

Density of States based on Dimensional Dilution Symmetry for
Disordered Hypercubic Lattices

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Abstract

Dilution symmetry of tight-binding hamiltonians in finite hypercubic lattices leads directly for pure systems to the convolution integral formula for the density of states in a given dimension. We explore consequences of this symmetry for the diagonally disordered models and propose approximate methods. We compare them numerically with the Dean's method. Our approach requires very little computer time and in spite of implicit approximations gives fairly good results.

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I. Introduction

Recently Pastawski and Wiecko¹ have pointed out a new view on a rather classical problem in solid state physics, namely that of a tight-binding hamiltonian on a finite hypercubic lattice. It was shown there that the matrix hamiltonian related to a finite system showed self-similarity or dilution symmetry as a function of dimension. This leads to a hierarchical tree for the eigenvalues which means that those corresponding to a higher dimension can be derived from those of the preceding one by a very simple and numerically cheap algorithm. For the density of states the method is equivalent to the convolution formula, namely:

$$N_d(E) = \int N_1(E-E') N_{d-1}(E') dE'$$

Where $N_d(E)$ is the density of states in d dimension. However, the method of Ref. 1 reduces it to finite sums.

The purpose of the present paper is to explore the above point of view in diagonally disordered systems.^{2,3} There, self-similarity is not perfect due to the randomness of the matrix elements. However, the structure, due to the fact that we are still dealing with a hypercubic lattice, is conserved, and at least on the average, the same dilution symmetries persist as in the pure case.

We develop approximate methods based on the dilution symmetry which start from the knowledge of eigenvalues in one dimension. Due to this, in a disordered system, as all the states are localized in one dimension,⁴ any approximate extension to higher

dimension cannot give information about mobility edges. On the other hand, as the methods derived in what follows start from exact results in one dimension and then build up results in higher dimensions, they will lead to results less exact with the growing dimension. Nevertheless, the qualitative features are correctly obtained in a 3-d as we will show below.

In section II we develop a new formulation based on a matrix representation of the tight-binding hamiltonian which leads to a description in terms of direct products of matrices associated with each dimension element (sites on a chain, rows in a plane, planes in a cube, ect.). We can think of a direct product taken in such a way as to be equivalent to the dilution symmetry pointed out in Ref. 1. We apply the formalism first to the ordered case and it leads there to the convolution formula for the density of states as pointed out above. Next we study another exact case, namely that where the diagonal energy elements are a sum of terms, each coming in a separate way from an isolated dimension. We call it the separable variable problem.

In section III we apply the formalism to the diagonal disorder problem. There, some approximations have to be introduced and we study several possibilities.

In section IV we show numerical results for the diagonal disorder case, both with the square box Anderson² distribution of disorder and with the gaussian one. Different approximations are compared with the numerical calculation by the classical method of Dean⁵ which gives exactly the integrated density of states using the negative eigenvalue theorem, both for the density of states

and for the tail behavior explicitly as shown by the integrated density of states.

In section V we present a different approximation scheme for the diagonal disorder case, which explicitly takes into account the localization properties of the states. It therefore gives excellent results for the minority component of the binary disordered alloy.

Numerical results are shown in section VI.

Finally we give the conclusions.

We must mention that the study in terms of direct products is on the same line of thought as the work of Schwalm and Schwalm⁶ performed for the Green's functions.

II. The formalism

The tight-binding hamiltonian in site representation reads:

$$H = \sum_{\bar{\ell}} \epsilon_{\bar{\ell}} |\bar{\ell}\rangle \langle \bar{\ell}| + \sum_{\bar{\ell}, \bar{\ell}'} V_{\bar{\ell}, \bar{\ell}'} \left[|\bar{\ell}'\rangle \langle \bar{\ell}| + |\bar{\ell}\rangle \langle \bar{\ell}'| \right] \quad (1)$$

where $\epsilon_{\bar{\ell}}$ is the on-site energy and $V_{\bar{\ell}, \bar{\ell}'}$ are the hopping integrals.

In what follows we will analyze the tridimensional case, but the generalization for other dimensions is straightforward. Thus, each site on a 3-d cubic lattice can be labelled as

$$\bar{\ell} = i, j, k \quad (2)$$

with i meaning sites, j meaning rows and k meaning planes. Therefore:

$$\varepsilon_{\bar{\ell}} \rightarrow \varepsilon_{i,j,k} \quad |\bar{\ell}\rangle \rightarrow |ijk\rangle \quad (3)$$

The hopping integrals are:

$$V_{ijk, i\pm 1 jk} \rightarrow \text{between sites}$$

$$V_{ijn, ij\pm 1k} \rightarrow \text{between rows}$$

$$V_{ijk, ijk\pm 1} \rightarrow \text{between planes}$$

Explicitly we get in this notation:

$$\begin{aligned} H = \sum_{ijk} \varepsilon_{ijk} |ijk\rangle\langle ijk| + V_{ijk, i+1jk} [|ijk\rangle\langle i+1jk| + |i+1jk\rangle\langle ijk|] \\ (4) \\ + V_{ijk, ij+1n} [|ijk\rangle\langle ij+1n| + |ij+1n\rangle\langle ijk|] + V_{ijk, ijk+1} [|ijk\rangle\langle ijk+1| \\ + |ijk+1\rangle\langle ijk|] \end{aligned}$$

We now define in terms of projectors the matrices:

$$A_i = |i\rangle\langle i| \quad (5)$$

$$B_i = |i\rangle\langle i+1| + |i+1\rangle\langle i|$$

In this notation the 1-d hamiltonian reads:

$$H^{(1)} = \sum_{i=1}^N \epsilon_i A_i + \sum_{i=1}^{N-1} V_{i,i+1} B_i \quad (6)$$

Now we go to 3-d and introduce the formalism of direct products which reflects the dilution symmetry of the hypercubic lattice. It means that we write projectors in terms of direct products:

$$|ijk\rangle = |i\rangle \otimes |j\rangle \otimes |k\rangle \quad (7)$$

and with the definition (5) the hamiltonian reads:

$$\begin{aligned} H^{(3)} = & \sum_{i=1}^N \sum_{j=1}^N \sum_{k=1}^N \epsilon_{ijk} A_k \otimes A_j \otimes A_i + \sum_{i=1}^{N-1} \sum_{j=1}^N \sum_{k=1}^N V_{ijk, i+1jk} A_k \otimes A_j \otimes B_i \\ & + \sum_{i=1}^N \sum_{j=1}^{N-1} \sum_{k=1}^N V_{ijk, ij+1k} A_k \otimes B_j \otimes A_i + \sum_{i=1}^N \sum_{j=1}^N \sum_{k=1}^{N-1} V_{ijk, ijk+1} B_k \otimes A_j \otimes A_i \end{aligned} \quad (8)$$

a) The ordered case

In the ordered case we have:

$$\epsilon_i = \epsilon \quad (9)$$

$$V_{ijk, i+1jk} = V_{ijk, ij+1k} = V_{ijk, ijk+1} = V$$

using the fact that $I = \sum_i A_i$ and taking $\epsilon = 0$, $V = 1$, the 3-d ordered hamiltonian reads:

$$H_o^{(3)} = I \otimes I \otimes H_o^{(1)} + I \otimes H_o^{(1)} \otimes I + H_o^{(1)} \otimes I \otimes I \quad (10)$$

where $H_o^{(1)}$ is the 1-d ordered hamiltonian.

As the members of sum (10) commute they can be diagonalized separately. If P is a unitary matrix and $D_o = P^{-1} H_o P$ with

$$D_o = \sum_i E_i^o A_i \quad (11)$$

where E_i^o are the eigenvalues, we get:

$$D_o^{(3)} = P^{(3)-1} H_o^{(3)} P^{(B)} = I \otimes I \otimes D_o + I \otimes D_o \otimes I + D_o \otimes I \otimes I \quad (12)$$

with

$$P^{(3)} = P \otimes P \otimes P \quad (13)$$

Using (11) we get:

$$D_o^{(3)} = \sum_{i=1}^N \sum_{j=1}^N \sum_{k=1}^N (E_i^o + E_j^o + E_k^o) A_k \otimes A_j \otimes A_i \quad (14)$$

Thus we have the result that the eigenvalues of the 3-d ordered case can be obtained as sums of eigenvalues of the 1-d ordered hamiltonian. This is equivalent to the result of Ref.(1).

From here it is immediate to say that the density of states of the high dimensional system is a convolution of lower dimensional systems:

$$\begin{aligned}
N_o^{(3)}(E) &= \int N_o^{(1)}(E') N_o^{(2)}(E-E') dE' = \\
&= \iint N_o^{(1)}(E') N_o^{(1)}(E'') N_o^{(1)}(E-E'-E'') dE' dE''
\end{aligned} \tag{15}$$

b) The separable variable problem

This problem consists in having:

$$\varepsilon_{ijk} = \alpha_i + \beta_j + \gamma_k \tag{16}$$

and

$$\begin{aligned}
V_{ijk, i+1jk} &= V_{ii+1}^\alpha \\
V_{ijk, ij+1k} &= V_{jj+1}^\beta \\
V_{ijk, ijk+1} &= V_{kk+1}^\gamma
\end{aligned} \tag{17}$$

In this case we have in 3-d:

$$\begin{aligned}
H_{sv}^{(3)} &= \sum_{ijk} \alpha_i A_k \otimes A_j \otimes A_i + \beta_j A_k \otimes A_j \otimes A_i + \gamma_k A_k \otimes A_j \otimes A_i \\
&+ V_{ii+1}^\alpha A_k \otimes A_j \otimes B_i + V_{jj+1}^\beta A_k \otimes B_j \otimes A_i + V_{kk+1}^\gamma B_k \otimes A_j \otimes A_i
\end{aligned} \tag{18}$$

Due to the separable energies (eq. 16), we get: /

$$H_{sv}^{(3)} = I \otimes I \otimes \left[\sum_{i=1}^N \alpha_i A_i + \sum_{i=1}^{N-1} V_{ii+1}^\alpha B_i \right] + I \otimes \left[\sum_{j=1}^N \beta_j A_j + \sum_{j=1}^{N-1} V_{jj+1}^\beta B_j \right] \otimes I \tag{19}$$

$$+ \left[\sum_{k=1}^N \gamma_k A_k + \sum_{k=1}^{N-1} v_{kk+1}^\gamma B_k \right] \otimes I \otimes I$$

We can gather the one dimensional hamiltonians from here:

$$H_\alpha^{(1)} = \sum_{i=1}^N \alpha_i A_i + \sum_{i=1}^{N-1} v_{ii+1}^\alpha B_i; \text{ etc.} \quad (20)$$

and get

$$H_{sv}^{(3)} = I \otimes I \otimes H_\alpha^{(1)} + I \otimes H_\beta^{(1)} \otimes I + H_\gamma^{(1)} \otimes I \otimes I \quad (21)$$

Again we can diagonalize each term separately due to the fact that they commute and get:

$$D_{sv}^{(3)} = P_{sv}^{(3)-1} H_{sv}^{(3)} P_{sv}^{(3)} = I \otimes I \otimes D_\alpha^{(1)} + I \otimes D_\beta^{(1)} \otimes I + D_\gamma^{(1)} \otimes I \otimes I \quad (22)$$

with

$$P_{sv}^{(3)} = P_\alpha \otimes P_\beta \otimes P_\gamma \quad (23)$$

and

$$D_{sv}^{(3)} = \sum_{ijk} \left[E_i^\alpha + E_j^\beta + E_k^\gamma \right] A_k \otimes A_j \otimes A_i \quad (24)$$

Again the density of states is the convolution:

$$N_{sv}^{(3)}(E) = \iint N_\alpha^{(1)}(E') N_\beta^{(1)}(E'') N_\gamma^{(1)}(E-E'-E'') dE' dE'' \quad (25)$$

In Ref. 1 a hierarchical tree as function of dimension was presented for the eigenvalues for the pure case. There, each 'generation' was given by the increasing dimension and the eigenvalues at each step were obtained by summing up to each eigenvalue of the immediately lower dimension the same set of eigenvalues of a 1-d chain. In the present case of the separable variable problem a hierarchical tree can be constructed as well. Now at each generation, however, different set of eigenvalues will be summed up.

A physical example of the separable variable problem is the superlattice where:

$$\beta_j = \gamma_k = \text{constant} \quad (28)$$

and α_i is a function of the site position i . In the superlattice we can have disorder or modulation in one direction and a translational symmetry in the other directions. Usually this problem is solved by reducing it to a 1-d problem through Fourier transforming in the ordered directions.

III. Application to the diagonal disorder case

After having discussed two models where through the property of the dilution symmetry the density of states can be generated by convolution of the 1-d problems exactly, we now proceed to study the possible approaches in the same spirit to the diagonally disordered tight-binding model.^{2,3}

The hamiltonian reads:

$$H_D^{(3)} = \sum_{ijk} \epsilon_{ijk} A_k \otimes A_j \otimes A_i + A_k \otimes A_j \otimes B_i + A_k \otimes B_j \otimes A_i + B_k \otimes A_j \otimes A_i \quad (27)$$

where ϵ_{ijk} are random numbers with $\langle \epsilon_{ijk} \rangle = 0$ and $\langle \epsilon_{ijk}^2 \rangle = W^2$,

In the disordered case we are forced to make some approximations. We make them through two different approaches leading to respectively two kinds of treatments.

One view is to propose successive approximations: 1) the convolution of the distribution of disorder with the density of states of the pure system; 2) the convolution of the 1-d disordered density of states with the one of the pure system in the immediately previous dimension (1-dimensional disorder approximation, 1-DDA);... n+1) the convolution of the n-dimensional disordered density of states with that of the d-n dimensional pure system (n-DDA); etc..

The other point of view consists in approximating the random sequence ϵ_{ijk} by one which can be expressed as a separable variable problem and then make the convolution as in eq.(25) (separable variable approximation, SVA).

Let us analyze them:

a1) Approximation of the convolution of the pure system with the distribution of disorder

We write:

$$H_D^{(3)} = \sum_{ijk} \epsilon_{ijk} A_k \otimes A_j \otimes A_i + H_o^{(3)} = H_D + H_o^{(3)} \quad (28)$$

supposing

$$\begin{bmatrix} H_D & H_o^{(3)} \end{bmatrix} \approx 0 \quad (29)$$

which is true if we average it in the disorder distribution. Then, within this assumption, we can diagonalize each hamiltonian, H_D and H_o , separately and take as an approximation for the eigenvalues the sum of the eigenvalues of the 3-d ordered case and the random sequence ϵ_{ijk} . It means:

$$E_D^{(3)} \approx (E_o^{(3)})_{ijk} + \epsilon_{ijk} = E_i^o + E_j^o + E_k^o + \epsilon_{ijk} \quad (30)$$

For the averaged density of states it means:

$$N_{D(E)}^{(3)} \approx \int N_o^{(3)}(E-E') \rho_w(E') dE' \quad (31)$$

where $\rho_w(E)$ is the probability distribution of the ϵ_{ijk} . This approximation is exact for the Lorentz distribution as was shown by Lloyd.⁷

a2) The one dimensional disorder approximation (1-DDA)

We can make a better approximation than the previous one by taking:

$$H_D^{(3)} = H_D^{(1)} + H_o^{(2)} \quad (32)$$

with

$$H_o^{(2)} = I \otimes H_o^{(1)} \otimes I + H_o^{(1)} \otimes I \otimes I \quad (33)$$

and

$$H_D^{(1)} = \sum_{jk} A_k \otimes A_j \otimes \left(\sum_i \varepsilon_{ijk} A_i + B_i \right) = \sum_{jk} A_k \otimes A_j \otimes H_{jk}^{(1)} \quad (34)$$

As $H_D^{(1)}$ represents an ensemble of non-interacting chains, we can diagonalize it with:

$$P_D^{(1)} = \sum_{jk} A_k \otimes A_j \otimes P_{jk} \quad (35)$$

with P_{jk} so that $P_{jk}^{-1} H_{jk}^{(1)} P_{jk} = D_{jk}$, which is a diagonal matrix with the eigenvalues of $H_{jk}^{(1)}$. The approximation we make here is to suppose that:

$$\left[H_D^{(1)}, H_o^{(2)} \right] \approx 0 \quad (36)$$

This is true when the configurational average is performed. Accepting the approximation, and proceeding as in the previous cases, we get:

$$E_D^{(3)} \approx (E_o^{(2)})_{jk} + (E_D^{(1)})_{ijk} = E_j^o + E_k^o + (E_D^{(1)})_{ijk} \quad (37)$$

and for the averaged density of states:

$$N_D^{(3)} \approx \int N_O^{(2)}(E') N_D^{(1)}(E-E') dE' \quad (38)$$

This method allows for the numerical evaluation of the density of states by the sum of eigenvalues (eq.(37)) or analytically from eq.(38) where the density of states of a one dimensional chain can be obtained from the formula of Dyson-Schmidt.⁸ In practice however, this also requires a numerical procedure as in the work of Gubernatis et al..⁹

In other words, the approximation consists in adding the disordered chain eigenvalues to each eigenvalue of the ordered 2-d system.

b) The separable variable approximation (SVA)

As discussed previously in section 2 the problem of separable variables can be solved exactly. We apply it now to the disordered system given by Eq.(27).

The approximation¹⁰ reads:

$$\epsilon_{ijk} \approx \alpha_i + \beta_j + \gamma_k \quad (39)$$

$$\langle \alpha_i \beta_j \rangle = \langle \beta_j \gamma_k \rangle = \langle \alpha_i \gamma_k \rangle = 0$$

This approximation for ϵ_{ijk} means to introduce correlations between sites whereas they are absent in the original model:

$$\langle \epsilon_{ijk} \epsilon_{i',j',k'} \rangle = \langle \alpha_i^2 \rangle \delta_{ii'} + \langle \beta_j^2 \rangle \delta_{jj'} + \langle \gamma_k^2 \rangle \delta_{kk'} \quad (40)$$

Taking

$$\langle \alpha_1^2 \rangle = \langle \beta_j^2 \rangle = \langle \gamma_k^2 \rangle = W_1^2 \quad (41)$$

we have

$$\langle \epsilon_{ijk}^2 \rangle = W_3^2 = 3W_1^2 \quad (42)$$

In this way the problem is solvable as shown in section 2.b. Thus, in this approximation the eigenvalues are obtained by adding three disordered one dimensional chains:

$$E_D^{(3)} \approx (E_D^{(1)})_i + (E_D^{(1)})_j + (E_D^{(1)})_k \quad (43)$$

In general the disorder distribution for ϵ_{ijk} is different than the distribution taken for $\alpha_1, \beta_j, \gamma_k$ of the starting chains. The approximation of eq. (39) requires that the probability distribution of the 3-d site energy variable should be the convolution of the probability distributions of the chain site energy variables. In the case of a gaussian distribution its form is conserved by successive convolutions with the only change of the standard deviation (i.e. when $\alpha_1, \beta_j, \gamma_k$ are random gaussian variables with width W , the resulting ϵ_{ijk} is also a gaussian but with width $\sqrt{3} \cdot W_1$).

Thus, when the disorder distribution is a gaussian of width W , the density of states in the SVA reads:

$$N_D^{(3)}(E, W) \approx \int dE' \int dE'' N_D^{(1)}(E', \frac{W}{\sqrt{3}}) N_D^{(1)}(E'', \frac{W}{\sqrt{3}}) \cdot N_D(E-E'-E'', \frac{W}{\sqrt{3}}) \quad (44)$$

IV. - Numerical Results for the Disordered problem by the 1-DDA and the SVA

Here we will check numerically the 1-DDA and the SVA proposed in the previous section.

First we will compare computational results for the 3-d density of states with the diagonal Anderson disorder.² The distribution of the on-site energies is:

$$\rho_W^A(\epsilon_{ijk}) = \begin{cases} 1/W & \text{if } |\epsilon_{ijk}| \leq \frac{W}{2} \\ 0 & \text{if } |\epsilon_{ijk}| > \frac{W}{2} \end{cases} \quad (45)$$

In Fig. 1 we show the results of the method 1-DDA and the method SVA for different values of disorder. These results can favourably compare with those given by Hu et al.¹¹ using the method of Dean⁵. For the central part of the density of states we find a very good agreement with Ref. 11. However, the tails in our treatment die less abruptly. We must point out that in the SVA the final distribution for the diagonal elements is not exactly the square box distribution and so we are in some way forcing the comparison. Nevertheless, the agreement is quite reasonable.

We next compare the methods for the gaussian distribution (where the SVA can be applied without problems) defined as:

$$\rho_W^G(E) = \frac{1}{\sqrt{2\pi} \cdot W} e^{-\varepsilon^2/2W^2} \quad (46)$$

with the exact numerical results obtained with the method of Dean.

In Fig. 2 we show the results of our approximations for the density of states for a given disorder W together with the exact result. In Fig. 3 we show the integrated density of states where some discrepancies in the tails can be evaluated for the two methods. Except these discrepancies in the tails, we see good agreement with the exact Dean's results for both approximations. Also we see, that the results get better with the increasing disorder, which is reasonable, due to the fact that our starting point in both methods is the 1-d disordered chain where all the states are localized⁴, and in 3-d we have localization for all the eigenstates above the Anderson transition ($W > W_c$).^{2,3}

The great advantage of our approximate methods with respect to the Dean's exact method is the enormous save of computer time (of about four orders of magnitude). In our examples we take relatively small samples in order to be able to compare with the Dean's method which is time consuming. But with our approximations we can perform the calculation on big samples with very reasonable computer times.

V.- The Alternative localized Eigenstates Approximation (LEA)

We want to present here an alternative method for the problem of diagonal disorder based explicitly on the localization properties of the states in one dimension. This method can be easily developed with the formalism introduced in section 2

although it does not lead to a convolution formula for the density of states.

We start with the hamiltonian for the diagonal disorder as defined in Eq. (27), and explicitly separate in it the block hamiltonians corresponding to chains in the x-direction of the terms including hopping between them in the other directions, by writing:

$$\begin{aligned}
 H_D^{(3)} &= \sum_{jk} A_k \otimes A_j \otimes \left[\sum_l \epsilon_{ljk} A_l + B_l \right] + \sum_{ljk} A_k \otimes B_j \otimes A_l + B_k \otimes A_j \otimes A_l \quad (47) \\
 &= \sum_{jk} A_k \otimes A_j \otimes H_{jk} + \sum_{ljk} A_k \otimes B_j \otimes A_l + B_k \otimes A_j \otimes A_l
 \end{aligned}$$

First we diagonalize these 1-d hamiltonians H_{jk} by:

$$P_{jk}^{-1} H_{jk} P_{jk} = D_{jk} = \sum_l \epsilon_{ljk}^{(1)} A_l \quad (48)$$

where we order the eigenvalues $\epsilon_{ljk}^{(1)}$ of a given jk -chain with the index l which corresponds to the site of localization of the respective eigenvector. In doing this we have made the hypothesis that all the eigenstates are localized on different sites.

Next we apply to the over-all hamiltonian of Eq.(47) the ortogonal transformation:

$$P^{(1)} = \sum_{jk} A_k \otimes A_j \otimes P_{jk} \quad (49)$$

where, due to the ordering we have taken for the eigenvalues, the rows of P_{jk} corresponding to eigenstates of H_{jk} are ordered according to its site of localization. After applying (49) we have:

$$\begin{aligned}
 H_D^{(3)'} = P^{(1)-1} H_D^{(3)} P^{(1)} = \sum_{\ell jk} \epsilon_{\ell jk}^{(1)} A_k \otimes A_j \otimes A_\ell + \sum_{jk} A_k \otimes L_j \otimes P_{jk}^{-1} \\
 + \sum_{jk} A_k \otimes R_j \otimes P_{jk}^{-1} P_{j+1k} + \sum_{jk} L_k \otimes A_j \otimes P_{jk+1}^{-1} P_{jk} + \sum_{jk} R_k \otimes A_j \otimes P_{jk}^{-1} P_{jk+1}
 \end{aligned} \quad (50)$$

with

$$L_j = |j+1\rangle\langle j| \quad (51)$$

$$R_j = |j\rangle\langle j+1|$$

Let us define the matrices:

$$Q_{jk, j+1k} = P_{jk}^{-1} P_{j+1k} \quad (52)$$

$$Q_{jk, jk+1} = P_{jk}^{-1} P_{jk+1}$$

and

$$A_{lm} = |l\rangle\langle m| \quad (53)$$

Now we have:

$$\begin{aligned}
H_D^{(3)} = & \sum_{ljk} \varepsilon_{ljk}^{(1)} A_k \otimes A_j \otimes A_l + \sum_{jk} \left[Q_{jk, j+1k} \right]_{lm} A_k \otimes R_j \otimes A_{lm} \\
& + \sum_{\substack{jk \\ lm}} \left[Q_{jk, j+1k} \right]_{ml} A_k \otimes L_j \otimes A_{lm} \\
& + \sum_{\substack{jk \\ lm}} \left[Q_{jk, jk+1} \right]_{lm} R_k \otimes A_j \otimes A_{lm} + \sum_{\substack{jk \\ lm}} \left[Q_{jk, jk+1} \right]_{ml} L_k \otimes A_j \otimes A_{lm} \quad (54)
\end{aligned}$$

This is the same hamiltonian $H_D^{(3)}$ given on a different basis. So up to now $H_D^{(3)}$ is exact but more complex. We have eliminated the term $A_k \otimes A_j \otimes B_l$ but we have added more complex couplings. It means that connections between neighbors into the row jk have disappeared but now multiple connections between different planes have been established through the Q matrices defined in Eq. (52).

Now due to the fact that eigenstates are localized in one dimension for any given disorder,⁴ the matrix elements $(A_{jk, j+1k})_{lm}$ decreases exponentially with $|l-m|$. The approximation LEA consists in neglecting all the off-diagonal elements of the Q matrices and taking all of them as the identity matrix, i.e.:

$$\left[Q_{jk, j+1k} \right]_{lm} \approx \delta_{lm} \quad (55)$$

This is a strong assumption which is true in the large disorder limit ($W \rightarrow \infty$).

So we will work with an effective hamiltonian H'_{eff} which corresponds to an ensemble of decoupled disordered planes:

$$\begin{aligned}
 H_D^{(3)'} \approx H'_{\text{eff}} &= \sum_{ljk} \epsilon_{ljk}^{(1)} A_k \otimes A_j \otimes A_l + \sum_{ljk} A_k \otimes B_j \otimes A_l + B_k \otimes A_j \otimes A_l \\
 &= \sum_l H_l \otimes A_l
 \end{aligned} \tag{56}$$

where H_l identifies each l -plane with random site energies given by the previously obtained eigenvalues $\epsilon_{ljk}^{(1)}$:

$$H_l = \sum_{jk} \epsilon_{ljk}^{(1)} A_k \otimes A_j + A_k \otimes B_j + B_k \otimes A_j \tag{57}$$

In the second step of the method we have to diagonalize first the bidimensional effective problem. To do this we proceed as above each H_l . Thus, after having diagonalized the rows lk in the planes with hamiltonian:

$$H_{ln} = \sum_j \epsilon_{ljk}^{(1)} A_j + B_j \tag{58}$$

and having made the approximation (55) for the resulting Q matrices, we have the new effective hamiltonian:

$$H_{\text{eff}}'' = \sum_{lmk} \epsilon_{lmk}^{(2)} A_k \otimes A_m \otimes A_l + B_k \otimes A_m \otimes A_l = \sum_{lm} H_{lm} \otimes A_m \otimes A_l \tag{59}$$

where $\epsilon_{lmk}^{(2)}$ is the eigenvalue of the hamiltonian H_{lk} corresponding

to a state localized on the site m of the $1k$ chain.

Now H''_{eff} is an ensemble of decoupled one dimensional chains and, in the third step of the method, it can be diagonalized by diagonalizing each one of them. So we finally obtain:

$$H''' = \sum_{lmn} \epsilon_{lmn}^{(3)} A_n \otimes A_m \otimes A_\ell \quad (60)$$

As a conclusion the $\epsilon_{lmn}^{(3)}$ are the eigenvalues used to determine the 3-d density of states. For d dimensions we have to perform d steps.

Physically the method means the following. We choose one direction in a cubic lattice and determine a basis of states corresponding to disordered chains in that direction. We write an effective hamiltonian in that basis for each perpendicular plane which couples all the localized states corresponding to that coordinate. Next on each plane two directions are chosen and the procedure is repeated.

Finally we remark that LEA is based on these two assumptions:

- a) the supposition that all the states localize on different sites in one dimension,
- b) the approximation of the matrices Q by identity matrices (Eq. (55)).

VI.- Numerical Results for the LEA method

In this section we will apply the LEA method to different models of disorder and compare it with the exact computational results of the Dean's method.

First we analyze the binary alloy model,³ i.e. the tight-binding model of a substitutional alloy of A and B components. In this case the hamiltonian (27) is given with:

$$\rho(\epsilon_{ijk}) = c \delta(\epsilon_{ijk} - \epsilon_A) + (1-c) \delta(\epsilon_{ijk} - \epsilon_B) \quad (61)$$

where we choose energy units such that:

$$\epsilon_A = -W, \quad \epsilon_B = W \quad (62)$$

and c is the concentration of A atoms.

In Fig. 4a,b we show the LEA results for low disorder ($W=2$) and two values of the impurity concentration ($c=0.1, c=0.4$). We see that the LEA accounts well for the over-all band shape for small concentrations. In particular it gives correctly the location of the secondary peak related with the minority component (i.e. the A atoms). However, for higher values of c the agreement with the exact results is not so good.

When W increases the agreement increases. In Fig. 4c,d the density of states is shown for $W = 5$ and $c = 0.1, 0.4$. In this case the A and B subbands are well separated and we can see that the method gives different results for each subband. While for the minority subband (i.e. the band related with the A component) the agreement is excellent, for the majority subband, although LEA gives correctly the band limits, it does not account for the shape of the density of states.

The fact that LEA works very well for the minority subband in

lower concentrations of A is in good accord with the idea of the method which is based on the localization properties of the states. This is because it is known that in the limit of large W and low c almost all the states of the minority subband are localized in 3-d¹⁵.

In this limit we show the detailed agreement of LEA with the exact density of states for the minority subband in Fig. 5. We can obtain with this method the characteristic three peaked structure (with some substructure) of this band. Physically,¹⁶ the central peak of the minority band is due to isolated impurities, while the two satellites arise from the bonding and antibonding levels of a nearest neighbour impurity pair cluster. Traditionally the density of states of disordered models is obtained through the application of the coherent potential approximation (CPA).¹² Since CPA is an approach based on an effective periodic medium it is incapable of describing the effects due to the local environment of the atoms, and then it cannot reproduce the peaked structure of the minority subband.¹³ Due to this, there has been in the past numerous attempts to generalize CPA including cluster effects.^{3,14} Many of these attempts have found problems in the analytic properties of the Green function in the high disorder limit or they require a hard computational effort (for a discussion of the CPA generalizations see the review of Elliot et al.).¹⁴ It is in this context that we think that the LEA method is relevant. We say that the LEA is complementary of CPA because it works well where CPA does not although it fails where CPA is good.

Recently Chu-liang and Wei-chao (17) developed a method based on the renormalization-group for the density of states of binary alloys. We want to point out that their method cannot account for the central peak in the alloy problem. Besides it has been performed only for two dimensional cases.

Now we evaluate the relevance of the approximations on which LEA is based as mentioned at the end of section V.

The first hypothesis of LEA is the supposition that all eigenstates localize in different sites for one-dimensional lattices. We check this hypothesis by diagonalizing an ensemble of disordered chains and taking the configurational average of the number of coincidences, $\langle N_c \rangle$, in the site of localization of the eigenstates of each sample. Then, LEA will be appropriate when $\langle N_c \rangle$ is small.

The second hypothesis of LEA is the approximation of eq.(55). To evaluate this we take the mean value of the Q matrices over an ensemble of chains, and calculate the ratio between the off-diagonal elements and the diagonal elements of $\langle Q \rangle$, obtaining what we call the concordance ratio:

$$C_r = \frac{1}{N-1} \frac{\sum_{i \neq j} \langle Q \rangle_{ij}}{\sum_i \langle Q \rangle_{ii}} \quad (63)$$

Then, when C_r is small we expect that LEA can be applied.

(Also we checked that the matrix elements $\langle Q \rangle_{lm}$ decrease exponentially with $|l-m|$).

In Fig. 6 we show the number of coincidences and the

concordance ratio for the binary alloy problem for different values of W and different concentrations. We see that $\langle N_c \rangle$ is independent of W and decreases with the concentration. On the other hand, C_r tends to decrease for small concentrations and also it appears that it slightly decreases with W . The fact that these two parameters behave in opposite directions explains the situation that we cannot reach an agreement with the exact results for both subbands simultaneously.

Finally we apply the LEA method for gaussian disorder as defined in Eq.(46). For small values of the disorder ($W < 2$) our results do not account for the shape of the density of states in the same way that LEA could not give correctly the majority band in the binary alloy case. For these values of W the methods 1-DDA and SVA analyzed in section 4 are better.

However, for larger values of disorder ($W > 2$) we see an excellent agreement of the LEA with the Dean's exact results as it is shown in figures 7 and 8. Here also the concordance of our results with the exact density of states increases with W . In this case the agreement is better than the 1-DDA and SVA results and LEA can also give correctly the band tail behavior of the integrated density of states (Fig. 8) when the other methods cannot. Here again the LEA works well in a region where CPA fails. Recently there has been a renewed interest in the behavior of the density of states near the band edges.^{18,19} This is because it can explain the exponential tail of the optical-absorption coefficient exponent measured on amorphous semiconductors and known as the Urbach tail.²⁰ All the theoretical and numerical¹⁹ work done in this area gives for the band tail the

law:

$$N(E) \sim e^{-|E|/2AW^2}$$

We have verified that the LEA method accounts correctly for this functional form for $W > 2$. Also we have compared our LEA calculations for big samples ($50 \times 50 \times 50$) of the factor A with previous exact numerical results¹⁹ and we found an agreement of the order of 5% with them.

Next, in Fig. 9 we show the number of coincidences and the concordance ratio for the gaussian model as function of the disorder. We see that both parameters decrease for increasing W taking values smaller than those we have obtained for the binary alloy case. The region of values of W where the parameters are small is in accordance with the range of W where we have seen the agreement of LEA with the exact results.

Also we have applied LEA for the Anderson square box disorder. For low disorder the agreement with the results of Hu et al.¹¹ is not so good and the 1-DDA and SVA methods are better. But for large values of disorder the LEA are better specially the tails fall more abruptly than with the other methods in accordance with the results of Ref. 11.

VII.- Conclusions

We have explored the consequences of the dilution symmetry of tight-binding hamiltonians in finite hypercubic lattices for models with different distributions of diagonal disorder. This

symmetry leads directly to the convolution formula for the density of states in low dimensions as has been studied in Ref. 1. For disordered models some approximations have to be introduced.

The dilution symmetry reflects itself naturally in the formalism based on the direct products of matrices coming from the 1-d problem as shown in the paper.

We have compared the results of our approximations with the exact results obtained by the Dean's method for the square box Anderson disorder, for the gaussian disorder, and for the binary alloy. The methods 1-DDA and SVA give good agreement for the first two disorder models. However we find some discrepancies in the tail behavior. The agreement improves with increasing disorder. For the binary alloy model these approximations give slight discrepancies in the gap positions.

Then we have proposed a different LEA method based explicitly on the localization of the states. This last method gives good results for all three models of disorder. In particular the minority component of the binary alloy model comes out with excellent agreement for the peaked structure which in general cannot be obtained by CPA calculations.

The most important feature of our approximations is that they require very short computer times in comparison with the Dean's method.

In conclusion, the dilution symmetry which implies that the eigenvalues of a problem in higher dimension can be obtained from eigenvalues in lower dimension can also be used in disordered systems. However, in the pure case this property is exact and

with disorder some approximation schemes have to be used.

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Figure Captions

Figure 1: Averaged density of states for the square box disordered model for different values of the disorder W . a) One dimensional disorder approximation (1-DDA), b) Separable variable approximation (SVA). The size of the cubic samples is $20 \times 20 \times 20$.

Figure 2: Density of states for the diagonal gaussian distribution of disorder with disorder strength $W = 3$. The numerical results obtained through a) 1-DDA and b) SVA methods (dotted line) are compared with the exact ones calculated by the Dean's method (full line). The oscillations are due to disorder fluctuations. The sample size is $10 \times 10 \times 10$.

Figure 3: Tail behavior of the integrated density of states (I.D.S.) for gaussian disorder of strength $W = 3$. The logarithmic scale magnifies the disagreement for high absolute energies between the exact results calculated by the Dean's method (full line) and the approaches of a) 1-DDA and b) SVA (dotted line). The sample size is $10 \times 10 \times 10$.

Figure 4: Density of states for the binary alloy model. We compare the exact results of the Dean's method (full line) with the curves obtained through the localized eigenstates approximation (LEA), (dotted line). a) $c = 0.1$, $W = 2$; b) $c = 0.4$, $W = 2$; c) $c = 0.1$, $W = 5$; d) $c = 0.4$, $W = 5$. The sample size is $10 \times 10 \times 10$. The oscillations are due to disorder fluctuations.

Figure 5: Density of states of the minority subband of a binary alloy with $c = 0.1$, $W = 10$. We show the agreement between the exact numerical results of the Dean's method (full line) and the results of the LEA (dotted line). The sample size is $10 \times 10 \times 10$.

Figure 6: Test of the validity of the hypothesis of LEA for the binary alloy model over an ensemble of 100 chains. a) Mean value of the number of coincidences in the site of localization $\langle N_c \rangle$ vs. the concentration c of A atoms. b) Concordance ratio Cr as defined in Eq. (63) vs. c . The error bars are of the same order magnitude of the point values. $\times W = 2$; $\circ W = 5$; $\square W = 10$.

Figure 7: Density of states for the gaussian disordered model. We compare the LEA results (dotted line) with the results of Dean's method (full line). the samples size is $10 \times 10 \times 10$. a) $W = 3$; b) $W = 10$.

Figure 8: Tail behavior of the integrated density of states (I.D.S.) for the gaussian disordered model. We show the agreement between the LEA results (dotted line) and the exact numerical results of Dean's method (full line). The sample size is $10 \times 10 \times 10$. a) $W = 3$ (compare with Fig. 3); b) $W = 10$.

Figure 9: Test of the validity of the hypothesis of LEA for the gaussian disordered model as function of the disorder strength W over an ensemble of 100 chains. a) Cr vs. W b) $\langle N_c \rangle$ vs. W . The error bars are of the same order of magnitude of the point values.

Fig. 1

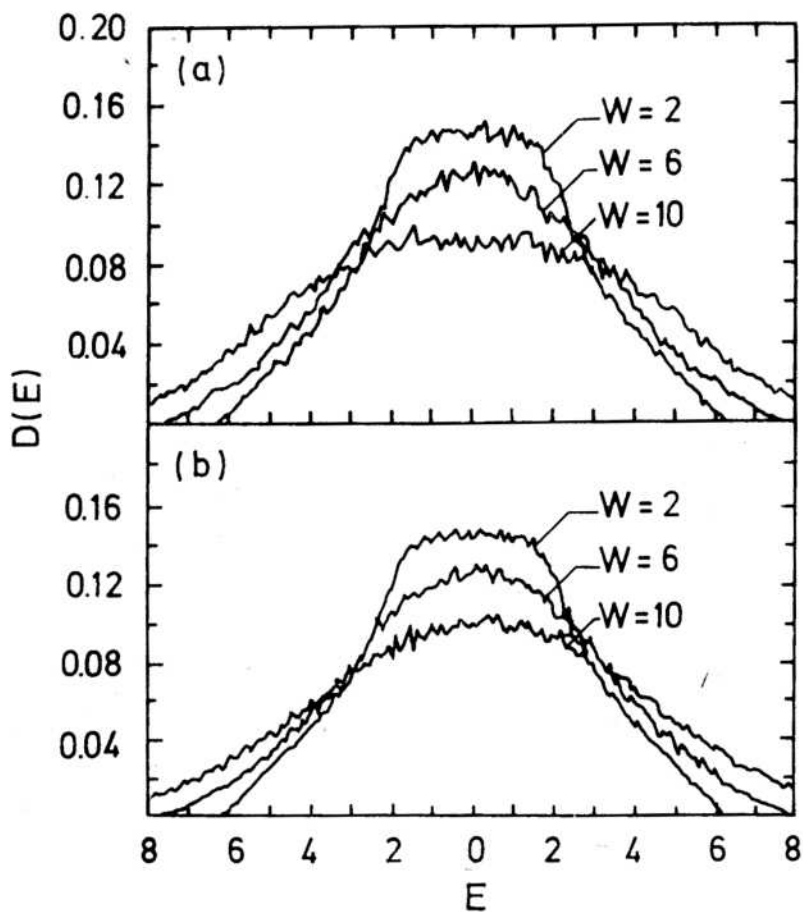
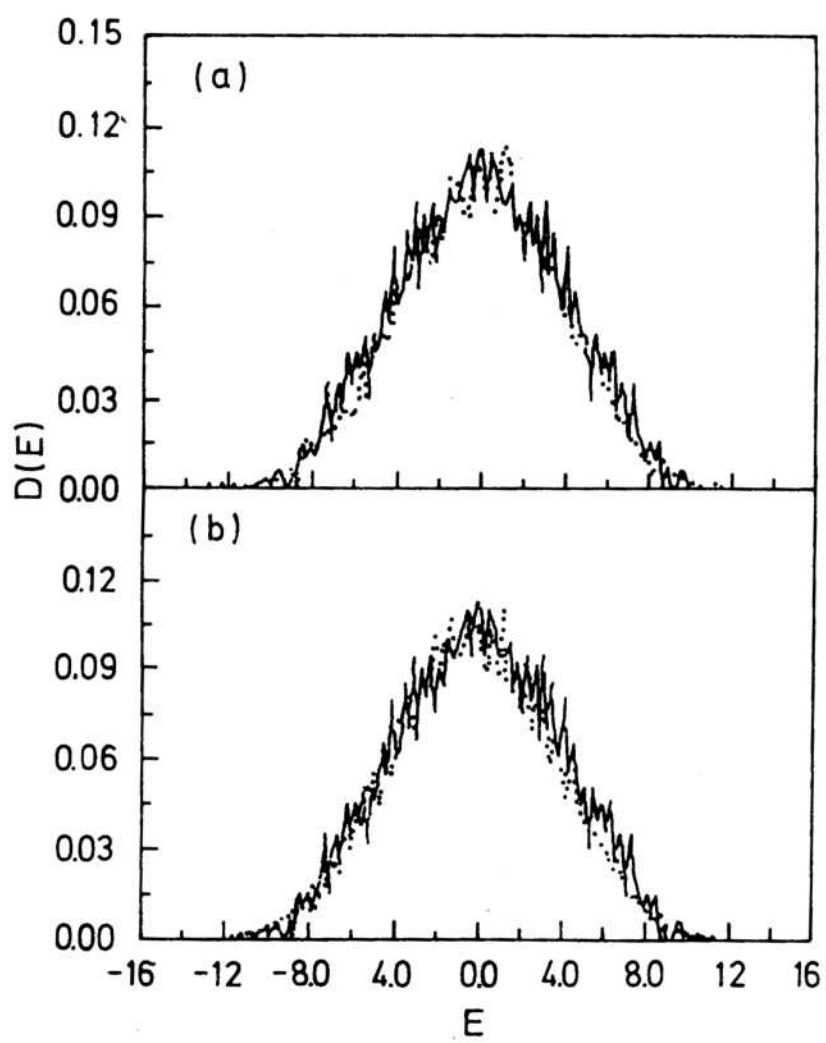


Fig. 2



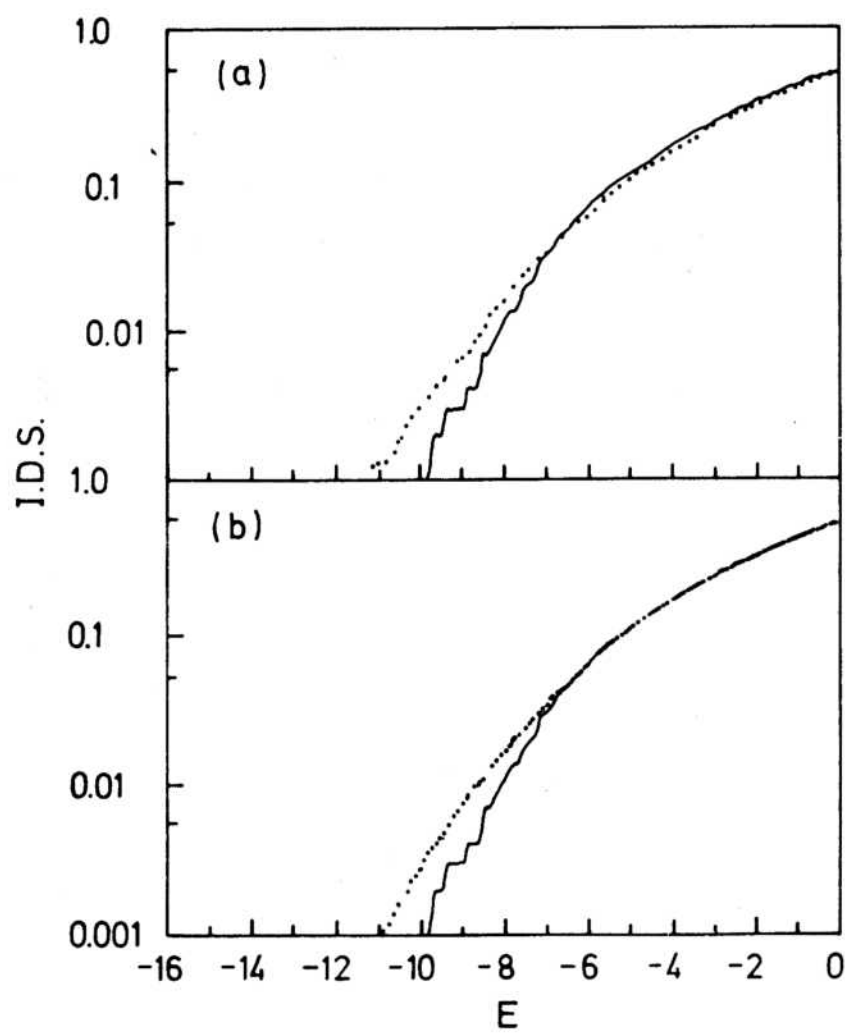


Fig. 4

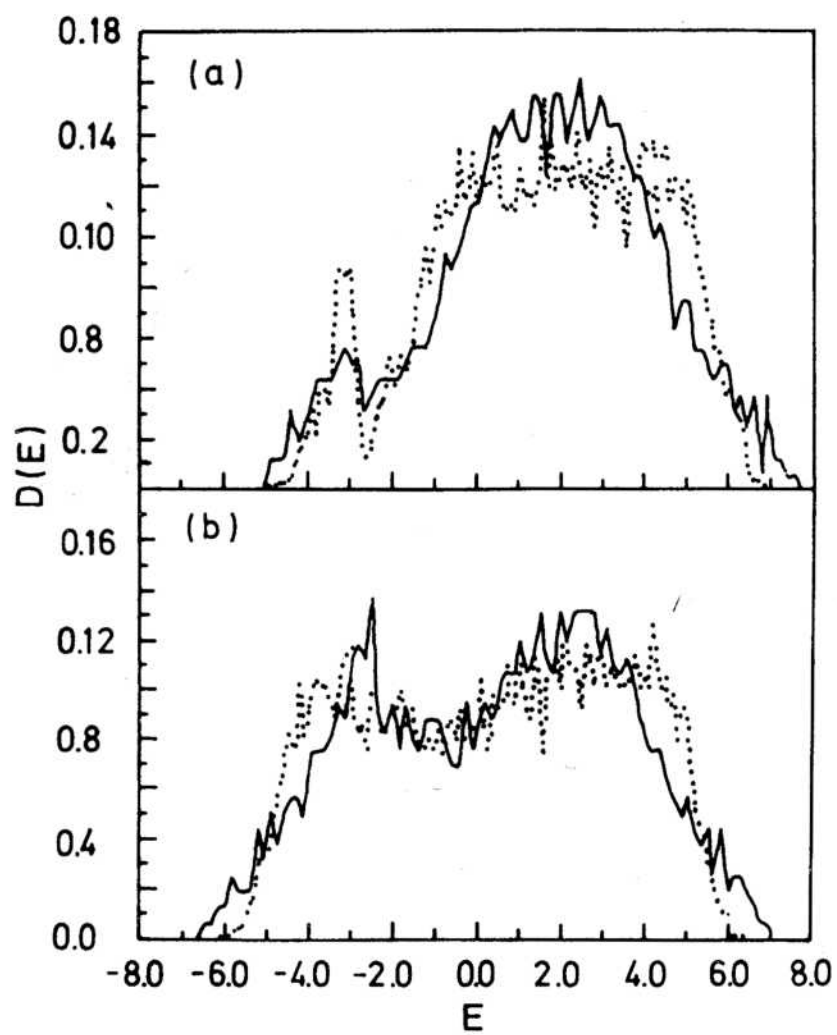


Fig 4

