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Anderson localization in a model binary alloy

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The equation-of-motion method is applied to a random binary alloy represented by a simple tight-binding Hamiltonian in the split-band limit. The results suggest that Anderson localization occurs well above the percolation threshold, which was not predicted by previous analytic studies.

I. INTRODUCTION

In this paper we examine the problem of Anderson localization in a model binary-alloy system. The simplest Hamiltonian which may be applied to this problem is that of Anderson,[1] with diagonal elements taking two values, $\pm\frac{1}{2}\delta$, at randomly distributed A and B sites. We shall be dealing only with the limit of infinite δ, with attention focused on the A subband only. This will consist of states confined to the A sites and the Hamiltonian therefore takes the simple form

$$H_{AA} = \sum_{\substack{A \text{ atoms only} \\ i,j \text{ nearest} \\ \text{neighbors}}} V\,|\,i\rangle\langle j\,| . \tag{1.1}$$

The B atoms are thus formally removed from the problem. There is a critical concentration x_c of A atoms, below which they form only finite clusters. This is the well-known "percolation threshold."[2] For $x < x_c$ all states of the A subband are (trivially) localized. Above x_c, there is an infinitely connected network of A atoms but this still may not sustain extended eigenstates. Hence a second critical concentration, x_c', is expected, at which extended states first appear. The available estimates[3,4] of x_c' fall *below* x_c, which is clearly unacceptable.

We have applied the equation-of-motion method, as developed by Weaire and Williams,[5] to this problem, and have arrived at estimates of x_c' which fall well above the percolation threshold.

Before presenting the calculations we shall give a brief discussion of the special type of localized states described by Kirkpatrick and Eggarter.[6] These are peculiar to the case considered here and complicate, at least in principle, the interpretation of the results.

II. KIRKPATRICK-EGGARTER STATES AND THE PROBLEM OF DEGENERACY

In addition to the states which are confined to a finite cluster and those which are (exponentially) localized by disorder on an infinite cluster, one can have sharply localized states of the type illustrated in Fig. 1, whenever there are favorable configurations of B sites surrounding an A cluster. These particular examples are states at $E = 0$ and $\pm V$, but it is easy to see that such states can occur *anywhere* within the band (see also Hede and Tong[7]). It seems therefore that one must have localized and extended states coexisting in the same range of energy in this system, which is not thought to be possible for more general Hamiltonians.

These "hopscotch" states can be degenerate, which is not usually possible in a disordered system. In the adaptation of the equation-of-motion method to the localization problem,[5] it was assumed that there was no such degeneracy, so it is necessary to consider how it affects the results.

It was previously shown[5,8] that band averages of

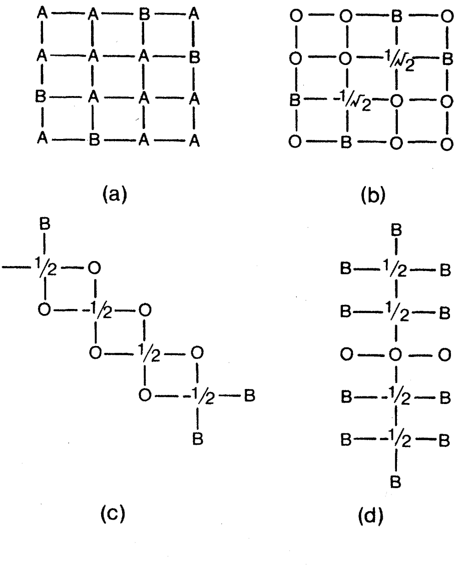

FIG. 1. Sketches of Kirkpatrick-Eggarter-type localized states in two dimensions. (a) A possible local configuration of A atoms is shown which is not isolated but supports a localized eigenstate, whose wave function is shown in (b). In (c) and (d) wave functions of larger localized eigenstates are shown.

the inverse participation number (the mean fourth power of the modulus of a wave function) could be calculated in terms of time averages of a randomly specified wave function. Specifically

$$\mathcal{P} = \frac{N}{2} \sum_i \left(2\langle p_i\rangle^2 - \langle p_i^2\rangle\right), \tag{2.1}$$

gives the average inverse participation number in terms of the average squared probabilities associated with sites i. Angular brackets, $\langle\,\rangle$, denote the time averaging.

It should first be noted that for a degenerate set of states the average inverse participation number is not invariant with respect to the choice of basis states for the set. In those cases, such as that of isolated atoms (giving degenerate states at $E=0$) for which *nonoverlapping* basis states can be chosen, the method gives the average inverse participation number of this particular set. Degenerate states not satisfying this condition will be comparatively rare, so they are perhaps not worthy of a detailed analysis. In fact, it can be shown that in general the method yields

$$c_1\mathcal{P}_1 + 2c_2\mathcal{P}_2 + 3c_3\mathcal{P}_3 + \ldots, \tag{2.2}$$

where there is a fraction c_1 of nondegenerate states and $\mathcal{P}_1$ is their average inverse participation number, a fraction c_2 of doubly degenerate states, etc. Here "average" includes the average with respect to choice of basis states.

This suffices to show all that is really necessary for the interpretation of results, namely that localization is diagnosed by this method as the departure of $\mathcal{P}$ from zero [or, more precisely, from $O(1/N)$].

III. STATES LOCALIZED ON ONE OR TWO ATOMS

We are working in the extreme split band limit ($\delta=\infty$) and x is the concentration of A atoms, hence x is also the total number of states per atom in the A subband. In the case of a square lattice xy^4 is the contribution of isolated A atoms to this total, where $y = 1-x$. It follows that

$$\mathcal{P}_1 = y^4. \tag{3.1}$$

States localized on two atoms are of two types, namely, those associated with isolated pairs of A atoms and the Kirkpatrick-Eggarter states. Following Kirkpatrick and Eggarter we obtain the contributions to $\mathcal{P}$ from all such two-site states,

$$\mathcal{P}_2 = xy^4(1-y^2) + x^2y^6 + xy^6. \tag{3.2}$$

Figure 2 shows these contributions as a function of x in the region of interest.

The single-site states can all be separated in the sense of Sec. II and so will be correctly included in our calculation. The same holds for the states on

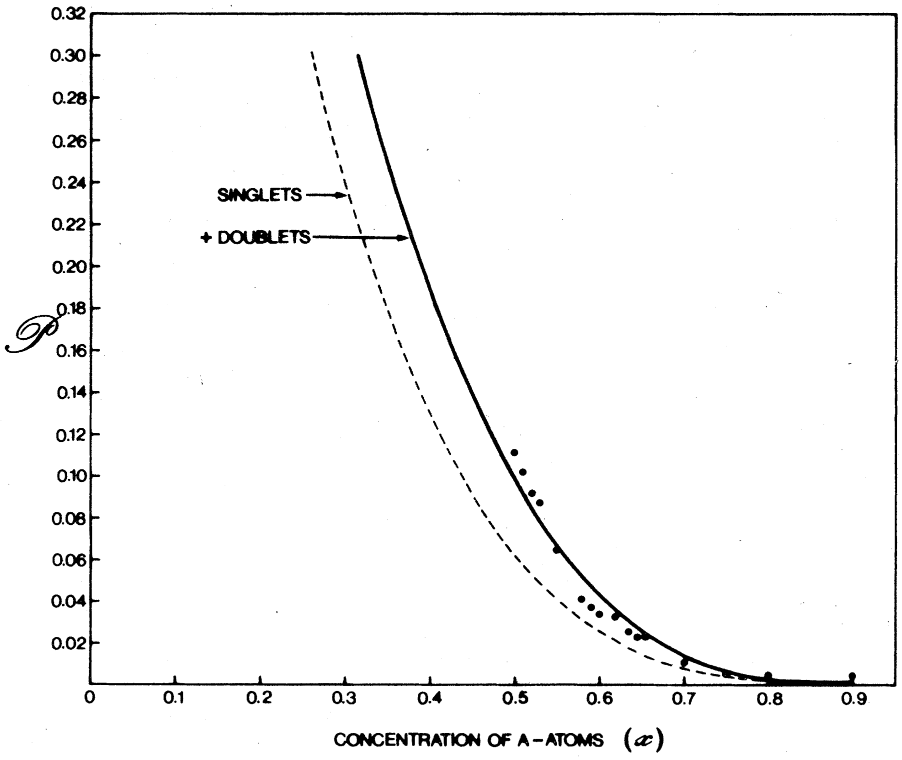

FIG. 2. Various crude numerical and analytical estimates of $\mathcal{P}$ (average of the inverse of number of sites participating in an eigenstate). Dotted line: contributions of isolated singlets; solid line: singlets together with doublets associated with isolated pairs and the Kirkpatrick-Eggarter states. The isolated points correspond to the enumerations of expression (3.3) with the help of computer generated random samples of size 25×27.

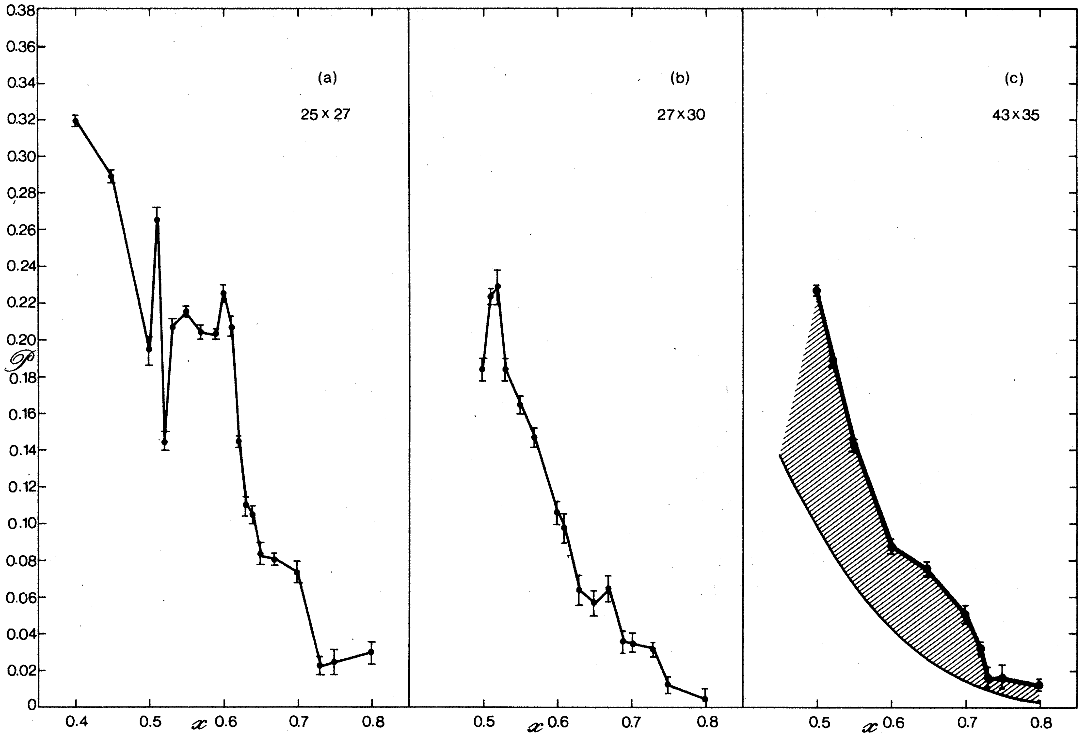

FIG. 3. The inverse participation number $\mathcal{P}$ averaged over the whole band of eigenenergies, vs x, the concentration of A atoms, for a square lattice of cell sizes 25×27, 27×30, and 43×35. The lighter curve in (c) is the estimate of the contribution of singlets and doublets to $\mathcal{P}$ as given in Fig. 2. The hatched area is indicative of the contribution to $\mathcal{P}$ from the states localized by disorder.

isolated pairs of sites that are degenerate at $E=\pm V$. Some of the two-site "hopscotch" states will not satisfy this condition but the proportion should be small. Degenerate sets arising from larger clusters or hopscotch configurations are relatively rare. Some indication of this is given by the points shown in Fig. 2 which are numerically calculated from

$$\mathcal{P}=n^{-1}, \tag{3.3}$$

where n is the average number of sites per cluster, for randomly generated samples of the system. This formula is obtained if we assume that each cluster of n sites supports n states uniformly distributed over it. This does not take account of the hopscotch states yet the agreement of the points with the solid line ($\mathcal{P}_1+\mathcal{P}_2$) is good.

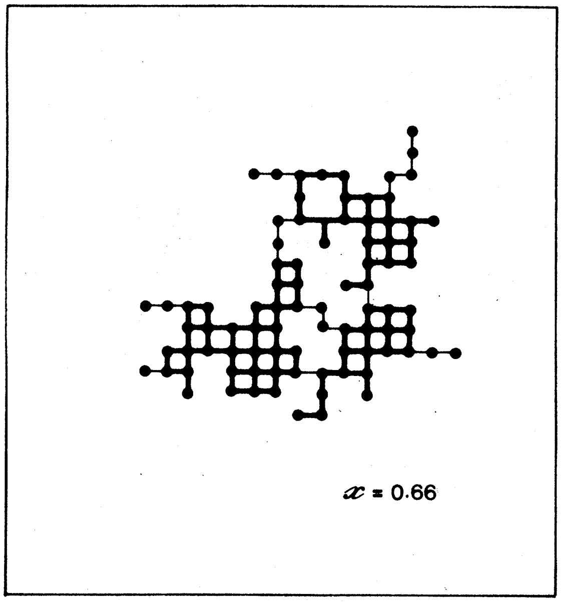

FIG. 4. Part of a computer generated random array with $x=0.66$. The A sites are shown by dots and the B sites are omitted. The thick lines denote the nearest neighbor bonding among the sites in a cluster. The clusters are weakly bonded with each other as indicated by the thin lines.

IV. RESULTS OF THE EQUATION-OF-MOTION METHOD

Figure 3 shows the variation of $\mathcal{P}$ [Eq. (2.1)] with concentration x of A atoms in samples of a square lattice of size 25×27, 27×30, and 43×35 with periodic boundary conditions. The dependence of the results on cell size was not systematic enough to enable us to extrapolate usefully to $N=\infty$. In interpreting the results we therefore focus on the largest system. It is seen that the calculated values of $\mathcal{P}$ significantly exceed the estimates given in the previous section, based on single-site and two-site states. This is especially true above the percolation threshold $x_c=0.59$.[2] We interpret this as indicating that extended states do not appear until $x_c' \simeq 0.73$, well above the percolation threshold.

How is this to be understood? If we take $x=0.66$, which lies in the range in question, the distribution of A sites is typically as in Fig. 4. Thus, although there is an infinite cluster, it is easily dissected into fairly compact (but irregular) clusters of about 20 sites which are very weakly connected. In the case shown, the clusters interact with about four other clusters, and these interactions are *via* only one nearest-neighbor interactions, or occasionally two. If we consider the coupling of eigenstates of individual clusters, assuming only those closest in energy need be included (in the style of Thouless[9]) we arrive at the following crude estimate of the strength of disorder in this transformed version of the problem.

$$\frac{\tilde{w}}{\tilde{z}\tilde{v}} \approx \frac{8V}{4V} \approx 2, \tag{4.1}$$

where $\tilde{w}$ is the width of distribution of energy levels which are coupled, $\tilde{z}$ is the number of nearest neighbors and $\tilde{v}$ is the coupling strength. Previous investigations[8] have shown that, in two dimensions, the critical value for Anderson transition is about 1.5. The estimate (4.1) exceeds this value, hence we may conclude that states are localized. The size of the constituent clusters sets the basic scale of this localization, which is consistent with our results.

The above argument is quantitatively crude but provides, we believe, a useful picture of Anderson localization above the percolation threshold.

We have also performed calculations for a 3*d* cubic lattice with cell size $9\times 10\times 11$, which gives rather similar but somewhat noisier results. We would deduce $x_c' \simeq 0.47$, in comparison with the percolation threshold[2] $x_c=0.31$.

We have examined the calculations in detail, to gain a better understanding of the statistical noise which is evident in Fig. 3. This appears to be associated with the sudden appearance or disappearance of small isolated clusters at particular values of x. It could, of course, be removed by a numerical average over different computer generated samples, but we have not yet done this.

V. CONCLUSION

Because of the average which is involved in the definition of the quantity we have calculated, our conclusion must remain tentative since it is possible that a small proportion of extended states appears at a lower value of x_c' than that which we proposed. More detailed calculations will be necessary in order to rule this out.

Finally we comment on the previous analytical results of Economou and co-workers.[3,4] Using the so-called $F(E)$ formula they found $x_c'=0.17$ and 0.12, respectively, for square and simple cubic lattices.[4] Later a modified formula[3] gave $x_c'=0.42$ and 0.25. The approximations involved in the use of coherent-potential-approximation self-energy[4] and coherent-potential-approximation Green's function[3] may be the reasons for such low values of x_c'. The coherent-potential approximation is well known to break down in the split band limit. Errors arising from the use of the coherent-potential-approximation Green's function in the localization problem were shown by Srivastava *et al.*[10]

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