

What determines the spreading of a wave packet?

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The multifractal dimensions D_2^μ and D_2^ψ of the energy spectrum and eigenfunctions, resp., are shown to determine the asymptotic scaling of the width of a spreading wave packet. For systems where the shape of the wave packet is preserved the k -th moment increases as $t^{k\beta}$ with $\beta = D_2^\mu/D_2^\psi$, while in general $t^{k\beta}$ is an optimal lower bound. Furthermore, we show that in d dimensions asymptotically in time the center of any wave packet decreases spatially as a power law with exponent $D_2^\psi - d$ and present numerical support for these results.

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For the case of a free particle, the spreading of a quantum mechanical wave packet is a textbook example. One finds that asymptotically the width increases linearly in time and the corresponding energy spectrum is absolutely continuous. In the case of a point spectrum, on the other hand, there is asymptotically no increase of the width of a wave packet, if the eigenfunctions are semi-uniformly localized [1]. Between these extremes flourishes the world of quantum systems with fractal energy spectra and eigenfunctions. They include systems studied in the early days of quantum mechanics, like Bloch electrons in a magnetic field [2] as well as quasicrystals [3] and disordered systems, e.g. at the Anderson transition [4] or in the Quantum Hall regime [5]. A natural question then arises: What determines their long-time dynamical properties, e.g. the spreading of wave packets (quantum diffusion) and the decay of temporal correlations?

Very few rigorous and general answers are known so far. Temporal correlations decay as $t^{-D_2^\mu}$ [6], where D_2^μ is the correlation dimension of the spectral measure μ (i.e. the local density of states). For the spreading of a wave packet, on the other hand, two *inequalities* were derived by Guarneri. The growth of the k -th moment $m_k(t) \sim t^{k\beta_k}$ is bounded from below by $D_1^\mu \leq \beta_k$ [7] and the entropic width grows faster than $t^{D_1^\mu}$ [8], where D_1^μ is another generalized dimension of the spectral measure.

In search for *equalities*, relating the growth of the moments of a wave packet to fractal properties of the spectrum, numerical studies of the Harper model [9,10], the Fibonacci model [11,12], and the kicked Harper model [13] were performed, suggesting, e.g. $\beta_2 = D_0$, in agreement with a heuristic argument [7,10], where D_0 is the fractal (box-counting) dimension of the spectrum. More recently, numerical studies [14,15] showed that this simple relation does not hold exactly. These studies also revealed that one often finds multiscaling in time [16], i.e. β_k varies with k . For a restricted class of systems, Mantica showed that $\beta_k = D_{1-k}^\mu$, whereas in general it is at best approximate [17]. The similar relation $\beta_k = D_{1-k}$,

now with the multifractal dimension of the ("global") density of states, was proposed to hold after averaging the dynamics of *all* wave packets started at different initial sites [18]. Therefore, the basic question, of what determines the spreading of a *single* wave packet, still remains open.

In this paper we derive a partial answer to this question (Fig. 1), by including, for the first time, fractal properties of the eigenfunctions. For systems where asymptotically the k -th moment of a wave packet increases proportional to $t^{k\beta}$, we show

$$\beta = D_2^\mu/D_2^\psi, \quad (1)$$

where D_2^ψ is the correlation dimension of the (suitably averaged) eigenfunctions. For the more general case of multiscaling in time we derive an optimal lower bound for positive moments under reasonable assumptions:

$$\beta_k \geq D_2^\mu/D_2^\psi. \quad (2)$$

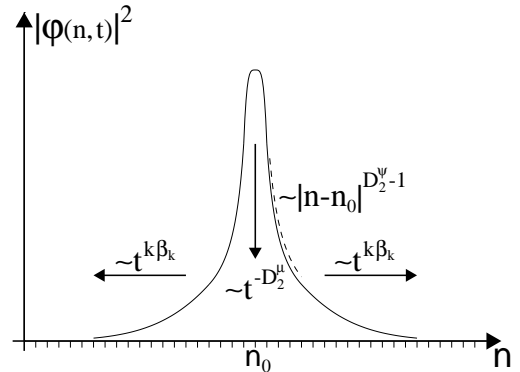


FIG. 1. Quantum diffusion of a wave packet initially started at site n_0 . The staying probability decays as $t^{-D_2^\mu}$, whereas the k -th moment increases as $t^{k\beta_k}$. If the form of the wave packet remains unchanged (uniform scaling) Eq. (1) leads to $\beta_k = \beta \equiv D_2^\mu/D_2^\psi$ for $k > 0$. For the case of multiscaling dynamics we find the lower bound $\beta \leq \beta_k$ for $k > 0$ (Eq. (2)). In any case, the center of the wave packet spatially decreases as $|n - n_0|^{D_2^\psi - 1}$ for $|n - n_0| \ll t^\beta$.

We verify these results numerically for the on-site Fibonacci model and the Harper model, where it is a much better lower bound than the previously obtained D_1^μ [7], which did not make use of fractal properties of the eigenfunctions. Surprisingly, we find from these dynamical properties that in d dimensions asymptotically in time the center of any wave packet decreases spatially like a power law with an exponent $D_2^\psi - d$ (see Fig. 1).

The moments of a wave packet $\varphi(n, t)$, initially located on site n_0 , are given by $m_k(t) = \sum_{n \neq n_0} |n - n_0|^k |\varphi(n, t)|^2$, where for convenience we use a finite one-dimensional lattice. To derive the scaling properties of the moments we need a relation between the integrated wave packet

$$g(x, t) = \sum_{|n-n_0|<x} |\varphi(n, t)|^2 \quad (3)$$

and the spectral function [19]

$$S(x, \omega) = \sum_{\substack{i,j \\ |E_i - E_j| < \omega}} \sum_{|n-n_0|<x} \psi_i^*(n_0) \psi_j(n_0) \psi_i(n) \psi_j^*(n) \quad (4)$$

with E_i and ψ_i denoting eigenenergies and eigenfunctions, respectively. For systems described by a real symmetric matrix these are simply related by

$$g(x, t) = \int_0^\infty d\omega \cos \omega t \frac{d}{d\omega} S(x, \omega) \quad (5)$$

and

$$S(x, \omega) = \frac{2}{\pi} \int_0^\infty dt \frac{\sin \omega t}{t} g(x, t). \quad (6)$$

For the special case $x = 1$ the spectral function simplifies and we assume the following scaling behavior [20]:

$$S(x = 1, \omega) = \sum_{\substack{i,j \\ |E_i - E_j| < \omega}} |\psi_i(n_0)|^2 |\psi_j(n_0)|^2 \sim \omega^{D_2^\mu} \quad (7)$$

and

$$S(x, \omega = \omega_{\min}) \sim x^{D_2^\psi}, \quad (8)$$

where ω_{\min} is the smallest energy scale where the scaling of Eq. (7) still holds for a given finite system. Physically, ω_{\min} is the inverse of the time when a wave packet reaches the boundary and when the power-law moment growth is modified. D_2^μ is the (standard) correlation dimension of the spectral measure and D_2^ψ denotes the correlation dimension of the averaged eigenfunctions [21].

We will first study the special case that the overall shape of the wave packet stays the same during its time evolution, with, of course, a scaling in width and

amplitude. Assuming a power-law scaling one therefore has a function G of a single variable defined by $G(x/t^\beta) = g(x, t)$. This is equivalent to the property that the positive ($k \geq 0$) moments scale as $m_k(t) \sim t^{k\beta}$, which we call uniform scaling. From Eq. (6) and the properties of G we find that $S(x, \omega)$ is a function of $x\omega^\beta$ only. Together with the scaling behaviors of Eqs. (7) and (8) one easily finds the result $\beta = D_2^\mu/D_2^\psi$ (Eq. (1)). From Eq. (5) we can thus even determine all negative moments: $m_k(t) \sim t^{k\beta}$ for $k \geq -D_2^\psi$, whereas $m_k(t) \sim t^{-D_2^\psi}$ for $k \leq -D_2^\psi$.

Secondly, we now want to study the case of multiscaling dynamics. We cannot do this in the most general form, but need two reasonable assumptions. We first assume that for $x\omega^\beta \ll 1$ the spectral function $S(x, \omega)$ is determined by its limiting scaling behaviors (Eqs. (7) and (8)), namely $S(x, \omega) \sim x^{D_2^\mu} \omega^{D_2^\mu}$ [22]. Using Eqs. (5) and (6) this implies uniform scaling for the center of the wave packet only, i.e. $g(x, t) = G(x/t^\beta)$ for $x \ll t^\beta$. In fact, it follows $g(x, t) \sim x^{D_2^\mu} t^{-D_2^\mu}$ for $x \ll t^\beta$. Remarkably, this even determines the shape of the center of the wave packet, namely, an algebraic decay $|n - n_0|^{D_2^\psi - 1}$ for $|n - n_0| \ll t^\beta$. In addition, we assume that outside this region it decays faster than $|n - n_0|^{D_2^\psi - 1}$, which it certainly has to do asymptotically in order to stay normalized. Under these assumptions, it follows that for a large enough time T there exists an X such that $g(x, T) \propto x^{D_2^\psi}$ for $x \leq X$ and that for all $t > T$ with $g(\xi(t), t) = g(X, T)$ the relation $\xi(t)/t^\beta \geq X/T^\beta$ must hold. Using a result by Guarneri and Mantica [7], stating that all β_k (for $k \geq 0$) are larger than the scaling exponent of $\xi(t)$, it then follows that all positive moments scale as $t^{k\beta_k}$ with $\beta_k \geq \beta$. Therefore β is a lower bound on the scaling of the positive moments that incorporates multifractal properties of the eigenfunctions. In fact, for negative moments ($k < 0$) we find that $\beta \geq \beta_k$ is an upper bound. In that sense β is an optimal lower bound for all positive moments.

Furthermore, note that this analysis can be readily extended to systems in higher dimensions d by appropriately generalizing the definitions of g and S . Under the condition $D_2^\mu < 1$ Eqs. (1) and (2) remain unchanged and the spatial decay of the center of the wave packet has an exponent $D_2^\psi - d$. Finally, this formalism can easily describe the averaged dynamics of wave packets started at different initial sites n_0 . To this end we introduce an average in Eqs. (7) and (8) defining exponents \bar{D}_2^μ and \bar{D}_2^ψ , which replace D_2^μ and D_2^ψ in the above results [23].

One can try to understand the derived results in an intuitive way: The temporal decay of the center of the wave packet is known to be given by $t^{-D_2^\mu}$ [6]. Naively, normalization then requires a spreading described by an exponent $\beta = D_2^\mu/d$ in d dimensions. If the spreading, however, takes place in a space with an effectively reduced dimension D_2^ψ instead of d [5], we have $\beta = D_2^\mu/D_2^\psi$. Sim-

ilarly, the integrated wave packet $g(x, t)$, which usually increases initially as x^d , here increases with $x^{D_2^\psi}$ instead. This leads immediately to a power-law decay $|n - n_0|^{D_2^\psi - d}$ for the center of the wave packet in the d -dimensional embedding space.

In the remainder, we want to give examples and numerical evidence supporting the above analysis [24].

For disordered systems at the metal-insulator transition in 2 (with strong magnetic field or symplectic symmetry) and 3 dimensions Eq. (1) is already known. These systems are simpler in the sense that the fractal dimension D_0 of the spectrum is 1 and it was shown that $D_2^\psi = dD_2^\mu$ holds [5,25,26], where $d = 2, 3$ is the spatial dimension. On the other hand, $\beta = 1/d$ follows from the non-fractal value of D_0 using heuristic arguments, as in Refs. [7,10,12], and was numerically confirmed for the second moment [5,27]. The prediction that the asymptotic shape of the wave packet follows the power law $|n - n_0|^{D_2^\psi - d}$ waits to be observed in disordered systems.

We now consider the on-site Fibonacci chain, which is a one-dimensional model of a quasicrystal [3] given by a tight-binding Hamiltonian where the on-site energy V_n takes the values $+V$ and $-V$, arranged according to the Fibonacci sequence. Figs. 2 and 3 show that the ratio $\beta = D_2^\mu/D_2^\psi = 0.477$ coincides, within the numerical accuracy, with the scaling behavior of the moments, thus confirming Eq. (1) [28].

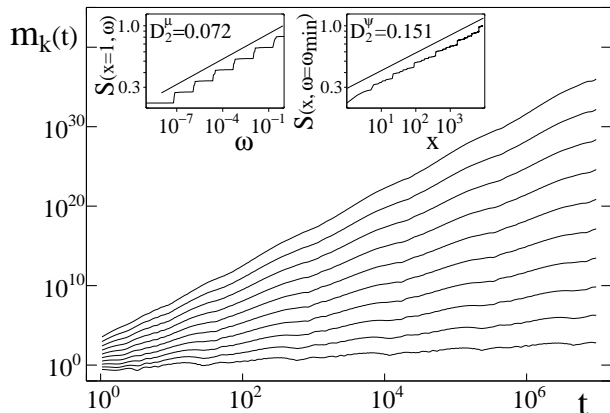


FIG. 2. The moments $m_k(t)$ for $k = 1, 2, \dots, 10$ of a wave packet initially started at a symmetric site of a Fibonacci chain with $V = 2$ and 17711 sites. The insets show the determination of $D_2^\psi = 0.072$ (left) and $D_2^\psi = 0.151$ (right) from the limiting scaling behavior of $S(x, \omega)$ yielding $\beta = D_2^\mu/D_2^\psi = 0.477$, which is much larger than the information dimension $D_1^\mu = 0.153$.

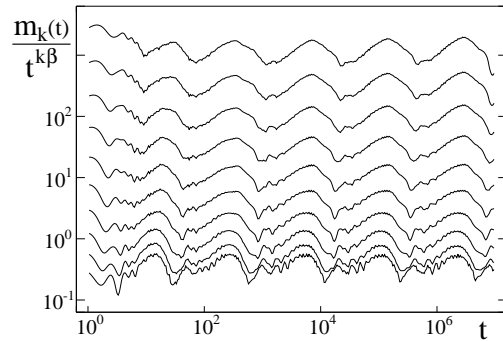


FIG. 3. The scaled moments $m_k(t)/t^{k\beta}$ of a Fibonacci chain corresponding to the parameters of Fig. 2 are (on average) constant, thus confirming Eq. (1).

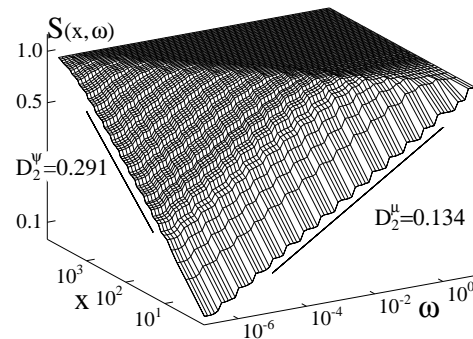


FIG. 4. The spectral function $S(x, \omega)$ for the Harper model with $\sigma = 6765/10946$, an approximant of the golden mean, and $\nu = 0$ of a wave packet initially started at $n = 0$. It shows the scaling behavior $\sim x^{D_2^\psi} \omega^{D_2^\mu}$ for small x and ω , as we have it assumed for deriving Eq. (2). (Deviations close to $S(x, \omega) = 1$ might be the cause for multiscaling in time.) We find $D_2^\mu = 0.134$ and $D_2^\psi = 0.291$.

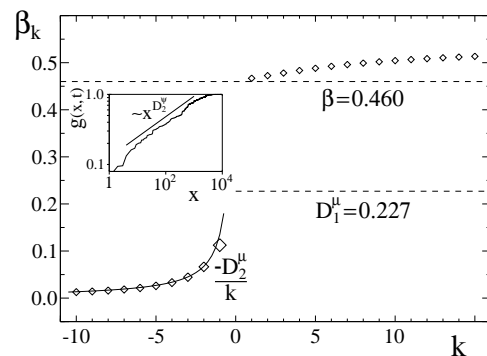


FIG. 5. The values β_k (diamonds) of the power-law scaling moments $m_k(t) \sim t^{k\beta_k}$ of the Harper model with $\sigma = 10946/17711$ and $\nu = 0$ of a wave packet initially started at $n = 0$. One can see that $\beta = D_2^\mu/D_2^\psi = 0.460$ is a much better lower bound for all positive moments than $D_1^\mu = 0.227$. For negative moments, $k \leq -1$, we find $k\beta_k = -D_2^\mu$. The inset shows the power-law behavior of the integrated wave packet $g(x, t = 3 \times 10^6) \sim x^{D_2^\psi}$ corresponding to a power-law decay $|\varphi(n, t)|^2 \sim |n - n_0|^{D_2^\psi - 1}$.

In general, though, quantum systems with a fractal energy spectrum generate multiscaling dynamics [14–16]. As an example we consider the Harper model [29], describing an electron in a two-dimensional periodic potential and a perpendicular magnetic field [2]. For σ the number of magnetic flux quanta per unit cell it is given by a tight-binding Hamiltonian, where now $V_n = 2 \cos(2\pi\sigma n + \nu)$ holds. Fig. 4 shows that the scaling assumption for $S(x, \omega)$ is fulfilled [30] and Fig. 5 shows that $\beta \leq \beta_k$ is a good lower bound for the positive moments. We have verified $\beta \leq \beta_k$ also for wave packets started at other sites n_0 as well as for a few other irrational σ . In fact, in all cases β considerably improves the lower bound D_1^μ deduced from spectral properties [7]. In addition, we have confirmed the prediction for the shape of the center of the wave packet, namely a power-law decay with exponent $D_2^\psi - 1$, i.e. $g(x, t) \sim x^{D_2^\psi}$ (Fig. 5 inset).

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* Present address.

- [1] R. del Rio et al., Phys. Rev. Lett. **75**, 117 (1995).
- [2] R. Peierls, Z. Phys. **80**, 763 (1933).
- [3] D. Shechtman et al., Phys. Rev. Lett. **53**, 1951 (1984).
- [4] M. Schreiber and H. Grussbach, Phys. Rev. Lett. **67**, 607 (1991).
- [5] B. Huckestein and L. Schweitzer, Phys. Rev. Lett. **72**, 713 (1994).
- [6] R. Ketzmerick, G. Petschel, and T. Geisel, Phys. Rev. Lett. **69**, 695 (1992); subsequent derivations in the mathematical literature were given by M. Holschneider, Comm. Math. Phys. **160**, 457 (1994); C. A. Guerin and M. Holschneider, J. Stat. Phys. **86**, 707 (1997); J. X. Zhong and R. Mosseri, J. Phys.: Condens. Matt. **7**, 8383 (1995); J. M. Barbaroux, J. M. Combes, and R. Montcho, preprint CPT-96/P.3303.
- [7] I. Guarneri, Europhys. Lett. **10**, 95 (1989); I. Guarneri, Europhys. Lett. **21**, 729 (1993); generalizations of this result were given by J. M. Combes, in *Differential Equations with Applications to Mathematical Physics*, edited by W. F. Ames, E. M. Harrell, J. V. Herod (Academic Press, Boston, 1993); I. Guarneri and G. Mantica, Ann. Inst. H. Poincaré **61**, 369 (1994); Y. Last, to appear in J. Func. Anal.
- [8] I. Guarneri and M. Di Meo, J. Phys. A: Math. Gen. **28**, 2717 (1995); and I. Guarneri, private communication.
- [9] H. Hiramoto and S. Abe, J. Phys. Soc. Jpn. **57**, 1365 (1988).
- [10] T. Geisel, R. Ketzmerick, G. Petschel, Phys. Rev. Lett. **66**, 1651 (1991).
- [11] H. Hiramoto and S. Abe, J. Phys. Soc. Jpn. **57**, 230 (1988).
- [12] T. Geisel, R. Ketzmerick, G. Petschel, in *Quantum Chaos - Theory and Experiment*, edited by P. Cvitanovic, I. C. Percival, A. Wirzba (Kluwer, Dordrecht, 1992).
- [13] R. Lima, D. Shepelyansky, Phys. Rev. Lett. **67**, 1377 (1991); T. Geisel, R. Ketzmerick, G. Petschel, Phys. Rev. Lett. **67**, 3635 (1991); R. Artuso, G. Casati, and D. Shepelyansky, Phys. Rev. Lett. **68**, 3826 (1992); R. Artuso et al., Phys. Rev. Lett. **69**, 3302 (1992).
- [14] I. Guarneri and G. Mantica, Phys. Rev. Lett. **73**, 3379 (1994).
- [15] M. Wilkinson and J. Austin, Phys. Rev. B **50**, 1420 (1994).
- [16] S. N. Evangelou and D. E. Katsanos, J. Phys. A **26**, L1243 (1993).
- [17] G. Mantica, to appear in Physica D, 1996.
- [18] F. Piéchon, Phys. Rev. Lett. **76**, 4372 (1996).
- [19] In order to smooth out fluctuations we have added two sums compared to the definition in J. T. Chalker and G. J. Daniell, Phys. Rev. Lett. **61**, 593 (1988), where a disorder averaging was used.
- [20] From Eq. (7) follows for the temporal correlation decay $C(t) \equiv \frac{1}{t} \int_0^t dt' g(1, t') \sim t^{-D_2^\mu}$ as was shown in Ref. [6].
- [21] Actually, D_2^μ is defined by the box-counting method [T. C. Halsey et al., Phys. Rev. A **33**, 1141 (1986).], where the spectrum is divided into boxes of size ω and the scaling of the sum $\sum_s p_s^2 \sim \omega^{D_2^\mu}$ determines D_2^μ . Here $p_s = \sum_{i \in B_s} |\psi_i(n_0)|^2$ is the probability to be in box B_s and thus $\sum_s p_s^2 = \sum_s \sum_{i,j \in B_s} |\psi_i(n_0)|^2 |\psi_j(n_0)|^2$ has the same scaling behavior as Eq. (7). A similar argument holds for D_2^ψ in the case where ω_{\min} is the smallest level spacing and the spectral function simplifies to $S(x, \omega = \omega_{\min}) = \sum_i \sum_{|n-n_0| < x} |\psi_i(n_0)|^2 |\psi_i(n)|^2$. For convenience we use the notation D_2^ψ in Eq. (8) also for general ω_{\min} .
- [22] Under this condition the value of D_2^ψ in Eq. (8) does not depend on the exact choice of ω_{\min} , as long as it is in the scaling regime of $S(x, \omega)$.
- [23] For the Harper model with σ the golden mean we find $\bar{D}_2^\mu = 0.265$ explaining the averaged temporal correlation decay $\bar{C}(t) \sim t^{-0.25}$ found in Ref. [16].
- [24] Ref. [1] gives a surprising example showing that a point spectrum with exponentially localized eigenfunctions can coexist with moment growth at rates that are arbitrarily close to ballistic. Unfortunately, we cannot numerically check our results for this model due to the specially chosen irrational.
- [25] L. Schweitzer, J. Phys.: Condens. Matt. **7**, L281 (1995).
- [26] T. Brandes, B. Huckestein, and L. Schweitzer, Ann. Phys. **5**, 633 (1996).
- [27] T. Ohtsuki and T. Kawarabayashi, J. Phys. Soc. Jpn. **66**, 314 (1997).
- [28] If the on-site Fibonacci model for the chosen initial condition were not a uniform scaling system, but a very weakly multiscaling system, the data would still confirm the more general Eq. (2) within the numerical accuracy.
- [29] P. G. Harper, Proc. R. Soc. London A **68**, 874 (1955); M. Ya. Azbel', Zh. Eksp. Teor. Fiz. **46**, 429 (1964) [Sov. Phys. JETP **19**, 634 (1964)]; D. R. Hofstadter, Phys. Rev. B **14**, 2239 (1976).
- [30] For the parameters of Fig. 4 the finite system size destroys the scaling behavior $S(x, \omega) \sim x^{D_2^\psi} \omega^{D_2^\mu}$ below $\omega_{\min} = 10^{-7}$. In fact, for $\omega < \omega_{\min}$ one finds a different power law exponent in x .