

Density of states based on dimensional dilution symmetry for disordered hypercubic lattices

D. Domínguez and C. Wiecko

Centro Atómico Bariloche, 8400 S.C. de Bariloche, Rio Negro, Argentina

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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 results obtained by exact diagonalization of small tridimensional samples. Our approach requires very little computer time and, in spite of implicit approximations, gives fairly good results.

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 which 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 dimensions. 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 a 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 three dimensions as we will show below.

In Sec. 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, etc.). We can

think of a direct product taken in such a way as 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 (SV) problem.

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

In Sec. 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 Sec. 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 Sec. 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

$$H = \sum_{\bar{l}} \epsilon_{\bar{l}} |\bar{l}\rangle \langle \bar{l}| + \sum_{\bar{l}, \bar{l}'} V_{\bar{l}, \bar{l}'} (|\bar{l}'\rangle \langle \bar{l}| + |\bar{l}\rangle \langle \bar{l}'|), \quad (1)$$

where $\epsilon_{\bar{l}}$ is the on-site energy and $V_{\bar{l}, \bar{l}'}$ 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 three-dimensional (3D) cubic lattice can be labeled as

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

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

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

$$H = \sum_{ijk} \varepsilon_{ijk} |ijk\rangle \langle ijk| + V_{ijk,i+1jk} (|ijk\rangle \langle i+1jk| + |i+1jk\rangle \langle ijk|) \\ + V_{ijk,ij+1k} (|ijk\rangle \langle ij+1k| + |ij+1k\rangle \langle ijk|) + V_{ijk,ijk+1} (|ijk\rangle \langle ijk+1| + |ijk+1\rangle \langle ijk|). \quad (4)$$

We now define the matrices in terms of projectors

$$A_i = |i\rangle \langle i|, \quad (5) \\ B_i = |i\rangle \langle i+1| + |i+1\rangle \langle i|.$$

In this notation the 1D Hamiltonian reads

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

Now we go to three dimensions 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

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

A. The ordered case

In the ordered case we have

$$\varepsilon_i = \varepsilon, \quad (9) \\ V_{ijk,i+1jk} = V_{ijk,ij+1k} = V_{ijk,ijk+1} = V,$$

$$N_0^{(3)}(E) = \int N_0^{(1)}(E') N_0^{(2)}(E - E') dE' \\ = \int \int N_0^{(1)}(E') N_0^{(1)}(E'') N_0^{(1)}(E - E' - E'') dE' dE''. \quad (15)$$

B. The separable-variable problem

This problem consists in having

$$\varepsilon_{ijk} = \alpha_i + \beta_j + \gamma_k \quad (16)$$

and

The hopping integrals are

$$V_{ijk,i\pm 1jk} \rightarrow \text{between sites}, \\ V_{ijn,ij\pm 1k} \rightarrow \text{between rows}, \\ V_{ijk,ijk\pm 1} \rightarrow \text{between planes}.$$

Explicitly in this notation we get

using the fact that $I = \sum_i A_i$ and taking $\varepsilon=0$, $V=1$, the 3D ordered Hamiltonian reads

$$H_0^{(3)} = I \otimes I \otimes H_0^{(1)} + I \otimes H_0^{(1)} \otimes I + H_0^{(1)} \otimes I \otimes I, \quad (10)$$

where $H_0^{(1)}$ is the 1D ordered Hamiltonian.

As the members of sum (10) commute they can be diagonalized separately. If P is a unitary matrix and $D_0 = P^{-1} H_0 P$ with

$$D_0 = \sum_i E_i^0 A_i, \quad (11)$$

where E_i^0 are the eigenvalues, we get

$$D_0^{(3)} = P^{(3-1)} H_0^{(3)} P^{(3)} \\ = I \otimes I \otimes D_0 + I \otimes D_0 \otimes I + D_0 \otimes I \otimes I \quad (12)$$

with

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

Using (11) we get

$$D_0^{(3)} = \sum_{i=1}^N \sum_{j=1}^N \sum_{k=1}^N (E_i^0 + E_j^0 + E_k^0) A_k \otimes A_j \otimes A_i. \quad (14)$$

Thus, we have the result that the eigenvalues of the 3D ordered case can be obtained as sums of eigenvalues of the 1d 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:

$$V_{ijk,i+1jk} = V_{ii+1}^\alpha, \\ V_{ijk,ij+1k} = V_{jj+1}^\beta, \\ V_{ijk,ijk+1} = V_{kk+1}^\gamma. \quad (17)$$

In this case we have in three dimensions,

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

Due to the separable energies [Eq. (16)], we get

$$\begin{aligned}
H_{SV}^{(3)} = & I \otimes I \otimes \left[\sum_{i=1}^N \alpha_i A_i + \sum_{i=1}^{N-1} V_{ii+1}^\alpha B_i \right] \\
& + I \otimes \left[\sum_{j=1}^N \beta_j A_j + \sum_{j=1}^{N-1} V_{jj+1}^\beta B_j \right] \otimes I \\
& + \left[\sum_{k=1}^N \gamma_k A_k + \sum_{k=1}^{N-1} V_{kk+1}^\gamma B_k \right] \otimes I \otimes I . \quad (19)
\end{aligned}$$

We can gather the one-dimensional Hamiltonians from here:

$$H_\alpha^{(1)} = \sum_{i=1}^N \alpha_i A_i + \sum_{i=1}^{N-1} V_{ii+1}^\alpha B_i , \quad (20)$$

etc., 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

$$\begin{aligned}
D_{SV}^{(3)} = & P_{SV}^{(3)-1} H_{SV}^{(3)} P_{SV}^{(3)} \\
= & I \otimes I \otimes D_\alpha^{(1)} + I \otimes D_\beta^{(1)} \otimes I + D_\gamma^{(1)} \otimes I \otimes I \quad (22)
\end{aligned}$$

with

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

and

$$D_{SV}^{(3)} = \sum_{ijk} (E_i^\alpha + E_j^\beta + E_k^\gamma) A_k \otimes A_j \otimes A_i . \quad (24)$$

Again the density of states is the convolution

$$\begin{aligned}
N_{SV}^{(3)}(E) = & \int \int N_\alpha^{(1)}(E') N_\beta^{(1)}(E'') \\
& \times N_\gamma^{(1)}(E - E' - E'') dE' dE'' . \quad (25)
\end{aligned}$$

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 1D chain. In the present case of the separable-variable problem a hierarchical tree can be constructed as well. Now at each generation, however, a different set of eigenvalues will be summed up.

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

$$\beta_j = \gamma_k = \text{const} \quad (26)$$

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 1D 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 1D 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

$$\begin{aligned}
H_D^{(3)} = & \sum_{ijk} \varepsilon_{ijk} A_k \otimes A_j \otimes A_i + A_k \otimes A_j \otimes B_i \\
& + A_k \otimes B_j \otimes A_i + B_k \otimes A_j \otimes A_i , \quad (27)
\end{aligned}$$

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

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 1D disordered density of states with the one of the pure system in the immediately previous dimension [one-dimensional disorder approximation (1DDA)], $(n+1)$ 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.

A. n -dimensional disorder approximations (n DDA)

1. Approximation of the convolution of the pure system with the distribution of disorder

We rewrite Eq. (27) as

$$H_D^{(3)} = \sum_{ijk} \varepsilon_{ijk} A_k \otimes A_j \otimes A_i + H_0^{(3)} = H_D^{(0)} + H_0^{(3)} . \quad (28)$$

Supposing

$$[H_D^{(0)}, H_0^{(3)}] \approx 0 , \quad (29)$$

which is true if we average it in the disorder distribution, we can diagonalize each Hamiltonian, $H_D^{(0)}$ and $H_0^{(3)}$, separately and take as an approximation for the eigenvalues the sum of the eigenvalues of the 3D ordered case and the random sequence ε_{ijk} . It means

$$E_D^{(3)} \approx (E_0^{(3)})_{ijk} + \varepsilon_{ijk} = E_i^0 + E_j^0 + E_k^0 + \varepsilon_{ijk} . \quad (30)$$

For the averaged density of states it means

$$N_D^{(3)}(E) \approx \int N_0^{(3)}(E - E') \rho_W(E') dE', \quad (31)$$

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

2. The one-dimensional disorder approximation

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

$$H_D^{(3)} = H_D^{(1)} + H_0^{(2)} \quad (32)$$

with

$$H_0^{(2)} = I \otimes H_0^{(1)} \otimes I + H_0^{(1)} \otimes I \otimes I \quad (33)$$

and

$$\begin{aligned} H_D^{(1)} &= \sum_{jk} A_k \otimes A_j \otimes \left[\sum_i \varepsilon_{ijk} A_i + B_i \right] \\ &= \sum_{jk} A_k \otimes A_j \otimes H_{jk}^{(1)}. \end{aligned} \quad (34)$$

As $H_D^{(1)}$ represents an ensemble of noninteracting 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

$$[H_D^{(1)}, H_0^{(2)}] \approx 0. \quad (36)$$

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

$$\begin{aligned} E_D^{(3)} &\approx (E_0^{(2)})_{jk} + (E_D^{(1)})_{ijk} \\ &= E_j^0 + E_k^0 + (E_D^{(1)})_{ijk} \end{aligned} \quad (37)$$

and for the averaged density of states we get

$$N_D^{(3)} \approx \int N_0^{(2)}(E') N_D^{(1)}(E - E') dE'. \quad (38)$$

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 disordered chain eigenvalues to each eigenvalue of the ordered 2D system.

B. The separable-variable approximation

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

The approximation¹⁰ reads

$$\begin{aligned} \varepsilon_{ijk} &\approx \alpha_i + \beta_j + \gamma_k, \\ \langle \alpha_i \beta_j \rangle &= \langle \beta_j \gamma_k \rangle = \langle \alpha_i \gamma_k \rangle = 0. \end{aligned} \quad (39)$$

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

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

Taking

$$\langle \alpha_i^2 \rangle = \langle \beta_j^2 \rangle = \langle \gamma_k^2 \rangle = W^2, \quad (41)$$

we have

$$\langle \varepsilon_{ijk}^2 \rangle = W^2 = 3W_1^2, \quad (42)$$

In this way the problem is solvable as shown in Sec. II 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 from the distribution taken for $\alpha_i, \beta_j, \gamma_k$ of the starting chains. The approximation of Eq. (39) requires that the probability distribution of the 3D 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 only the change of the standard deviation (i.e., when $\alpha_i, \beta_j, \gamma_k$ are random Gaussian variables with width W_j , the resulting ε_{ijk} is also a Gaussian but with width $\sqrt{3}W_1$).

Thus, when the disorder distribution is a Gaussian of width W , the density of states in the separable-variable approximation reads

$$\begin{aligned} N_D^{(3)}(E, W) &\approx \int dE' \int dE'' N_D^{(1)} \left[E', \frac{W}{\sqrt{3}} \right] \\ &\quad \times N_D^{(1)} \left[E'', \frac{W}{\sqrt{3}} \right] \\ &\quad \times N_D \left[E - E' - E'', \frac{W}{\sqrt{3}} \right]. \end{aligned} \quad (44)$$

IV. NUMERICAL RESULTS FOR THE ONE-DIMENSIONAL DISORDER APPROXIMATION AND FOR THE SEPARABLE-VARIABLE APPROXIMATION

Here we will check numerically the 1DDA and the SVA proposed in the previous section. First we will compare computational results for the 3D density of states with the diagonal Anderson disorder.² The distribution of the on-site energies is

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

In Fig. 1 we show the results of the method 1DDA and the SVA method for different values of disorder for a 3D cubic lattice. These results can favorably compare with those given by Hu *et al.*¹¹ using the method of Dean.⁵ 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

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

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 three dimensions. In Fig. 3 we show the integrated density of states where some discrepancies in the tails can be evaluated for the two methods. Except for these discrepancies in the tails, we see good agreement with 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 1D disordered chain where all the states are localized,⁴ and in three dimensions we have localization for all the eigenstates above the Anderson transition ($W > W_c$).^{2,3}

In our examples we take relatively small samples in order to be able to compare with Dean's method which is time consuming. But with both approximations we can perform the calculation on big samples with very reasonable computer times.

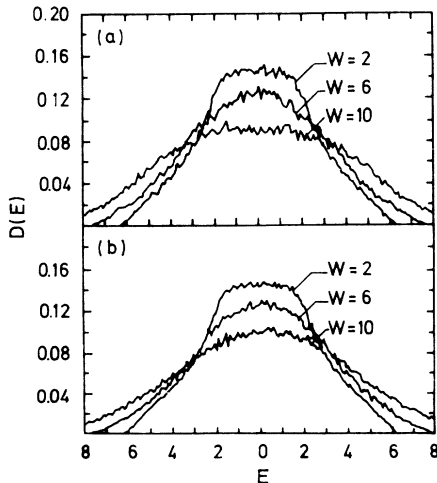


FIG. 1. Averaged density of states for the square box disordered model for different values of the disorder W . (a) one-dimensional disorder approximation (1DDA), (b) separable-variable approximation (SVA). The size of the cubic samples is $20 \times 20 \times 20$.

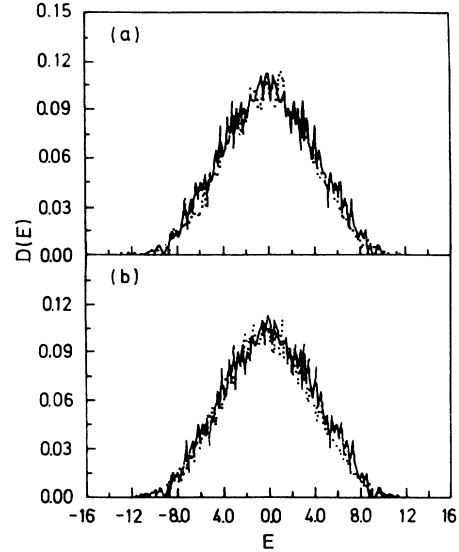


FIG. 2. Density of states for the diagonal Gaussian distribution of disorder with disorder strength $W=3$. The numerical results obtained through (a) 1DDA and (b) SVA methods (dotted line) are compared with the exact ones calculated by Dean's method (solid line). The oscillations are due to disorder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

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 Sec. II although it does not lead to a convolu-

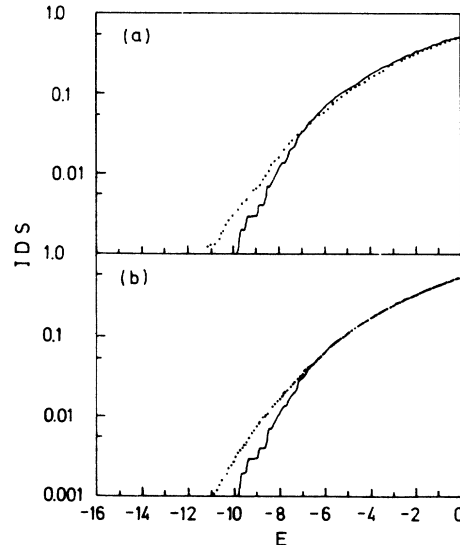


FIG. 3. Tail behavior of the integrated density of states (IDS) for Gaussian disorder of strength $W=3$. The logarithmic scale magnifies the disagreement for high absolute energies between the exact results calculated by Dean's method (solid line) and the approaches of (a) 1DDA and (b) SVA (dotted line). The samples size is $10 \times 10 \times 10$ (3D cubic lattice).

tion 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

$$\begin{aligned} H_D^{(3)} &= \sum_{jk} A_k \otimes A_j \otimes \left[\sum_i \varepsilon_{ijk} A_i + B_i \right] \\ &+ \sum_{ijk} A_k \otimes B_j \otimes A_i + B_k \otimes A_j \otimes A_i \\ &= \sum_{jk} A_k \otimes A_j \otimes H_{jk}^{(1)} + \sum_{ijk} A_k \otimes B_j \otimes A_i \\ &+ B_k \otimes A_j \otimes A_i . \end{aligned} \quad (47)$$

First we diagonalize these 1D Hamiltonians $H_{jk}^{(1)}$ by

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

with

$$\begin{aligned} L_j &= |j+1\rangle\langle j| , \\ R_j &= |j\rangle\langle j+1| . \end{aligned} \quad (51)$$

Let us define the matrices

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

and

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

Now we have

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

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 $A_k \otimes A_j \otimes B_i$ but we have added more complex couplings. It means that connections between neighbors into the rows jk have disappeared but new 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 $(A_{jk,j+1k})_{lm}$ decrease exponentially with $|l-m|$. The LEA consists in neglecting all the off-diagonal elements of the Q matrices and taking all of them as the identity matrix, i.e.,

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

where we order the eigenvalues $\varepsilon_{ljk}^{(1)}$ 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 overall Hamiltonian of Eq. (47) the orthogonal 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 $H_{jk}^{(1)}$ are ordered according to its site of localization. After applying (49) we have

$$(Q_{jk,j+1k})_{lm} \approx \delta_{lm} . \quad (55)$$

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

$$\begin{aligned} H_D^{(3)'} &\approx H'_{\text{eff}} = \sum_{ljk} \varepsilon_{ljk}^{(1)} A_k \otimes A_j \otimes A_l \\ &+ \sum_{ljk} A_k \otimes B_j \otimes A_l + B_k \otimes A_j \otimes A_l \\ &= \sum_l H_l^{(2)} \otimes A_l , \end{aligned} \quad (56)$$

where $H_l^{(2)}$ identifies each l plane with random site energies given by the previously obtained eigenvalues $\epsilon_{ijk}^{(1)}$:

$$H_l^{(2)} = \sum_{jk} \epsilon_{ijk}^{(1)} A_k \otimes A_j + A_k \otimes B_j + B_k \otimes A_j . \quad (57)$$

In the second step of the method we have to first diagonalize the bidimensional effective problems. To do this we proceed as above for each $H_l^{(2)}$. Thus, after having diagonalized the rows lk in the planes with the Hamiltonian

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

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

$$\begin{aligned} H_{\text{eff}}'' &= \sum_{lmk} \epsilon_{lmk}^{(2)} A_k \otimes A_m \otimes A_l + B_k \otimes A_m \otimes A_l \\ &= \sum_{lm} H_{lm}^{(1)} \otimes A_m \otimes A_l , \end{aligned} \quad (59)$$

where $\epsilon_{lmk}^{(2)}$ is the eigenvalue of the Hamiltonian $H_{lk}^{(1)}$ corresponding to a state localized on the site m of the lk 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

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

As a conclusion the $\epsilon_{lmn}^{(3)}$ are the eigenvalues used to determine the 3D 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 the LEA is based on these two assumptions: (a) the supposition that all the states localize on different sites in one dimension, and (b) the approximation of the matrices Q by identity matrices [Eq. (55)].

VI. NUMERICAL RESULTS FOR THE LOCALIZED EIGENSTATE APPROXIMATION

In this section we will apply the LEA method to different models of disorder and compare it with the exact computational results of 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 Figs. 4(a) and 4(b) we show the LEA results for low disorder ($W=2$) and two values of the impurity concentration ($c=0.1$ and 0.4) on a 3D cubic lattice. We see that the LEA accounts well for the overall 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 Figs. 4(c) and 4(d) the density of states is shown for $W=5$ and $c=0.1$ and 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),

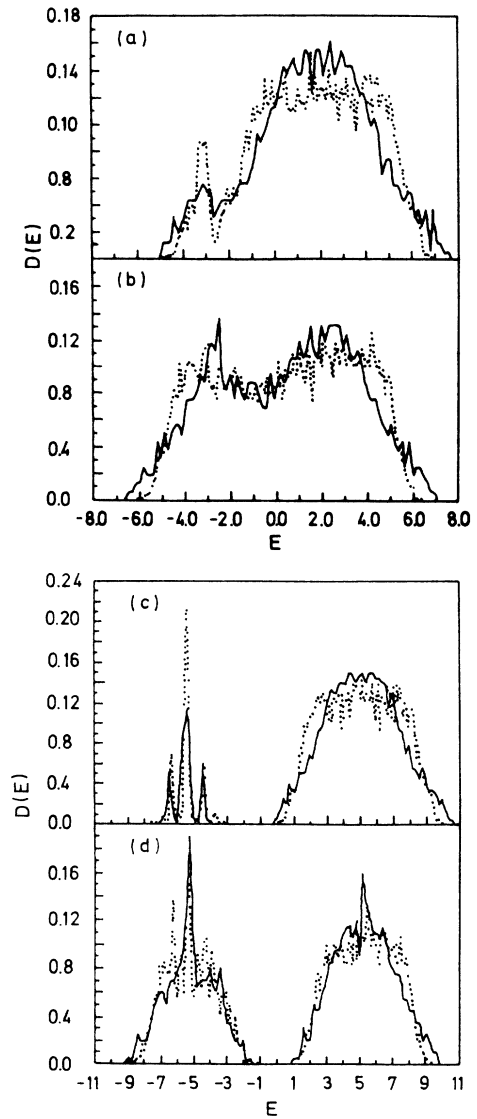


FIG. 4. Density of states for the binary-alloy model. We compare the exact results of Dean's method (solid line) with the curves obtained through the localized eigenstates approximation (LEA) (dotted line). (a) $c=0.1$, $W=2$; (b) $c=0.4$, $W=2$; (c) $c=0.1$, $W=5$; (d) $c=0.4$, $W=5$. The sample size is $10 \times 10 \times 10$ (3D cubic lattice). The oscillations are due to disorder fluctuations.

the agreement is excellent, for the majority subband, although the LEA correctly gives the band limits, it does not account for the shape of the density of states.

The fact that the 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 three dimensions.¹²

In this limit we show the detailed agreement of the 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,¹³ 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-neighbor impurity pair cluster. Traditionally the density of states of disordered models is obtained through the application of the coherent-potential approximation (CPA).¹⁴ Since the 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.¹⁵ Due to this, there has been, in the past, numerous attempts to generalize the CPA including cluster effects.¹⁶ Many of these attempts have found problems in the analytic properties of the Green's 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.*).¹⁶ It is in this context that we think that the LEA method is relevant. We say that the LEA is complementary of the CPA because it works well where the CPA does not, although it fails where the CPA is good.

Recently Chu-Liang and Wei-Liao¹⁷ 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

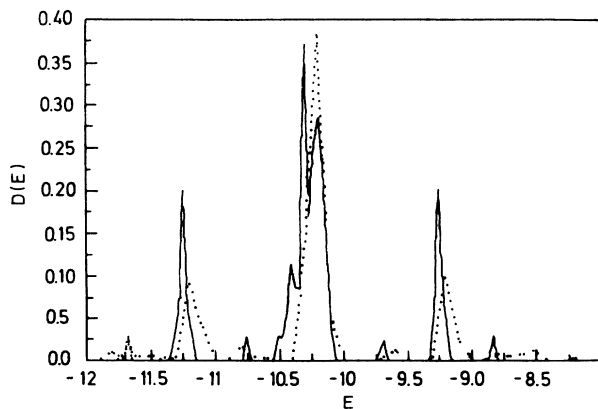


FIG. 5. Density of states of the minority subband of a binary alloy with $c=0.1$, $W=10$. We show the agreement between the exact numerical results of Dean's method (solid line) and the results of the LEA (dotted line). The sample size is $10 \times 10 \times 10$ (3D cubic lattice).

two-dimensional cases. Now we evaluate the relevance of the approximations on which the LEA is based as mentioned at the end of Sec. V.

The first hypothesis of the 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, the LEA will be appropriate when $\langle N_c \rangle$ is small.

The second hypothesis of the 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

$$C_r = \frac{1}{N-1} \left[\frac{\sum_{i \neq j} \langle Q \rangle_{ij}}{\sum_i \langle Q_{ii} \rangle} \right]. \quad (63)$$

Then, when C_r is small we expect that the 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 situa-

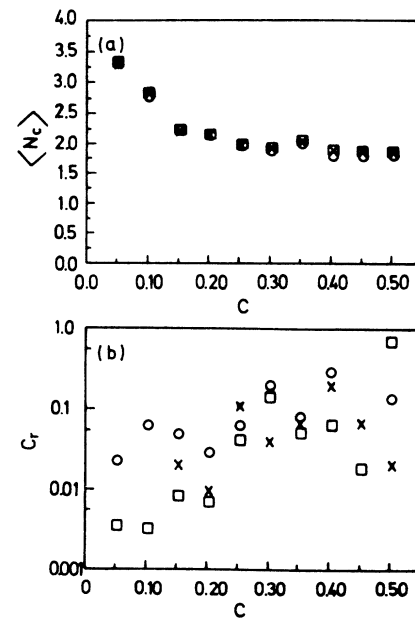


FIG. 6. Test of the validity of the hypothesis of the LEA for the binary-alloy model over an ensemble of 100 chains. (a) Mean value of the number of coincidences in the site of localization $\langle N_c \rangle$ vs the concentration c of A atoms. (b) Concordance ratio C_r , as defined in Eq. (63) vs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

tion 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 ($W \lesssim 2$) our results do not account for the shape of the density of states in the same way that the LEA could not give correctly the majority band in the binary-alloy case. For these values of W the 1DDA and SVA methods analyzed in Sec. IV are better.

However, for larger values of disorder ($W \gtrsim 2$) we see an excellent agreement of the LEA with Dean's exact results as it is shown in Figs. 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 1DDA and SVA results and the LEA can also correctly give the band-tail behavior of the integrated density of states (Fig. 8) when the other methods cannot. Also we have compared our LEA calculations for big samples ($50 \times 50 \times 50$) with the exact numerical diagonalization performed in the work of Li *et al.*¹⁸ There they have fitted a previously proposed law of exponential decay for the tail of the density of states:⁹

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

We have done the same fitting in our results obtaining an agreement of the order of 5% with the values of the factor A calculated in Ref. 18. Here again the LEA works well in a region where the CPA fails.

Next, in Fig. 9, we show the number of coincidences and the concordance ratio for the Gaussian model as a 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 re-

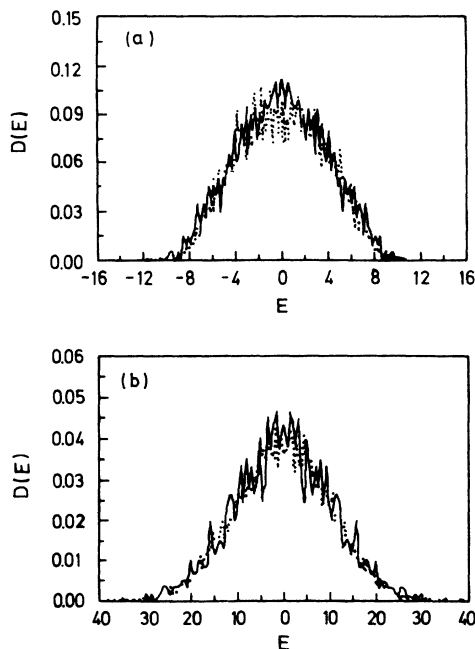


FIG. 7. Density of states for the Gaussian disordered model. We compare the LEA results (dotted line) with the results of Dean's method (solid line). The samples size is $10 \times 10 \times 10$ (3D cubic lattice). (a) $W = 3$, (b) $W = 10$.

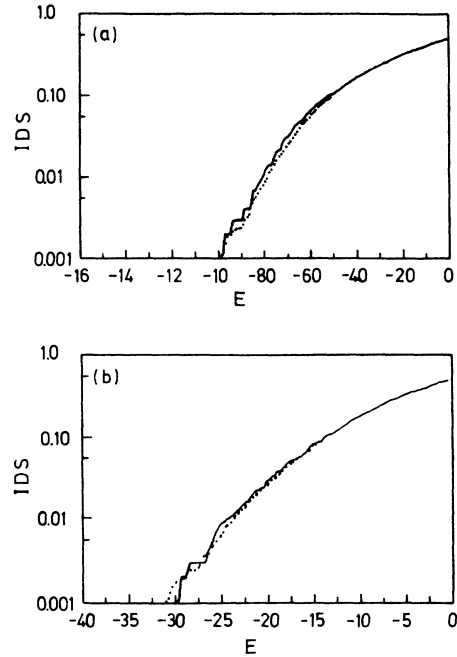


FIG. 8. Tail behavior of the integrated density of states for the Gaussian disordered model. We show the agreement between the LEA results (dotted line) and the exact numerical results of Dean's method (solid line). The sample size is $10 \times 10 \times 10$. (a) $W = 3$ (compare with Fig. 3), (b) $W = 10$.

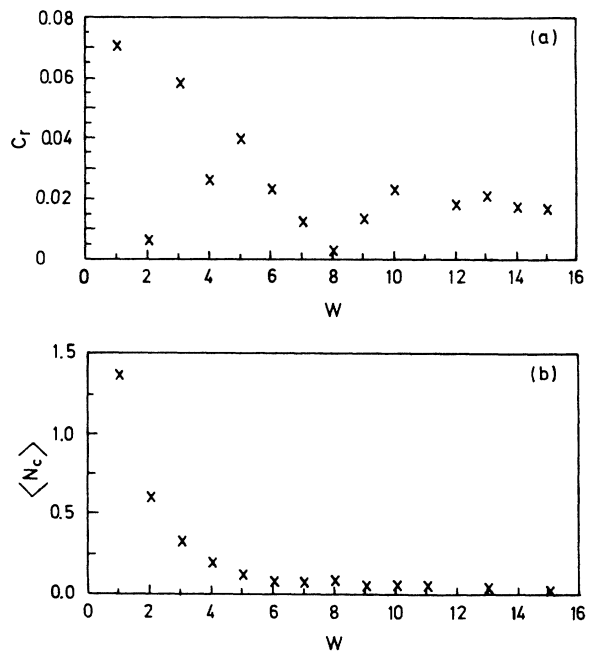


FIG. 9. Test of the validity of the hypothesis of the LEA for the Gaussian disordered model as function of the disorder strength W over an ensemble of 100 chains. (a) C_r vs W , (b) $\langle N_c \rangle$ vs W . The error bars are of the same order of magnitude of the point values.

gion of values of W where the parameters are small is in accordance with the range of W where we have seen the agreement of the LEA with the exact results.

Also we have applied the LEA for the Anderson square box disorder. For low disorder the agreement with the results of Hu *et al.*¹¹ is not as good and the 1DDA and SVA methods are better, but for large values of disorder the LEA results are better, and the tails fall off 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 1D problem as shown in this paper.

We have compared the results of our approximation with the exact results obtained by Dean's method for the square box Anderson disorder, for the Gaussian disorder, and for the binary alloy. The one-dimensional disorder approximation and the separable-variable approximation give a 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 method: the localized eigenstates approximation based explicitly on the lo-

calization 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 the CPA calculations.

An interesting feature of our approximations is that they require short computer times. The SVA and 1DDA methods are very fast (they require few minutes of CPU of a μ VAX) meanwhile the LEA requires a bit more of CPU due to the calculation of the site of localization of the eigenvectors. Compared with other standard methods, such as the equation of motion method¹⁵ or the recursion method,²⁰ the localized eigenstate approximation needs about the same order of computer time. However, these are not precise at the band tails (due to the termination of the continuous fraction in the recursion method, and due to the cutoff in the time of integration in the equation of motion method), then, in this case and for large disorder, the LEA method is more reliable.

In conclusion, the dilution symmetry which implies that the eigenvalues of a problem in a higher dimension can be obtained from eigenvalues in a 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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