$ . In the case where the energy is negative, which is the normal procedure for treating the tight-binding limit, the terms are all real and so the imaginary part only arises as a result of the divergence of the series. Thus the theoretical requirement is the identification of the most divergent sequence of terms. This paper attempts to identify those terms in a manner which follows a formulation of the substitutional alloy problem developed earlier by one of us [10, 11].

The defining equations are

$$\rho(\mathbf{k}, E) = -\frac{1}{\pi} \frac{1}{[E - k^2]^2} \text{Im}(\mathbf{T}) \quad (1)$$

where

$$\mathbf{T} = \sum_i \mathbf{t}_i + \sum_{i \neq j} \mathbf{t}_i \cdot \mathbf{G}_{ij} \cdot \mathbf{t}_j + \dots \quad (2)$$

With suitable algebraic manipulations [12] the  $\mathbf{t}$ -matrices in this equation can be replaced by energy-dependent functions derived from solving the wave equation in the given potential. These functions will still be labelled  $\mathbf{t}$  in the following discussion. The use of matrix notation in this equation allows for the case where the scattering potential has more than one angular momentum component. It is simpler in setting out the analysis which follows to consider only an s-wave scatterer so that the scattering may be represented by a scalar factor,  $t$ , which, of course, still depends upon energy. The full result can be obtained by taking the expressions at the end of the derivation which follows and reinstating the matrix notation.

As noted above, higher terms in the series (2) may be regarded as describing a path through the system of atoms and the simplest approximation in the disordered case is to assume that each scattering is entirely independent. This leads to the average  $t$ -matrix approximation (ATA) [13]. This is obviously incorrect when the scattering path includes more than one visit to the same site and indeed the predicted density of states is severely flawed in this model when the bandwidth is large compared to the splitting of the bound state energies of the constituent site potentials. To avoid this deficiency, there must be a correction for those paths which visit any site more than once and, in the more general case of local order, a correction is also required

when the path revisits the neighbourhood of a previous scattering site. Since, as noted, the imaginary part in (1) can only arise from the divergence of the series in (2), the task is to identify an approximation to the series which has similar divergences.

The approach to be explored in this paper is guided by a diagrammatic representation of the series and, in particular, the paths which include repeated scattering or their generalization in the case of local order. This is a problem which has been the subject of a number of different approaches over recent years [14–21]. For simplicity, local order will not be considered in the following discussion; it will be briefly considered later. In the absence of local order the probability function for the type of atom at a site can be defined in terms of the statistical ensemble representing the alloy under study. It will be supposed that there is a probability  $c_\alpha$  that the type of atom on any site is  $\alpha$ .

Consider a general term of the series (2) with a scattering sequence involving atoms  $i, j, k$ , etc. This must be averaged with the appropriate probability distribution, as indicated by the angular brackets in (1). If  $i, j, k \dots$  are all different, then the average will involve the probability distributions for the sites concerned. If, on the other hand, some of the sites are the same, say  $i = k$ , then a different set of probability distributions will be needed, the distribution of atom types at the *independent* sites in question. To put this into a formal expression, the type of atom at site  $i$  will be denoted  $a_i$ . The probability distribution for  $a_i$  is given by

$$p(a_i) = \sum_{\alpha} c_{\alpha} \delta_{a_i, \alpha}. \tag{3}$$

The equivalent expression for several sites is then

$$P(a_i, a_j, a_k, \dots) = \prod'_i p(a_i) \tag{4}$$

where the prime on the product means that only the independent sites  $i$  in the set  $i, j, k, \dots$  are included. Identification of the independent sites in the various terms of the expansion (2) is the principal requirement of the theory. The starting point for this work is to rewrite (4) in the form

$$\begin{aligned} P(a_i, a_j, a_k, \dots) &= \prod'_i p(a_i) \prod''_m [p(a_m) + 1 - p(a_m)] \\ &= \prod_i p(a_i) \prod''_m \left( 1 + \frac{1 - p(a_m)}{p(a_m)} \right) \end{aligned} \tag{5}$$

where the double prime indicates that the product, which is simply unity in the first line, runs over all of the dependent sites  $m$ . The final factor in the second line of this equation then takes direct account of the sequence of sites containing particular sites more than once. This dependent site product can be expanded to give

$$\prod''_m \left( 1 + \frac{1 - p(a_m)}{p(a_m)} \right) = 1 + \sum_m \left( \frac{1 - p(a_m)}{p(a_m)} \right) + \sum_{m,n} \left( \frac{1 - p(a_m)}{p(a_m)} \right) \left( \frac{1 - p(a_n)}{p(a_n)} \right) + \dots \tag{6}$$

where now  $m$  and  $n$  are different members of the sequence of dependent sites. The various terms of the expansion in (6) represent corrections to the treatment in which each scattering site is independent, and the identification of the most significant terms is the aim of the theory. Calculations based on this equation and using a diagrammatic approach were set out in [10] and were shown to give self-consistent results similar to those of the CPA. A specific method, closely related to that work, will be presented in the following section. Diagrammatic techniques have been widely used in dealing with this problem [7, 14] but the procedure just explained, with loops connecting dependent sites, shows particularly clearly the nature of the geometric problem.

### 3. Formal procedure

A random walk on a lattice in three dimensions will tend to move away from its initial site and so it can be qualitatively argued that diagrams containing multiple repeats will be less in number than those with fewer repeats. The larger the number of neighbours, the less likely the repeat sequence, so this is already a  $1/Z$  argument, where  $Z$  is the number of near neighbours. It is then possible to begin the calculation by concentrating on those diagrams which include multiple visits to one site only. If these were correctly accounted for, i.e. the probability distribution of equation (4) used, then the further corrections which would need to be included would have site sequences of the form  $i, j, i, j$  in which repeated visits to different sites are interleaved in some way. The terms requiring correction are only a small subset of the total number of site sequences, so it might be expected that they would not have a qualitative or even a large quantitative effect on the result.

To develop this approach, consider first a term with a sequence of sites which does not include any repeats, i.e. the set of dependent sites in (6) is empty. Retaining only these terms is simply the ATA. With such a sequence can be associated further sequences in which any particular site, say  $i$ , appears twice. The scatterings at  $i$ , together with the sequences of sites from  $i$  to  $i$  between scatterings, constitute a correction to the scattering at  $i$  in the first sequence. Further corrections arise from sequences with three, four or more appearances of site  $i$ . Taken together, these repeated visits to site  $i$  constitute a renormalization of the scattering at site  $i$  from  $t$  to an effective scattering,  $\tau$ , given schematically by

$$\tau + \tau S_- \tau + \tau S_- \tau S_- \tau + \dots = \langle t + t S_- t + t S_- t S_- t + \dots \rangle \quad (7)$$

where  $S_-$  describes the terms of the sequence between the two appearances of site  $i$  and will be discussed in the next paragraph. When  $t$  is replaced by  $\tau$  in this way it allows the scattering at site  $i$  to be represented without the need to determine whether it is the first or a subsequent appearance in the sequence. The first approximation to the required result is then to assume that every time  $t_i$  appears in a sequence it can be replaced by  $\tau$ . But site  $i$  was chosen arbitrarily and so the substitution can be made for every site in each scattering path. The  $T$ -matrix can then be written

$$T = \tau + \tau G \tau + \tau G \tau G \tau + \dots = \tau / (1 - G \tau) \quad (8)$$

and the density of states derived. The propagator or hopping components,  $G$ , are composed of factors such as  $G_{j,l} = G(\mathbf{R}_j - \mathbf{R}_l)$  and these represent the motion of an electron from one site to another. In these equations  $G$  corresponds to free particle motion. The process in equation (7) is self-consistent because of the implicit appearance of  $\tau$  in  $S_-$  as will now be explained.

The factor  $S_-$  represents the sum over all sequences which start and end at a particular site, such as  $i$ , but do not include intermediate returns to that site. Terms are of the general form  $G t G \dots t G$  and all intermediate sites are summed over. The primary assumption of this approach is that self-consistency can be achieved by replacing each  $t$ -matrix factor in the sequence by  $\tau$ , regardless of which site it refers to. Using the definition

$$G(\mathbf{k}) = \sum G(\mathbf{R}) \exp(i\mathbf{k} \cdot \mathbf{R}) \quad (9)$$

where the sum is over all lattice vectors, then the inverse transform can be written

$$G(\mathbf{R}) = \int G(\mathbf{k}) \exp(-i\mathbf{k} \cdot \mathbf{R}) \, d\mathbf{k} / v \quad (10)$$

provided that the lattice structure is perfectly ordered. The  $\mathbf{k}$ -integral is over the Brillouin zone of volume  $v$ . It is then straightforward to show that the sum over all returning diagrams which *do include* intermediate returns to the site  $i$ ,  $S_+$ , is given by

$$S_+ = \frac{1}{v} \int G^2(\mathbf{k}) \tau / [1 - \tau G(\mathbf{k})] \, d\mathbf{k}. \quad (11)$$

The required factor in which the sequences *do not include* returns to site  $i$  can then be evaluated from the remark that paths which do have intermediate returns to  $i$  can be made up from sequences of paths without intermediate returns. Inverting that result gives immediately

$$S_- = S_+ / [1 + \tau S_+] \quad (12)$$

remembering that each scattering factor at the site has been replaced by  $\tau$ . This result can be inserted into equation (7) to give the required effective scattering in this first approximation. Note that the energy is fixed in these equations so that only the values of the functions at a particular energy are required to solve the equations for that energy.

The difference between this approach and that of the CPA is readily illustrated in the tight-binding limit, in which case the inverse  $t$ -matrix is given to within a constant, which can be subsumed into the propagator, by  $t_i^{-1} = E - E_i$ . Then equation (7) can be written

$$1/(\tau^{-1} - S_-) = c_A/(E - E_A - S_-) + c_B/(E - E_B - S_-) \quad (13)$$

for a two-component alloy. This is the same equation as is used in the definition of the CPA, for example in equation (3.72) of [7]. However, in the CPA  $S_-$  is eliminated in order to give directly an equation for

$$\langle G(0) \rangle = 1/(\tau^{-1} - S_-). \quad (14)$$

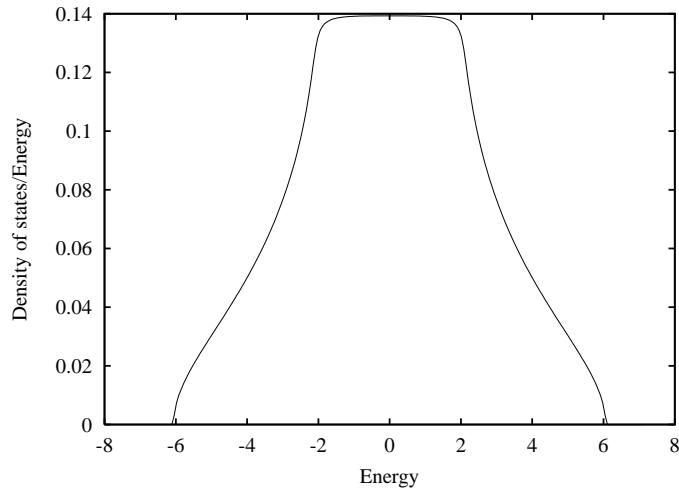
In this work, equations (9)–(13) are solved to give  $S_-$  and then  $\langle G(0) \rangle$  is subsequently calculated from equation (14). The self-consistency arises because of the dependence of  $S_-$  on  $\tau$ .

#### 4. Averaging and self-consistency

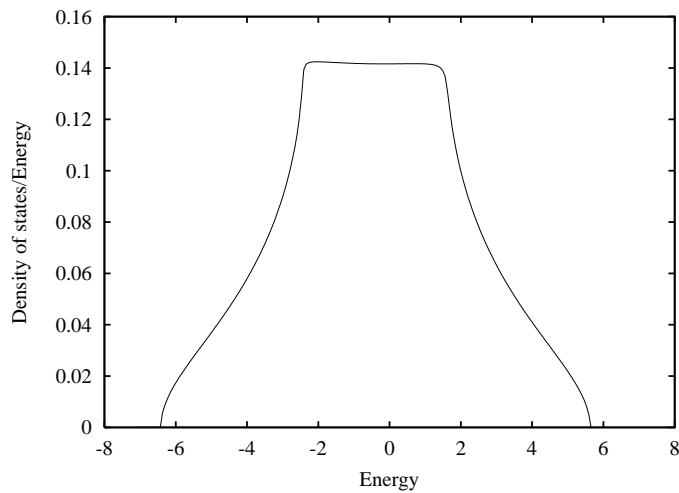
In the case where there is no correlation between the occupancy of sites, scattering at any site on a path can be treated independently. In the lowest order approximation this would mean using the average scattering, similar to the first-order term in (2). However, the analysis given in the previous section showed how the contributions of scattering paths involving returns to a site can be added to the scattering at that site to give an effective scattering, after averaging, of  $\tau$  as defined in equation (7). The use of  $\tau$  in place of  $t$  in equations (11) and (12) at sites other than the initial, particular site  $i$  is a self-consistent treatment which, as has already been noted, is very similar to the CPA. Physically, this represents the concept that as the electron moves through the lattice, it moves in a way that takes account of the presence of the neighbourhood of each scattering atom. In CPA terms this movement would be defined in terms of an effective potential.  $\tau$  may be complex, because of the denominator inside the integral (11).

The method shares a number of properties of the CPA. It does not distinguish between constituent atoms and so in the binary alloy case it is symmetric between  $c$  and  $(1 - c)$ . It gives a density of states which is properly normalized. If the bandwidth becomes small relative to the energy differences in a multi-component alloy then  $S_-$  becomes small and the density of states becomes a set of narrow bands about the energy levels each holding the number of states given by the appropriate concentration. The correction terms become smaller as  $Z$  increases, although, as discussed in the next section, the critical step of evaluating  $S_+$  requires a real lattice structure so that the large  $Z$  limit applies only by going to dimensions greater than three.

The approximation just described requires correction for those diagrams in which multiple visits to more than one site are interleaved. It can be noted that the first of these corrections in the present theory is the sequence  $i, j, i, j$  which is fourth order in  $t$  and is also the lowest order in which the CPA is not exact. However, this similarity does not imply that the approximations are the same, because the density of states is determined primarily by the divergence of higher terms in the series, which are treated differently in this work. The terms which are only approximate



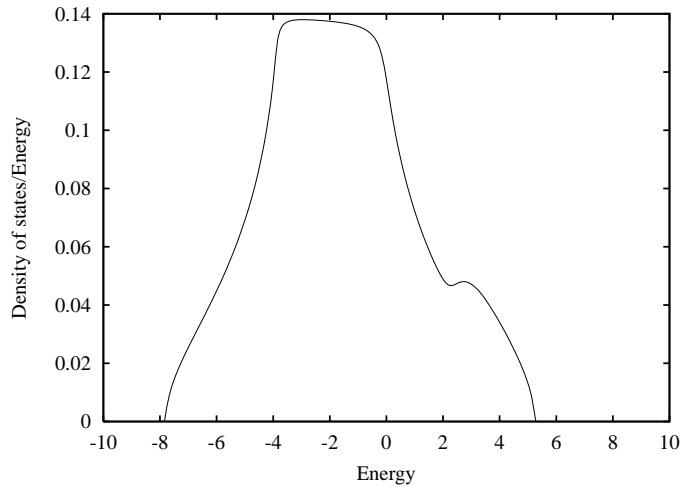
**Figure 1.** Density of states for a binary alloy;  $c_1 = c_2 = 0.5$ ,  $E_1 = 0.5$ ,  $E_2 = -0.5$ .



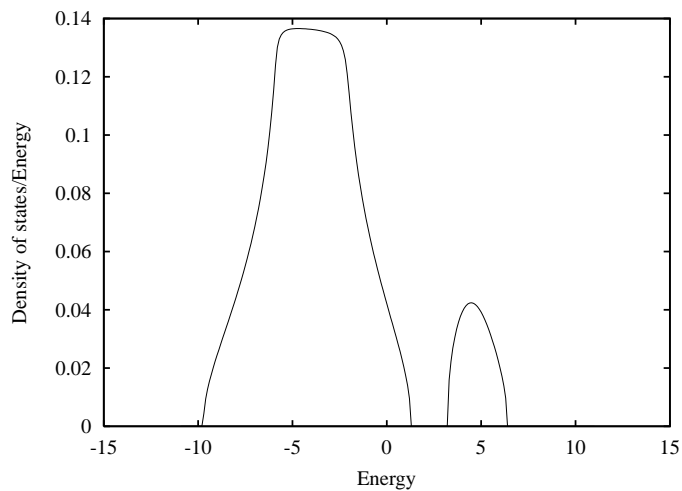
**Figure 2.** Density of states for a binary alloy;  $c_1 = 0.9$ ,  $c_2 = 0.1$ ,  $E_1 = 0.5$ ,  $E_2 = -0.5$ .

can be corrected using the diagram expansion which is derived from equation (6) and this constitutes the  $1/Z$  expansion already mentioned. This will lead both to a renormalization of  $\tau$  when applied to paths returning to the initial site and of  $G$  for paths terminating at a different site. The former renormalization is not too difficult and, in particular, continues to use the free particle propagator. Accordingly it is believed that this can be a useful step in improving the approximation, both in the presence and in the absence of local order. The renormalization of  $G$  is more complex, both algebraically and numerically, and the relative significance of this compared to modifying  $\tau$  has not yet been established. An important feature in this context is that the method allows a systematic development of increasingly accurate approximations. We intend to discuss this generalization of the approach in a future paper.

However, as will be shown in the next section, the lowest order approximation represented by equations (7), (11) and (12) is already very satisfactory. It gives densities of states with



**Figure 3.** Density of states for a binary alloy;  $c_1 = 0.9$ ,  $c_2 = 0.1$ ,  $E_1 = 2.0$ ,  $E_2 = -2.0$ .



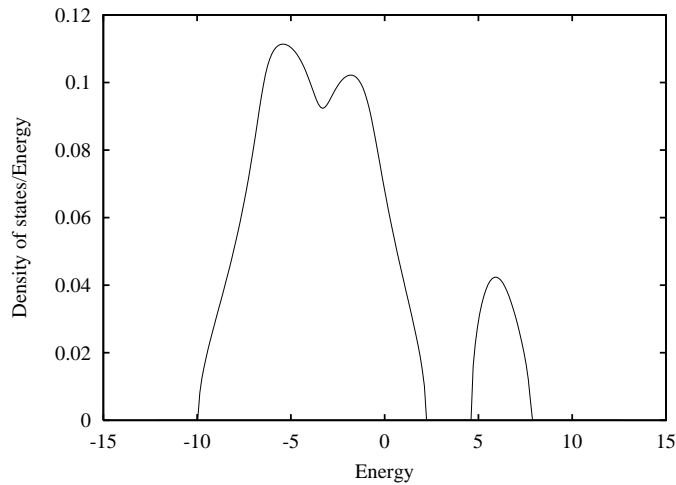
**Figure 4.** Density of states for a binary alloy;  $c_1 = 0.9$ ,  $c_2 = 0.1$ ,  $E_1 = -4.0$ ,  $E_2 = 4.0$ .

the expected characteristics and the self-consistency is easily achieved by a primitive iteration. Although the examples will be based on the tight-binding approximation, none of the numerical methods are dependent on that model.

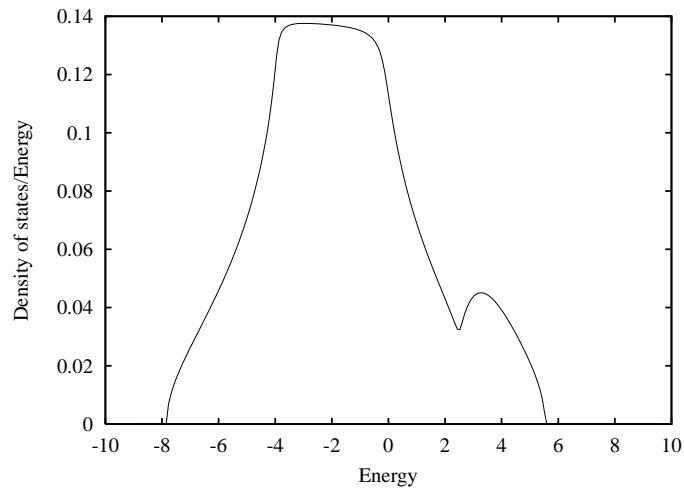
## 5. Numerical results

The density of states can be determined from the result (1) once a suitable approximation for  $\langle T \rangle$  has been established. It requires an integral over all  $\mathbf{k}$  corresponding to the fact that the electron wave functions have components with various  $\mathbf{k}$ -values differing by reciprocal lattice vectors. This integral can be simplified by taking the extreme tight-binding limit, in which case only the first Brillouin zone wave vectors contribute. Away from the tight-binding limit the  $\mathbf{k}$ -integral requires factors related to the radial wavefunction at the energy under consideration,





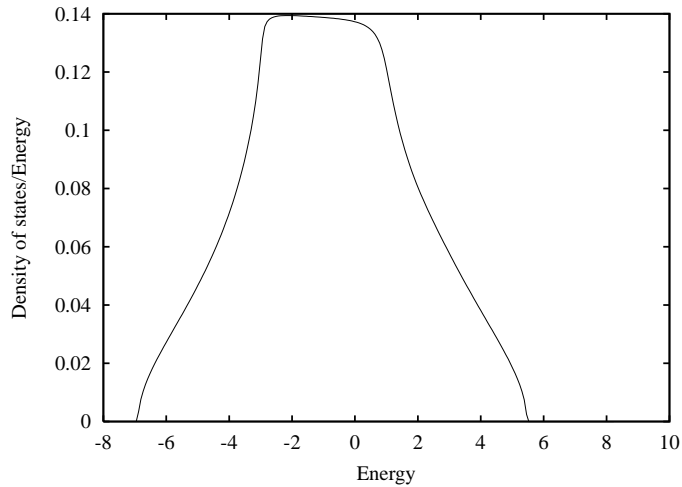
**Figure 5.** Density of states for a ternary alloy;  $c_1 = 0.5$ ,  $c_2 = 0.4$ ,  $c_3 = 0.1$ ,  $E_1 = -5.1$ ,  $E_2 = -2.0$ ,  $E_3 = 5.5$ .



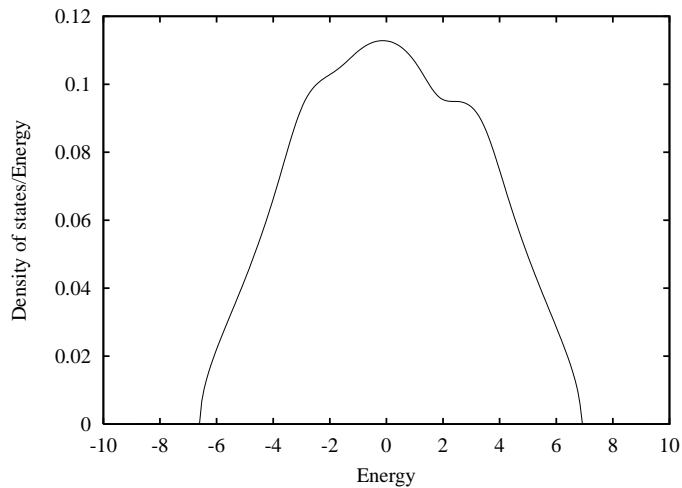
**Figure 6.** Density of states for a ternary alloy;  $c_1 = 0.5$ ,  $c_2 = 0.4$ ,  $c_3 = 0.1$ ,  $E_1 = -2.1$ ,  $E_2 = -2.0$ ,  $E_3 = 2.5$ .

as formulated in [12] but, as noted in sections 2 and 3, the self-consistent equations require only the values of the  $t$ -functions at the given energy. Thus the examples to be given below using the tight-binding limit are properly representative of the nature of this approach.

There are two energy scales in the binary alloy case—the bandwidth  $W$  and the splitting between the bound state energies  $\Delta E$ . When  $W/\Delta E$  is small, two separated bands are expected and when  $W/\Delta E$  is large, a single common band is expected. This is indeed shown by the numerical results using the first approximation of this paper. For simplicity a simple cubic lattice is used with unit hopping, so that the half-bandwidth is six. The calculation is begun for each value of energy by using a value for  $\tau$  which has an imaginary part. This is used to find  $S_-$  and hence a new value for  $\tau$ . After a few iterations this converges to a final value for  $\tau$  which is independent of the starting choice and from which the density of states can be



**Figure 7.** Density of states for a ternary alloy;  $c_1 = 0.5$ ,  $c_2 = 0.4$ ,  $c_3 = 0.1$ ,  $E_1 = -1.1$ ,  $E_2 = -1.0$ ,  $E_3 = 1.5$ .



**Figure 8.** Density of states for a ternary alloy;  $c_1 = 0.3$ ,  $c_2 = 0.4$ ,  $c_3 = 0.3$ ,  $E_1 = -2.1$ ,  $E_2 = 0.0$ ,  $E_3 = 2.5$ .

calculated. The integrals over the Brillouin zone can be simplified by calculating the function

$$p(h) = \int \delta(h - G(\mathbf{k})) d\mathbf{k} \quad (15)$$

which is independent of energy and only needs to be evaluated once.  $p(h)$  is, of course, the tight-binding density of states for the lattice used.

The results for binary alloys are presented in figures 1 to 4. Figure 1 is for a two-component alloy with equal concentrations.  $W/\Delta E = 12$  and the figure shows the band with a very similar shape to that of a perfect simple cubic lattice. Figures 2 to 4 show an alloy with  $c_1 = 0.9$ ,  $c_2 = 0.1$  with  $W/\Delta E = 12$ , 3 and 1.5 respectively. These show how the common band splits and the two halves pull apart, exactly as expected qualitatively. The iteration is not problematic in any of these cases although it does require a few more stages near band edges.

Figures 5 to 8 show some calculations for ternary alloys. In figure 5 the concentrations are 0.5, 0.4 and 0.1 with bound state energies  $-5.1$ ,  $-2.0$ ,  $+5.5$ . The figure shows a common band at the lower energy separated from the narrow band at the higher energy. When the energies are changed to  $-2.1$ ,  $-2.0$  and  $+2.5$  the bands begin to coalesce, as in figure 6, and when the energies are  $-1.1$ ,  $-1.0$  and  $+1.5$  there is a single common band. Figure 8 illustrates the case for different concentrations, 0.3, 0.4 and 0.3 with energies  $-2.1$ ,  $+0.0$  and  $+2.5$ . Again, these results give no problems with convergence of the iteration.

It is not straightforward to compare these results with those of the CPA. Although the method of this paper has iterated directly to a solution for all lattices tried, it fails for the artificial density of states on which most early papers were based [7, 14, 18]. Presumably this is because that function does not represent a true lattice so that  $S_+$  is not well defined. It can be seen from figures 2 to 4 that the dependence on  $W/\Delta E$  is the same as that for the published calculations, with the same ratio for the bands to separate.

If the  $t$ -matrix is not simply that of an s-scatterer, then the equations used are changed only by the replacement of the scalar variables  $\tau$ ,  $G$ ,  $t$ ,  $S_+$  and  $S_-$  by their appropriate matrix equivalents. No part of the derivation relied on the scalar properties.

## 6. Discussion

A simple approximation to allow calculations of the density of states in substitutional alloys, based on the lowest terms of a systematic treatment, has been derived. This has proved to be simple to use and to give good densities of states for a variety of alloys to which it has been applied. The theory has been developed in such a way that it can be extended to more complex systems, such as those with local ordering, and is not restricted to the tight-binding limit. Since each iteration takes place at a fixed energy all that needs to be known is the value of the  $t$ -matrix for each constituent at that energy. It is believed that the approach will be of value in those calculations of alloy properties which currently rely on the CPA.

## Acknowledgment

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