Self-similar dependence on dimension of Hamiltonians on hypercubic lattices

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We point out the existence of self-similarity as a function of dimension for the system of Schrödinger equations or of the matrix elements of the tight-binding Hamiltonian in site representation on a discrete hypercubic lattice of finite size. We show how this property of self-similarity can generate an efficient algorithm for the explicit calculation of eigenvalues and densities of states in any dimension.

Self-similarity or dilution symmetry is a fashionable topic. It is discussed in connection with non-Euclidean geometrical objects currently called fractals.[1] The idea of this concept is that there is a certain pattern on a small scale which organizes itself in such a way as to form a larger structure, and that the whole, analyzed on scales of different lengths, looks exactly like the initial pattern. Fractal objects can be defined as having this self-similar property without having translational invariance, even when real world examples of fractals usually have both upper and lower cutoff scales for the self-similar invariance. Recently physicists have shown interest in studying critical phenomena and statistical mechanics on a set of self-similar lattices such as the Sierpinski gaskets or Berker lattice.[2–6] Self-similarity has also been discussed in connection with eigenfunctions in incommensurate and disordered systems and with densities of states for those models.[7–9]

In this paper we want to show the striking self-similar organization as function of dimension of the system of Schrödinger equations on a discrete hypercubic lattice of finite size, or of the matrix elements of the tight-binding Hamiltonian in site representation on the same type of lattices. We will limit ourselves to regular systems for which this approach not only allows an intuitive hierarchical organization of the spectrum and its connection with eigenstates, but also allows us to derive a very practical procedure for the calculation of density of states in any dimension. Of course, as the explicit dispersion relations can be obtained for these infinite lattices by Fourier transformations, our method in this case has the sole advantage of being very practical. For the densities of states in two and three dimensions (3D) analytical results are known, expressable in terms of special functions. We reproduce them to our procedure with a very fast numerical algorithm. Also we show results in higher dimensions which, to our knowledge, have not been explicitly evaluated before. We think that the application of the ideas presented here can be extended to some kinds of problems with disorder and we are currently working upon the algorithms suitable for those cases.

Let us consider a nearest-neighbor hopping Hamiltonian of the form,

$$\hat{\mathcal{H}}=\sum_i E\,|i\rangle\langle i|+\sum_{[i,j]}(V\,|i\rangle\langle j|+V\,|j\rangle\langle i|)\,,$$

where $|i\rangle$ are local site functions with energy E and $[i,j]$ is a pair of nearest-neighbor sites on a given lattice. We will restrict ourselves here to regular lattices of finite size of a hypercubic type. In constructing the corresponding matrices we will choose the hopping V as the unit of energy.

As an illustration of our ideas we will discuss in some detail a very small system. In Fig. 1 we show a square lattice of 4×4 sites. The sites are numbered following the order shown there. Then, the complete Hamiltonian matrix of that system becomes

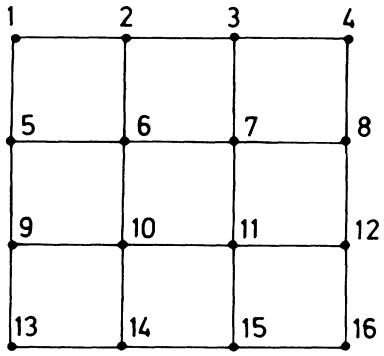

FIG. 1. Labeling order of site states for a 4×4 example.

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$$\mathbf{H}=\left[\begin{array}{cccc|cccc|cccc|cccc}
E & 1 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
1 & E & 1 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 1 & E & 1 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 1 & E & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
\hline
1 & 0 & 0 & 0 & E & 1 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 1 & 0 & 0 & 1 & E & 1 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 1 & 0 & 0 & 1 & E & 1 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 1 & 0 & 0 & 1 & E & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\
\hline
0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & E & 1 & 0 & 0 & 1 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & E & 1 & 0 & 0 & 1 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 1 & E & 1 & 0 & 0 & 1 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 1 & E & 0 & 0 & 0 & 1 \\
\hline
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & E & 1 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 1 & E & 1 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 1 & E & 1 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 1 & E
\end{array}\right] .$$

We can look at this matrix as follows. The states corresponding to the one-dimensional problem (the linear chain of four sites) form a 4×4 submatrix which we will call a "pattern" of the problem,

$$\mathbf{E}=\begin{bmatrix} E & 1 & 0 & 0 \\ 1 & E & 1 & 0 \\ 0 & 1 & E & 1 \\ 0 & 0 & 1 & E \end{bmatrix} .$$

In this case the pattern has four diagonal sites, two of which are "surface" sites. Because of the free boundary conditions, the nondiagonal matrix elements connect these only to one neighbor. The central point of the argument is that the whole matrix (the finite 2D problem based on that particular 1D problem) is obtained by repeating the pattern in an enlarged version,

$$\mathbf{H}=\begin{bmatrix} \mathbf{E} & \mathbf{I} & \mathbf{0} & \mathbf{0} \\ \mathbf{I} & \mathbf{E} & \mathbf{I} & \mathbf{0} \\ \mathbf{0} & \mathbf{I} & \mathbf{E} & \mathbf{I} \\ \mathbf{0} & \mathbf{0} & \mathbf{I} & \mathbf{E} \end{bmatrix} ,$$

with

$$\mathbf{I}=\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}$$

and

$$\mathbf{0}=\begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix} .$$

That is, each nondiagonal element of the pattern is replaced either by a unit or a null matrix (of a size corresponding to the size of the 1D problem) following the same sequence as given in the pattern and the diagonal elements of the pattern are replaced by the pattern itself.

Let us comment on how this self-similar structure looks in 3D for the problem of $4\times4\times4$ sites. These are numbered following the sequence shown in Fig. 1 for the first square and then repeating it for the subsequent planes in the same order. A straightforward construction will show a matrix with the same structure as that discussed above. If we forget for a moment the details on a scale lower than 4×4, we will recognize a 16×16 submatrix with the structure of the finite 2D problem already discussed. By recovering the 64×64 scale vision we will recognize that the diagonal elements correspond to the finite 1D problem, which we called the pattern, while hopping is represented by 4×4 unit matrices. Proceeding by induction we can easily visualize the matrix of an hypercubic cluster of any dimension.

Different rules for the enumeration of states may lead to different patterns. An example is obtained from the matrix of the 4×4 square system, taking the order obtained by performing decimation[5] on this small system. We first separate the system of Fig. 1 into two groups, placing each second element in the same group and then performing the same procedure inside each subgroup, and so on. The order obtained may be put in correspondence with the old one, as follows:

new: (1,2,3,4;5,6,7,8;9,10,11,12;13,14,15,16)

old: (1,9,5,13;3,11,7,15;2,10,6,14;4,12,8,16) .

By writing the matrix we may observe that it is again self-similar, but now with a pattern given by the following matrix:

$$\begin{bmatrix} E & 0 & 1 & 0 \\ 0 & E & 1 & 1 \\ 1 & 1 & E & 0 \\ 0 & 1 & 0 & E \end{bmatrix} .$$

However, it must be pointed that even when the self-similarity of the matrices originates from a true topological symmetry of the problem, its obvious manifestation depends on the ordering of the site states. If we take an arbitrary enumeration of states, no self-similar structure becomes evident.

We already showed how the matrix elements for finite systems may present a striking self-similar organization. Now, it is interesting to inquire if this self-similarity as a function of dimension is a true property of the Hamiltonian. We look at the structures of the eigenvalues (ω's), as a function of dimension, because these are independent of the representation which is used. In Fig. 2 we show the distribution of eigenvalues for the problem generated by four sites as a function of the dimension. A regular hierarchical tree can be constructed. For 1D we have four eigenstates obtained for the regular finite chain of four sites. If we plot the center of mass of these values as 0D and join the values of 1D with it we have the pattern of how the tree ramifies at each node. The eigenvalues of 2D square of 4×4 site are obtained from those of 1D, performing the indicated ramification at each node. The same is done when going from 2D to 3D and so on. This means that each eigenvalue for a problem in a given dimension can be derived from an eigenvalue of the problem in the lower dimension, the same as the matrix elements were just the enlarged copy of the lower dimensional pattern. From Fig. 2 we see that the eigenvalues for a certain dimension can be grouped in clusters containing as many elements as the 1D problem, from which the hypercube was generated, and having the same distribution of eigenvalues as the 1D problem. The mean value of each cluster gives exactly the distribution of eigenvalues of the immediately lower dimension. This can be written symbolically as a convolution integral,

$$N_d(\omega)=\int N_1(\omega-\omega')N_{d-1}(\omega')d\omega' ,$$

where $N_d(\omega)$ is the distribution that gives the density of states per site as function of the energy ω for a given dimension d.

Dashed lines in Fig. 2 show the upper and lower bounds for the eigenvalues given by the Gershgorim theorem. These limits are obtained both for infinite samples and for finite hypercubes with periodic boundary conditions. However, this last situation involves a network of interactions with a topological dimension higher than d. We will discuss this point further ahead.

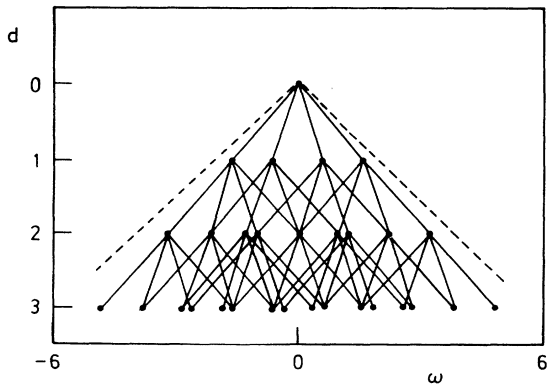

FIG. 2. The distribution of eigenvalues for the system generated by four sites as a function of dimension. Notice that some eigenvalues are degenerate.

Now, it is appropriate to discuss what is the effective dimension of a finite cluster with open boundary conditions. When considering, for example, the four sites chain it is obvious that it does not cover the whole 1D space. In fact, half of the sites are "surface" sites. So it is natural to seek a parameter which measures how a finite hypercube fails to fill the embedding d-dimensional space. The answer was suggested in Refs. 10 and 11 where an effective fractal dimensionality was defined in terms of the bandwidth B of the spectrum. For an hypercubic lattice this reads

$$d_{\text{eff}}=B/4V .$$

This fractal dimension approaches the embedding space dimension d when the ratio of surface sites to the bulk sites approaches zero.[12] Moreover, it allows an adequate interpolation between hypercubes of integer dimension. That is, it assigns an effective value $1<d_{\text{eff}}<2$ for a strip of finite width, a value $2<d_{\text{eff}}<3$ for an infinite bar of finite cross section, and so on. An interesting example which shows the coherence of our ideas is that of just one bar, namely, $L\Longrightarrow\infty$ sites in the first direction, two sites in the second direction and two sites in the third direction. Its effective fractal dimensionality is just 2, that of the cylinder, a two-dimensional object with periodic boundary conditions. In Fig. 3 we give the effective fractal dimension when accumulating L d-dimensional hypercubes of infinite size as function of L. As $L\Longrightarrow\infty$ ones gets a $(d+1)$-dimensional infinite hypercube.

As an application of the ideas explained, we calculate densities of states for large enough systems to be representative of true bulk densities of states for hypercubic lattices in any dimension. Starting from the eigenvalues of the 1D problem, we generate the eigenvalues of the higher dimensional problem following the initial pattern ramification and build the histogram. We must

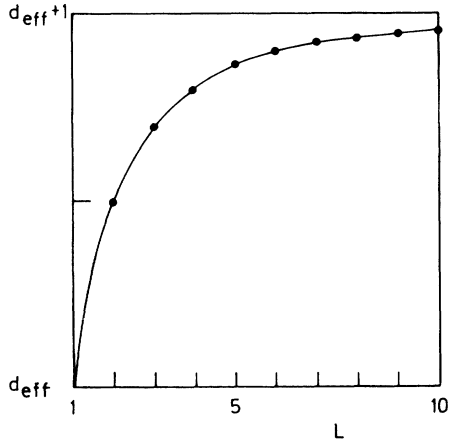

FIG. 3. Effective fractal dimension as defined in the text for L hypercubes of dimension d in a $(d+1)$-dimensional embedding space.

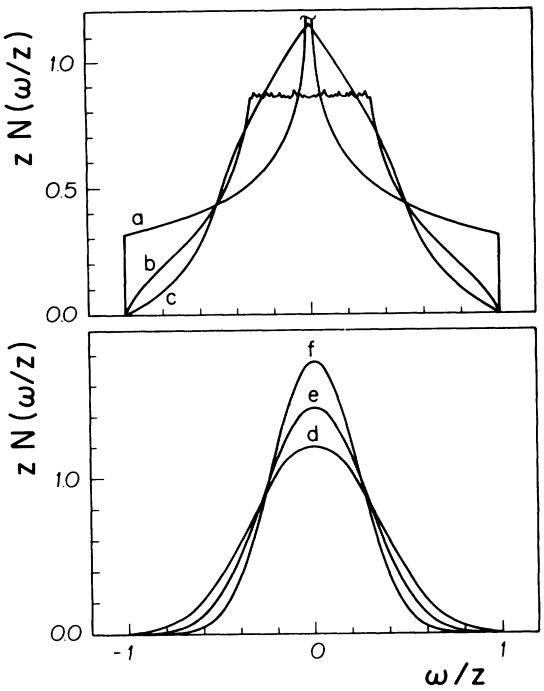

FIG. 4. The normalized density of states of a two- (curve *a*), three- (curve *b*), four- (curve *c*), five- (curve *d*), seven- (curve *e*), and ten- (curve *f*) dimensional hypercubic lattices generated by a pattern-repetition procedure from a 1D chain of 256 (curve *a*), 64 (curve *b*), and 128 (curves *c*–*f*) sites. *Z* is the number of nearest neighbors.

point out that since we want a histogram within a given ω/B precision, our method has no memory limitation and is very fast. In fact, all the results shown below imply very little time consumption.

In curve *a* of Fig. 4 we show the normalized density of states for 2D square lattice of 126×126 sites ($d_{\text{eff}}=1.9992$). In curve *b* of Fig. 4 we show the same function for a 3D simple cubic lattice originated from a 64 sites 1D chain ($d_{\text{eff}}=2.9925$). In both cases the densities of states are well known but they have to be obtained from special functions. With this procedure they can be generated very efficiently in a straightforward manner. The results shown here are in excellent agreement with the traditional ones. The vanHove singularities manifest themselves in the proper way. In curve *b* of Fig. 4 the small oscillations that appear in the graph are due to the fact that the system is not large enough. We show it explicitly in order to have a criteria for chosing the size of a system to represent the bulk density of states. It should be pointed that if we had used periodic boundary conditions the results would be much worse because of degeneracies imposed by the symmetries of this case. However, the densities of states at the band edges would improve slightly and one has a better fit to the law: $N_d(\omega)\sim|\omega-\omega_c|^{\nu}$, with $\nu=(d-2)/2$ and $\omega_c=\pm2dV$.

Let us show the densities of states corresponding to *d* dimensions, where $d>3$, which, to our knowledge, are not known. In curves *c*–*f* of Fig. 4 we show the density of states for four- , five- , seven- , and ten-dimensional hypercubes generated from the 1D system of 128 sites [$d_{\text{eff}}=d(1-3\times10^{-4})$]. The striking feature of these results is that no van Hove's singularities seem to appear in higher dimensions. The densities of states of *d* dimensions, where $d>4$ are smooth curves with continuous first derivatives, and a maximum at the band center with a relative width which gets smaller in relation to total bandwidth with increasing dimension.

In summary, we pointed out the striking self-similar organization as function of dimension of the system of Schrödinger equations on a discrete hypercube lattice of finite size or of the matrix elements of the tight-binding Hamiltonian in site representation on the same type of lattices. We showed how these problems can be written down just by enlarging in a proper way a certain pattern which is just the 1D system from which higher dimensional lattice is generated. This self-similarity property is a true symmetry of the problem since it also appears in the structure of the eigenvalues, which follows a regular hierarchical tree organization as function of dimension. This property gives a very efficient algorithm for calculating eigenvalues and densities of states for these problems. We showed the application of the algorithm by reproducing the well-known results for 2D and 3D lattices and evaluating explicitly the problems of densities of states of *d* dimensions, where $d>3$.

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[12]J. L. D'Amato and H. M. Pastawski (unpublished) have used this definition for the case of Sierpinski gaskets in two- and three-dimensional space. It is found that $d_{\text{eff}}=1.5$ and $d_{\text{eff}}=2$ which is in good agreement with the Haussdorff dimension of the corresponding lattices: $D=\ln3/\ln2=1.57\ldots$ and $D=\ln4/\ln2=2$.