RAPID COMMUNICATIONS

PHYSICAL REVIEW B VOLUME 28, NUMBER 8 15 OCTOBER 1983

Nature of eigenstates on fractal structures

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(Received 25 July 1983)

The density of states and the nature of the eigenstates of the tight-binding (or any general quadratic) Hamiltonian, on a d-dimensional Sierpinski gasket, are investigated. For $d > 1$, the spectral measure is the superposition of two distinct parts: a pure point measure of relative weight $d/(d+1)$, associated with "molecular" localized states, and a pure point measure, with a Cantor set support, associated with "hierarchical" states.

It has been recently shown[1] that fractals may represent, up to the correlation length, the main geometrical features of percolation clusters. However, this example of fractals is not an isolated one. A linear or branched polymer, and a random or self-avoiding walk in free space or on a periodic lattice, are other examples of fractals. The common feature of these structures is their dilation symmetry (scale invariance), in contrast with the translation symmetry possessed by standard Euclidean spaces. In this respect, fractals may bridge the gap between crystalline structures and disordered materials. In addition to the well-known fractal dimensionality $\bar{d}$, the new concept of spectral dimensionality $\tilde{d}$ was introduced recently in order to describe, among other effects, the classical diffusion on fractals.[2] The dimensions $\bar{d}$ and $\tilde{d}$ seem also to control many other physical phenomena: localization, self-avoidance of random walks, etc. The spectral dimensionality $\tilde{d}$ is naturally associated with the power-law behavior of the low-frequency density of states (e.g., for elastic vibrations): $\rho(\omega) \sim \omega^{\tilde{d}-1}$. From this viewpoint, Euclidean spaces, of dimension d, are special and degenerate cases because $\bar{d} = \tilde{d} = d$ in them and the energy spectrum of electron (or vibration) states consists of bands of extended eigenstates. In this Rapid Communication, we investigate the spectrum of the same type Hamiltonian, on a family of nontrivial fractal lattices: the d-dimensional Sierpinski gaskets.[3]

To construct a d-dimensional gasket, we begin with a d-dimensional hypertetrahedron G_0 (triangle for $d=2$) at stage $n=0$. G_{n+1} is obtained from G_n by juxtaposition of $(d+1)$ stage-n structures, at their external corners. The scaling factor is $b=2$ at each iteration and the fractal dimensionality of the gasket is easily found: $\bar{d} = \ln(d+1)/\ln 2$. Assume now a system of identical masses m placed at the sites of the gasket and connected by springs of strength K. The masses are allowed to move only in a direction orthogonal to the d-dimensional space of the gasket. Let us denote $\alpha = m\omega^2/K \equiv \omega^2/\omega_0^2$ the reduced squared frequency and let $\{U_j e^{i\omega t}\}$ be the eigenstate associated with a mode of frequency ω. The set of equations of motion for a given site is

$$\alpha U_i = \sum_j (U_i - U_j) \ , \tag{1}$$

where j denotes a neighboring site of i.[4]

Of particular interest for physical applications are the nature of the spectral measure, the spatial behavior of eigenmodes, and, finally, the topological feature of the spectrum. A first step in this program is to use the scale invariance of the gasket in order to renormalize Eq. (1). Starting from the equations of motion, one eliminates the amplitudes corresponding to the sites located at midpoint of hypertetrahedron edges at the lowest scale. This decimation procedure leads to a reduced set of equations, describing the same physics on a gasket, scaled down by a factor $b=2$. This exact renormalization leads to a renormalized frequency, and the dimensionless parameter α is simply replaced[5] by

$$\alpha' \equiv \phi(\alpha) = (d+3)\alpha - \alpha^2 \ . \tag{2}$$

The spectral dimensionality can then be deduced from the slope of $\phi(\alpha)$ as its trivial fixed point $\alpha = 0$ (Ref. 2):

$$\tilde{d} \equiv 2\bar{d} \ln b / |\ln \phi'(0)| = 2\ln(d+1)/\ln(d+3) \ . \tag{3}$$

The nature of the spectrum is closely related to the properties of the quadratic map $\phi(\alpha)$. Precise information is gained through the diagonal Green's function, which also gives the integrated density of states. If $N(\omega^2)$ is used to denote the fraction of modes, with squared frequency less than ω^2, it is well known that

$$N(\omega^2) = -(2/\pi)\,\mathrm{Im}\Phi(-\omega^2 + i\epsilon) \ , \tag{4}$$

where $\Phi(Z)$ is defined for complex numbers Z by

$$\Phi(Z) = -\tfrac{1}{2} \lim_{n\to\infty} \frac{1}{N_n} \sum_{j=1}^{N_n} \ln(Z + \omega_{j,n}^2) \ . \tag{5}$$

Here, $N_n = (d+1)[1+(d+1)^n]/2$ denotes the total number of sites at stage n, and $\{\omega_{j,n}\}$ is the set of N_n eigenfrequencies. Using a standard[6] integral representation for $\Phi(Z)$, we can derive a functional equation for Φ. This equation corresponds to a decimation, over hidden variables associated with the integral representation, and can be written as (the detailed algebra will be given elsewhere[5])

$$\Phi(Z) = \frac{\Phi(Z(Z+d+3))}{d+1} - \frac{d-1}{2(d+1)^2} \ln\left[\frac{(Z+d+3)(Z+2d+2)^{d+1}}{Z+2}\right] \ . \tag{6}$$

This nontrivial functional equation for $\Phi(Z)$ cannot be solved, in general, except for $d=1$, where known results

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for linear chains are reproduced. However, the spectrum can be deduced from Eq. (6). For instance, the edges of the spectrum are located at $\omega^2_{\min}=0$ and $\omega^2_{\max}=(2d+2)\omega_0^2$. On the other hand, $N(\alpha)$ is given by the discontinuities [Eq. (4)] of $\mathrm{Im}\Phi(Z)$ on the real negative axis. This leads to a spectrum completely determined by the boundary conditions

$$N(\alpha\leq 0)=0, \quad N(\alpha\geq 2d+2)=1 \ , \tag{7}$$

and the following two iteration equations:

$$N(\alpha)=\frac{N(\phi(\alpha))}{d+1}-\frac{d-1}{(d+2)^2}\Theta(\alpha-2) \tag{8a}$$

for $0<\alpha<(d+3)/2$, and

$$N(\alpha)=-\frac{d-1}{(d+1)^2}[\Theta(\alpha-2)-\Theta(\alpha-d-3)-(d+1)\Theta(\alpha-2d-2)]+\frac{2}{d+1}-\frac{N(\phi(\alpha))}{d+1} \tag{8b}$$

for $(d+3)/2<\alpha<\infty$, where $\Theta(x)$ is the step function [$\Theta(x)=0$, if $x<0$, $\Theta(x)=1$ if $x>0$]. Equations (7) and (8) suggest a natural procedure, illustrated in Fig. 1, for the determination of $N(\alpha)$, which is a non-negative monotonically increasing function but constant almost everywhere on the real axis. The behavior of this highly singular function is dictated by the properties of the map $\alpha\rightarrow\phi(\alpha)$, and its reverse $f_\pm$ defined by ($\delta=d+3$)

$$f_\pm(\alpha)=[\delta\pm(\delta^2-4\alpha)^{1/2}]/2 \ . \tag{9}$$

For instance, we deduce from the first iteration,

$$N(\alpha)=2/(d+1), \text{ for } (d+3)<\alpha<2(d+1) \ . \tag{10}$$

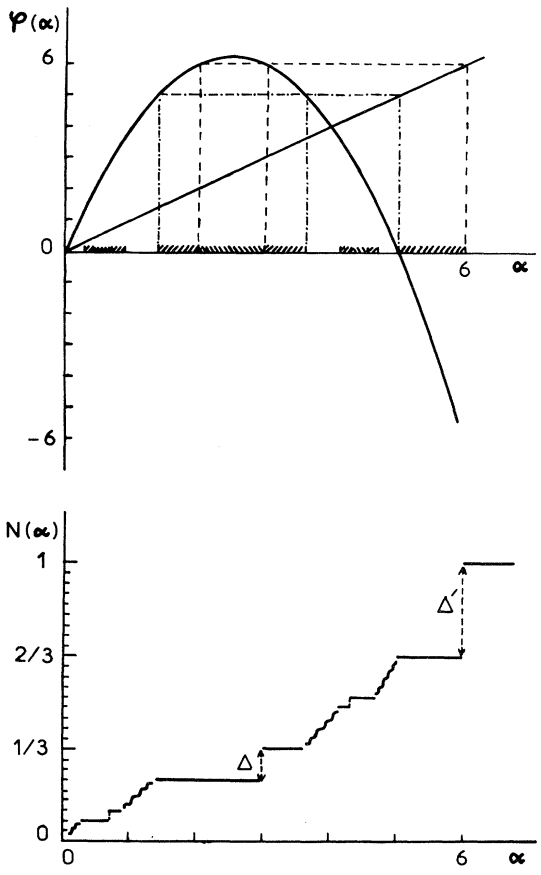

FIG. 1. Behavior of the integrated density of states $N(\alpha)$ obtained, as explained in the text, from the map $\phi(\alpha)$. Here, α denotes $\alpha=\omega^2/\omega_0^2$, the reduced squared frequency for the Sierpinski gasket at $d=2$.

A first jump, of height $\Delta'=(d-1)/(d+1)$, occurs at the upper edge of the spectrum. The next iteration shows the presence of another jump of $N(\alpha)$ at $\alpha=d+1$. The height of this jump is $\Delta_0=(d-1)/(d+1)^2$. The knowledge of $N(\alpha)$ on the interval $[0,d+3]$ is then reached by repeated application of $f_\pm$. At each stage of the iteration, every jump Δ_i gives rise to two new jumps, of equal magnitude $\Delta_{i+1}=\Delta_i/(d+1)$. The above construction thus generates a pure-point spectral measure, supported by a Cantor set of Lebesgue measure zero. The eigenfrequencies are located at $\alpha=2d+2$, and at $\alpha=d+1$, and its successive images by $f_\pm$. This part of the spectrum is self-similar by construction, and its relative weight is given by the sum ($d>1$)

$$\Delta'+\sum_{i=0}^{\infty}2^i\Delta_i=d/(d+1) \ . \tag{11}$$

The localized eigenstates associated with these frequencies are obtained iteratively, using $f_\pm$ (see Fig. 2). The amplitudes are nonzero only on a finite number of sites. We call

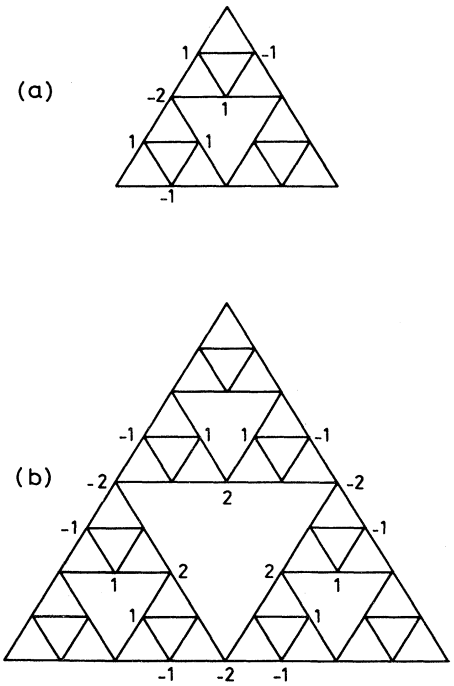

FIG. 2. Examples of "molecular" localized eigenmodes of the Sierpinski gasket at $d=2$. Only nonzero amplitudes are shown: (a) $\alpha=6$; (b) $\alpha=3$.

such states "molecular" modes. Their spatial extension can be measured, with a "localization" length $L(\alpha)$, such that $L^{\tilde{d}}(\alpha)$ corresponds to the "occupation volume" of the associated mode. A simple scaling argument gives the following relation for $L(\alpha)$:

$$L(\phi(\alpha)) = L(\alpha)/2 \ . \tag{12}$$

This length diverges at low frequency like $L(\omega) \sim \omega^{-\tilde{d}/\bar{d}}$, when the lower edge of the spectrum is approached.

The second part of the spectrum, of relative weight $1/(d+1)$, is given by the Julia set[7] associated with the map ϕ. This spectrum is invariant under the map ϕ and its reverses $f_{\pm}$. The spectrum (Cantor) is supported by a Cantor set C_δ of Lebesgue measure zero. The associated eigenfrequencies are coded naturally as

$$\alpha(\{\sigma\}) = \frac{\delta}{2} + \sigma_0[\lambda + \sigma_1(\lambda + \sigma_2 \cdots)^{1/2}]^{1/2} \ , \tag{13}$$

where $\{\sigma\} = (\sigma_0, \sigma_1, \ldots)$, $\sigma_i = \pm 1$, and $\lambda = \delta^2/4 - \delta/2 \geq 2$.

For instance, $\alpha = \delta$ ($\alpha = 0$) corresponds to the sequence $\sigma_i = +1$ (-1). To this spectrum [Eq. (13)] is associated a pure-point spectral measure of relative weight $1/d+1$ [the sum of $2^i\Delta_i$ as in Eq. (11)].

The above coding of eigenfrequencies exhibits the following properties:

$$\phi(\alpha\{\sigma\}) = T\{\sigma\} \ , \tag{14a}$$

$$f_{\pm}(\alpha(\{\sigma\})) = \alpha(\pm, \{\sigma\}) \ , \tag{14b}$$

expressing the invariance under ϕ and $f_{\pm}$. In Eqs. (14) we have used the shift operator T:

$$T(\sigma_0, \sigma_1, \ldots) = (-\sigma_1, \sigma_2, \sigma_3, \ldots) \tag{15a}$$

and

$$(\pm, \{\sigma\}) = (\pm, -\sigma_0, \sigma_1, \ldots) \tag{15b}$$

Further properties of this spectrum can be found in the mathematical literature.[8] To our knowledge, this kind of spectrum was first encountered in physical problems by Belissard, Bessis, and Moussa.[9] These authors have studied a one-dimensional crystallographic model: the "quadratic mapping Hamiltonian" which is almost periodic and admitting a spectrum similar to (13). Some results obtained in Ref. 8 were used here to obtain the eigenmodes associated with the second part of the spectrum of the gaskets. For this we use the sequence $\{P_n\}$ of polynomials, defined by the three-term recursion relation

$$\begin{aligned} &P_0 = 1, \quad P_1 = -\alpha + \delta/2, \\ &P_{n+1}(\alpha) = -(\alpha - \delta/2)P_n(\alpha) - R_n P_n(\alpha) \ , \end{aligned} \tag{16}$$

where R_n is defined recursively by

$$R_0 = 0, \quad R_1 = \lambda, \quad R_m = R_{2m} R_{2m-1}, \quad R_{2m} + R_{2m+1} = \lambda \ . \tag{17}$$

With the use of Eqs. (14), it is easy to check the following property:

$$P_{n,2^k}(\alpha) = P_n(\phi^{(k)}(\alpha)) \ , \tag{18}$$

where $\phi^{(k)}$ denotes the kth iterate of the map ϕ. This set of polynomials is appropriate for the dilation symmetry of the gasket, and is then the counterpart of Block waves in translation invariant systems. Equation (18) exhibits clearly this property. In particular, the $\{P_n\}$ reduce to the well-known Tchebyshev polynomials $\{T_n\}$ at $d=1$, where dilation and translation symmetries coexist. In this case, the spectrum is absolutely continuous (one band $0 \leq \alpha \leq 4$) and the eigenmodes can be expressed either as linear combination of polynomials $\{T_n\}$ or of Bloch waves.

In a similar manner, eigenmodes $\{U_n\}$ on the gasket are expressed as a linear combination of polynomials $\{P_n\}$. Of particular interest is their spatial behavior. For instance, if we choose a particular site, on an external edge of the gasket, as origin, it is easy to show using Eqs. (18) and (14):

$$U_{n,2^k}(\alpha) = U_n(\phi^{(k)}(\alpha)) = U_n(\alpha(T^k(\{\alpha\}))) \ , \tag{19}$$

where n denotes positions of sites along the chosen edge. This result is closely related to the scale invariance of the gasket and holds everywhere for a convenient labeling of sites.

Equation (19) can be used to obtain the set of eigenmodes corresponding to different $\alpha \in C_\delta$. For instance, starting from the uniform mode ($\alpha = 0$), amplitudes associated with $\alpha = \delta = f_+(0)$ are easily obtained. The remaining eigenmodes are deduced iteratively in a similar way. In general, U_n's vanish outside a finite region surrounding a hole arbitrarily chosen among the hierarchy of holes generated inside the gasket. For a fixed α, the relative degeneracy of each eigenstate decreases when the hole size increases. Therefore the eigenstates associated with C_δ can be viewed as localized modes with a hierarchy of localization lengths (hierarchical modes), standing from the lowest to the highest length scale on the gasket. However, if an "averaged" localization length is defined for each $\alpha \in C_\delta$, then a finite length is obtained which diverges only if $\alpha \to 0$.

In conclusion, we believe that some results obtained in this Rapid Communication are of generic nature and that similar features will be found to occur on other fractal structures. The map $\phi(\alpha)$ is expected to be a general rational function. It will also be quite useful to study other fractal structures, as simple as the gaskets, where $\tilde{d}$ would not be restricted to values smaller than 2.

After this work was submitted, we received a report of work prior to publication by Domany, Alexander, Bensimon, and Kadanoff.[10] Using a different approach, they study the cases $d=2$ and $d=3$, on finite systems, for which their main conclusions agree with those presented here.

ACKNOWLEDGMENTS

The author is indebted to Dr. G. Toulouse and Dr. B. Souillard for very useful discussions. It is a pleasure to thank Dr. S. Alexander for information about this work.

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