Multifractal Energy Spectra and Their Dynamical Implications

Italo Guarneri* and Giorgio Mantica†
Università di Milano, sede di Como, via Lucini 3, 22100 Como, Italy
(Received 11 January 1994)

We present a method for constructing lattice tridiagonal Hamiltonians having a preassigned multifractal measure as local spectrum. Using this construction we investigate how the fractal structure of the spectrum affects the motion of wave packets. We find that the quantum evolution is intermittent: The moments of particle's position on the lattice are characterized by a nontrivial scaling function, even when the spectrum is a one-scale, balanced Cantor set. Numerical data show that the minimum scaling exponent is always larger than the information dimension of the spectral measure, and qualitatively follows the behavior of this quantity, as the spectral measure is varied.

PACS numbers: 05.45.+b, 02.30.-f, 71.30.+h, 71.55.Jv

Until recently, the traditional classification of energy spectra in pure point and absolutely continuous has proven quite sufficient to describe quantum evolution. The third element exhausting this classification, singular continuous energy spectra, has been usually considered by physicists as a mathematical curiosity and overlooked. However, this exotic kind of spectra is now attracting a growing attention: In fact, it is generic (in a mathematical sense) for one-body Schrödinger operators [1] and appears fairly frequently in theoretical studies on quasiperiodic systems [2,3], on incommensurate structures [4], and on the electron dynamics of crystals in magnetic fields [5].

The success of fractals in various areas of physics has also invested this field, and the techniques of the thermodynamical formalism [6] have been applied to the systems just mentioned [7–9], although more often in a descriptive than in a predictive approach. Quite on the contrary, these spectra lead to dynamical behaviors of deep physical relevance; for instance, it has been found [10,11] that, for a particle moving on a one-dimensional lattice, the time-averaged probability of staying at the starting site decays in time asymptotically as t^{-D_2}, D_2 being the correlation dimension of the associated spectral measure. This is just one of the relations between dynamics and multifractal properties, which make the subject of this Letter.

The analysis of the Harper system [7,8] first brought into evidence a multifractal spectrum (with Hausdorff dimension close to $\frac{1}{2}$) associated with a pseudodiffusive evolution of wave packets initially focused at the origin: the expectation value of the square of the position of such packets grows (approximately) linearly in time. On the grounds of heuristic arguments [12,13] it has been conjectured [13] that the exponent β_2 ruling anomalous diffusion $\overline{\langle x^2\rangle}(t) \sim t^{2\beta_2}$ (the bar meaning time average), should coincide with the Hausdorff dimension D_H of the support of the spectral measure of the initial state. Although numerical data consistent with this surmise have been presented [9,13], quite recently some doubts on its generality have been put forward on the strength of other heuristic observations [14]; in summary, no decisive evidence in either sense has been provided so far.

A complete study of the scaling properties of wave-packet propagation can be centered around the behavior of the moments $\nu_\alpha(t) := \overline{\langle x^\alpha\rangle}(t)$ for real $\alpha > 0$. Under suitable circumstances, these moments behave like $t^{\alpha\beta}$, thereby defining a scaling function $\beta(\alpha)$ [15]. An exact analysis shows that $\beta(\alpha)$ must be larger than the information dimension D_1 of the spectral measure for any α [16,17]. The limit $\beta(0)$ can be defined, and it represents the lowest scaling exponent. In the general case, more precise results seem difficult to derive; at the same time a numerical investigation of the relations between the moment scaling function and the various fractal dimensions has to cope with the difficulties present in the accurate determination of both quantities.

For these reasons, in this Letter we take a different approach: Instead of studying a given Hamiltonian, and computing spectral properties and dynamics, we start from a given spectral measure, μ, arbitrarily chosen in a wide multifractal class, for which all fractal dimensions are explicitly computable. Then we show that a constructive procedure can be set to compute all matrix elements of a (tridiagonal) Hamiltonian H, which is the most natural operator processing μ as spectral measure. The related Schrödinger equation is then numerically solved via reliable procedures and $\beta(\alpha)$ extracted. We investigate various choices of the spectral measure and we find that the conjecture $\beta(2) \approx D_0$ is at best approximate; that the wave-packet propagation exhibits *multiscaling in time* (i.e., *intermittency*), in the sense that it is characterized by a nontrivial range of exponents $\beta(\alpha)$; and that intermittency is present even in the case of a homogeneous fractal measure, that is, multiscaling does not require multifractality.

The first step in our approach requires the solution of an inverse problem of the sort "can we build a drum with a given spectrum?" The "drum" is, in our case, a tridiagonal Hamiltonian matrix H of the tight-binding type widely used to model the dynamics of electrons in

0031-9007/94/73(25)/3379(4)$06.00

disordered solids:

$$H_{i,i} = A_i, \qquad H_{i,i+1} = H_{i+1,i} = r_{i+1} > 0, \qquad i = 0, 1, \ldots, \tag{1}$$

where A and r are site energies and hopping elements. We want to determine the real constants A_i and r_i (these latter, positive nonzero) in such a way that the spectral measure (also known to physicists as the local spectral density) of the vector $|0\rangle$ with respect to the Hamiltonian H defined in Eq. (1) coincides with a preassigned multifractal, normalized measure μ. This can be done as follows (see also [18,19]).

We assume that the support of μ is included in a finite interval $[a, b]$ and consider the Hilbert space $L^2_\mu([a, b])$ of square-summable functions with respect to the measure μ. In this space we consider the infinite sequence of orthogonal polynomials $p_n(x)$ associated with μ. Then, let us define H in L^2_μ as the multiplication by x: $H\psi(x) = x\psi(x)$. As is well known from the spectral theorem, the spectral measure of the vector $\psi(x) = 1$ with respect to H is none but μ itself. Moreover, it is immediate from the theory of orthogonal polynomials that $\langle p_n|H|p_m\rangle \neq 0$ only if $|m - n| \leq 1$, that is, the matrix of the operator H on the basis of the orthogonal polynomials has the form (1).

Determining the real coefficients A_n, r_n from the measure μ is generally a difficult endeavor [20] that we were able to accomplish for μ in the class of IFS (iterated function systems) [21,22]. IFS measures are invariant under a weighted set of affine renormalization transformations: for $j = 1, 2, \ldots, M$, let $w_j(x)$ be affine contracting real maps of the form $w_j(x) = \delta_j x + \beta_j$, $|\delta_j| < 1$. Associated with each map there exist weights $\pi_j > 0$, $\sum_j \pi_j = 1$. Then, μ is defined as the only positive measure such that the equality

$$\int f(x)\, d\mu(x) = \sum_{j=1}^{M} \pi_j \int f(w_j(x))\, d\mu(x) \tag{2}$$

holds for any continuous function f, and is also called the *balanced measure* of the IFS.

Measures in this class are rather general and versatile: for instance, they can approximate arbitrarily well any measure supported on a finite interval [23]. Of interest to our present application is the fact that their multifractal properties are exactly computable: The spectrum of generalized dimensions follows from the equation [24] $\sum_{j=1}^{M} \pi_j^q \delta_j^\tau = 1$, whose unique solution defines τ as a function of q. One then obtains $D_q = \frac{\tau(q)}{q-1}$.

It can be proved that the H-matrix elements for this class of measures form bounded sequences. Numerical evidence suggests a possible quasiperiodic behavior for which we do not have a theoretical proof at the moment.

Having thus determined the matrix H, we can solve Schrödinger's equation, $i\psi' = H\psi$ numerically for a wave packet initially concentrated at $|0\rangle$. We find

$$c_n(t) := \langle n|e^{-itH}|0\rangle = \int e^{-itx} p_n(x)\, d\mu(x)\,. \tag{3}$$

The second equality shows that the coefficients of the evolution are the Fourier transforms of the orthogonal polynomials *with respect to the spectral measure* μ. This is the basis of a numerical procedure we employed to compute $c_n(t)$, a Gaussian integration enhanced by Eq. (2). Other independent techniques we used for comparison are matrix diagonalization over a finite basis and direct solution of Schrödinger equation by an implicit Runge-Kutta method.

The asymptotic behavior of the coefficients can also be derived from Eq. (3): for small t, $\underline{|c_n(t)|^2} \sim t^{2n}$; in the infinite time limit, we obtain that $\overline{|c_n|^2}(t) \sim t^{-D_2}$ for all n, thereby generalizing the result of [13]. The position moments can be expressed as $\nu_\alpha(t) = \sum_n n^\alpha |c_n(t)|^2$. It is clear that their long-time asymptotics is governed by the nonuniformity in n of the behavior of each term in the summation.

The time is now ripe for introducing the results of our numerical experiments. Let us consider the IFS generated by two maps, with parameters $\delta_1 = \delta_2 = \frac{2}{5}$, $\beta_1 = 0$, $\beta_2 = \frac{3}{5}$, and $\pi_1 = \pi_2 = \frac{1}{2}$, corresponding to a "pure" Cantor set: $D_q = D_0 =$ log2/log5 − log2 for all q. The behavior of $\nu_\alpha(t)$ is power law, with superimposed log-periodic oscillations due to lacunarity (Figs. 1 and 2).

Because of these oscillations, care must be exerted in extracting the average exponent. Our data have been obtained with two different fitting techniques and are consistent within a few parts per thousand for values of α larger than 1. Reliability is just a little lower for α in between 0 and 1. The function $\beta(\alpha)$ (Fig. 3) is necessarily nondecreasing. In this example, it covers the range [0.773, 0.789] for α in [0, 2]. While the inequality $\beta(0) > D_1$ is validated, the Hausdorff dimension

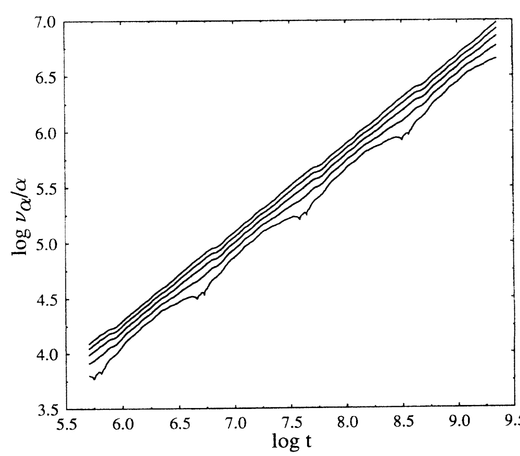

FIG. 1. Particle's moments ν_α versus time, in double logarithmic plot, for the IFS dynamics described in the text. The logarithm of each moment is divided by the corresponding value of α. The values of α are 0.5, 1, 1.5, 2, and 2.5, from the lowest curve to the highest.

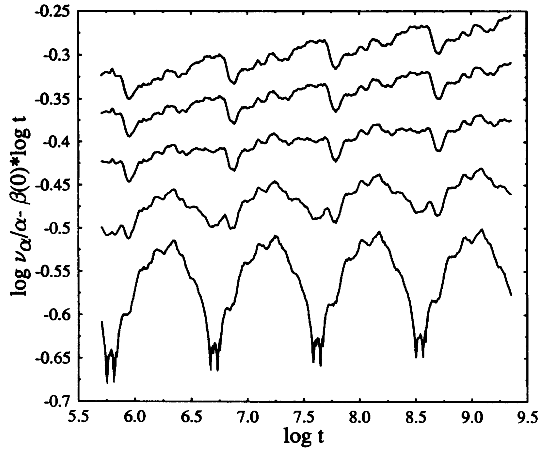

FIG. 2. Particle's moments ν_α versus time, as in Fig. 1, after subtraction of the behavior of the minimum scaling exponent, $\beta(0)\log t$, with $\beta(0) = 0.773$. The typical log-periodic oscillations appear now clearly, as well as the increasing slopes of the curves, which are still associated with the values $\alpha = 0.5$, 1, 1.5, 2, and 2.5, going from bottom to top.

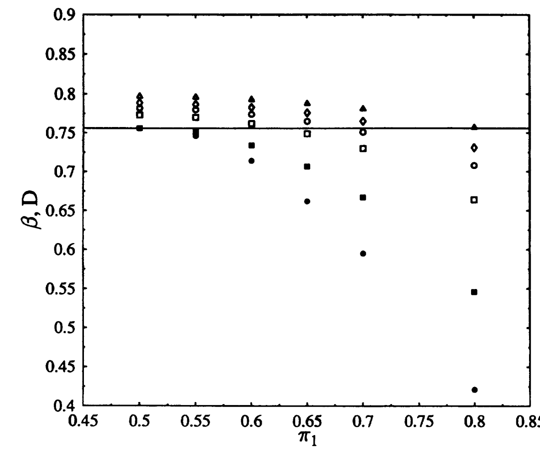

FIG. 4. Scaling exponents $\beta(0)$ (open squares), $\beta(1)$ (open circles), $\beta(2)$ (open diamonds), and $\beta(4)$ (open triangles) versus map weight π_1, for the IFS described in the text. Also plotted are D_1 (filled squares) and D_2 (filled circles). The horizontal line marks the value of D_0, which is here constant.

$D_H \simeq 0.7565$ (which coincides with D_0 for our class of fractals) is well below $\beta(2)$.

By varying the weight π_1 (and consequently π_2), while keeping the other parameters fixed, we can study spectral measures with the same support (hence, D_0) but different thermodynamics. Three main observations can be drawn from the data reported in Fig. 4: First, we notice that the minimum scaling exponent $\beta(0)$ is always *strictly* larger than its rigorous lower bound D_1, yet at the same time it follows qualitatively the behavior of the latter. Second, since D_0 is constant in π_1 while none of the β is such, the conjecture in the beginning is disproved. Third, as π_1 tends to 1, all generalized dimensions (except D_0) tend to zero, and the growth exponents do the same.

Alternatively, we elect to vary one of the contraction rates, δ_1, to study the general case of nonuniform, nonhomogeneous fractals. The other parameters defining the investigated IFS are $\delta_2 = \frac{2}{5}$, $\beta_1 = 0$, $\beta_2 = \frac{3}{5}$, $\pi_1 = \frac{3}{5}$, and $\pi_2 = \frac{2}{5}$. The range of variation of the exponents $\beta(0)$ is larger here than in the previous example (Fig. 5). They are still higher than their lower estimate D_1, although they show again the same trend.

We can therefore summarize our findings as follows: We have built and investigated a class of quantum models whose spectral properties are exactly known. We have found that the moment scaling function $\beta(\alpha)$ is never constant, not even for fractals characterized by a

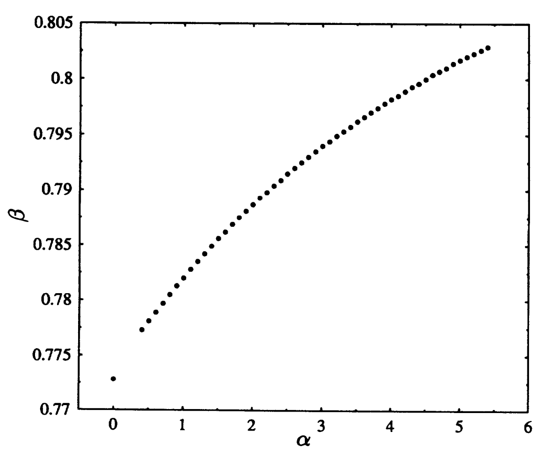

FIG. 3. Scaling exponent β versus α, for the IFS of Figs. 1 and 2.

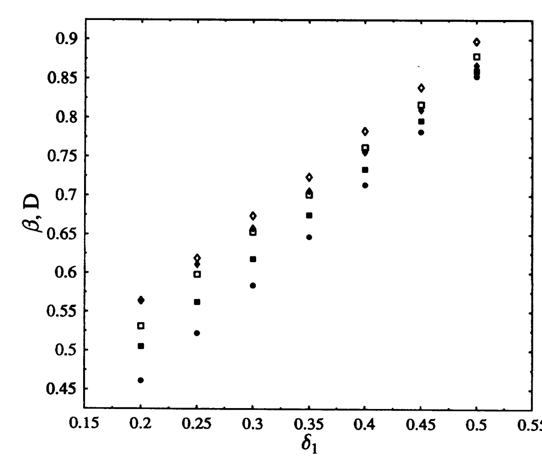

FIG. 5. Scaling exponents $\beta(0)$ (open squares), and $\beta(2)$ (open diamonds) versus map parameter δ_1, for the IFS described in the text. Also plotted are D_0 (filled diamonds), D_1 (filled squares), and D_2 (filled circles).

single dimension, thus preventing the existence of simple scaling relations for the dynamics; in this sense, quantum evolution of systems with fractal spectra is intermittent. Moment scaling exponents are somehow linked to the spectrum of generalized dimensions, the closest ties linking $\beta(0)$ and D_1, but no simple equality seems to hold. In particular, $\beta(2) \sim D_0$ is to be considered occasional, and typical (if validated) of a special model.

*Also atIstituto Nazionale di Fisica Nucleare, Sezione di Pavia, via Bassi 6, 27100 Pavia, Italy.
†Electronic address: mantica@milano.infn.it

[1] R. del Rio, S. Jitomirskaya, N. Makarov, and B. Simon, "Singular Continuous Spectrum is Generic" (to be published).
[2] B. Simon, Adv. App. Math. **3**, 463–490 (1982); S. Jitomirskaya and B. Simon (to be published).
[3] J. Bellissard, D. Bessis, and P. Moussa, Phys. Rev. Lett. **49**, 702–704 (1982).
[4] J.B. Sokolov, Phys. Rep. **126**, 189 (1985).
[5] P.G. Harper, Proc. R. Soc. London A **68**, 874 (1955); M. Ya.Az'bel, Sov. Phys. JETP **19**, 634 (1964); D.R. Hofstadter, Phys. Rev. B **14**, 2239 (1976); M. Wilkinson, Proc. R. Soc. London A **391**, 305 (1984), and J. Phys. A **20**, 4437 (1987).
[6] T.C. Halsey, M.H. Jensen, L.P. Kadanoff, I. Procaccia, and B.R. Shraiman, Phys. Rev. A **33**, 1141 (1986).
[7] C. Tang and M. Kohmoto, Phys. Rev. B **34**, 2041 (1986).
[8] H. Hiramoto and S. Abe, J. Phys. Soc. Jpn **57**, 230 (1988); **57**, 1365 (1988).
[9] R. Artuso, G. Casati, and D.L. Shepelyansky, Phys. Rev. Lett. **68**, 3826 (1992).
[10] R. Ketzmerick, G. Petschel, and T. Geisel, Phys. Rev. Lett. **69**, 695 (1992).
[11] M. Holschneider, Commun. Math. Phys. **160**, 457 (1994).
[12] I. Guarneri, Europhys. Lett. **10**, 95 (1989).
[13] T. Geisel, R. Ketzmerick, and G. Petschel, Phys. Rev. Lett. **66**, 1651 (1991); **67**, 3635 (1991).
[14] M. Wilkinson and E.J. Austin (to be published).
[15] S.N. Evangelou and D.E. Katsanos, J. Phys. A **26**, L1243 (1993).
[16] I. Guarneri, Europhys. Lett. **21**, 729 (1993).
[17] I. Guarneri and G. Mantica, Ann. Ist. H. Poincarè (to be published).
[18] K.M. Case and M. Kac, J. Math. Phys. **14**, 594 (1973).
[19] D. Bessis and G. Mantica, J. Comp. Appl. Math. **48**, 17–32 (1993).
[20] W. Gautschi, in *Orthogonal Polynomials,* edited by P. Nevai (Kluwer, Dordrecht, NL, 1990), pp. 181–216.
[21] J. Hutchinson, Indiana J. Math. **30**, 713–747 (1981); M.F. Barnsley and S.G. Demko, Proc. R. Soc. London A **399**, 243–275 (1985); M.F. Barnsley, *Fractals Everywhere* (Academic Press, New York, 1988).
[22] G. Mantica, "A Stieltjes Technique for Computing Jacobi Matrices Associated with Singular Measures" (to be published).
[23] C.R. Handy and G. Mantica, Physica (Amsterdam) **43D**, 17–36 (1990).
[24] This equation is valid for the disconnected IFS used in this Letter.