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Green function analysis of energy spectra scaling properties

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Abstract. The relation between the singularities of multifractal energy spectral measures and the behaviours of the Green function is studied in the framework of a tight-binding Hamiltonian. If the measure $\mu(E)$ has a scaling behaviour at energy E of the form $\Delta\mu(E) = \mu(E+\delta) - \mu(E-\delta) \propto \delta^{\alpha(E)}$, it is proved that the imaginary part of the Green function $P(E,\epsilon)$ scales as $P(E,\epsilon) \propto \epsilon^{\beta(E)}$ with $\beta(E) = \alpha(E)+1$, the reverse being also true. This is exemplified in the case of the density of states and the local density of states of the one-dimensional Fibonacci quasicrystalline chain.

1. Introduction

Singular measures are frequently met in physics, and much attention has been paid to their characterization in recent years. If $\mu(x)$ is such a measure, one can for instance consider the scaling behaviour of $\Delta\mu(x) = \int_x^{x+\Delta x} \mathrm{d}\mu(x)$ in the form

$$\Delta\mu(x) \propto \Delta x^{\alpha(x)} \qquad \Delta x \to 0. \tag{1}$$

A constant scaling exponent α corresponds to a homogeneous fractal measure. If, however, $\alpha(x)$ varies with x, the measure is said to be multifractal. Note that the above definition of the scaling behaviour can be sometimes ambiguous, due to the existence of subdominant terms which may play a role. We shall go back to this point below. In the multifractal case, one should also take care about the distribution of the exponent $\alpha(x)$. The usual approach to deal with (at least some of) these difficulties is the so-called 'thermodynamical' formalism [1], which focuses on the continuous spectrum of exponents $\alpha(x)$ and its density $f(\alpha)$, usually a smooth function in the range $[\alpha_{\min}, \alpha_{\max}]$. But $f(\alpha)$ only provides a global description of the scaling properties, and one might be interested in the spatial location of the singularities. Using wavelet transforms seems a promising tool to perform this task [2, 3].

The topic of this paper is the multifractal analysis of the spectral measure of a tight-binding Hamiltonian in the spirit of the wavelet analysis of reference [2]. Such singular continuous spectral measures have been widely studied in the last fifteen years. Their interest has become even sharper since the experimental discovery of quasicrystals [15], because quasiperiodic potentials often lead to singular spectral measures. Since electronic properties are associated with the nature of the spectrum, the investigation of its singularities is

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therefore of great importance. For instance, the electronic specific heat is directly connected to the scaling of the density of states (DOS) spectral measure at the Fermi level. Singularities in the local density of states (LDOS) measure can also greatly influence the electronic transport properties. Most of the works in this field were devoted to the determination of the global scaling distribution function $f(\alpha)$ for the DOS measure [4]. In this paper, we show that, for such systems, the Green function can be used to reveal the scaling exponent distribution both for the DOS and the LDOS, directly in the energy space.

2. Relation between the measure singularities and the Green function behaviour

The resolvent operator is defined by

$$G(Z) = 1/(Z - H) \tag{2}$$

with $Z = E + \mathrm{i}\epsilon$, where H denotes the Hamiltonian of the system, E is the energy, and ϵ a small positive value. For a tight-binding Hamiltonian

$$H = \sum_i v_i \, |i><i| + \sum_{i,j} t_{ij} \, |i><j| \tag{3}$$

where v_i is the ith site energy, t_{ij} the hopping integral between the ith and jth sites; the Green function satisfies the following equation:

$$(Z - v_i)G_{ij} = \delta_{ij} + \sum_k t_{ik} G_{kj}. \tag{4}$$

Let us define $P(E, \epsilon) = -(1/N\pi)\mathrm{Im}\sum_i^N G_{ii}(Z)$ in the case of DOS or $P(E, \epsilon) = -(1/\pi)\mathrm{Im}\, G_{ii}(Z)$ for the LDOS at the ith site with E real, real $\epsilon \in [0, 1]$, and N is the number of sites.

According to the above definition (2), $P(E, \epsilon)$ is related to the spectral measure by

$$P(E, \epsilon) = \frac{1}{\pi} \int_{-\infty}^{+\infty} \frac{\epsilon}{(E' - E)^2 + \epsilon^2} \, \mathrm{d}\mu(E') \tag{5}$$

and

$$\mu(E) = \lim_{\epsilon \to 0} \int_{-\infty}^{E} P(E', \epsilon) \, \mathrm{d}E' \tag{6}$$

where $\mu(E)$ is the measure for the DOS or the LDOS,

$$\mu(E) = \int_{-\infty}^{E} \mathrm{d}\mu(E') \tag{7}$$

with $0 \leqslant \mu(E) \leqslant 1$ and $\int_{-\infty}^{+\infty} \mathrm{d}\mu(E) = 1$.

Before discussing the relation between the measure singularities and the Green function behaviour, we need to give a clear definition of the scaling exponent α. For a positive function $g(\epsilon)$ in [0, 1], we consider the following integral:

$$J_g(\alpha') = \int_0^1 \frac{g(\epsilon)}{\epsilon^{1+\alpha'}} \, \mathrm{d}\epsilon \tag{8}$$

We shall say that $g(\epsilon) \propto \epsilon^{\alpha}$, if $J_g(\alpha')$ converges for $\alpha' < \alpha$ and diverges $\alpha' > \alpha$. For $\alpha'_1 \leqslant \alpha'_2$, we have $J_g(\alpha'_1) \leqslant J_g(\alpha'_2)$. Then if $g(\epsilon) \propto \epsilon^{\alpha}$, the scaling exponent α can be defined by

$$\alpha = \mathrm{Sup}\{\alpha', J_g(\alpha') < +\infty\}. \tag{9}$$

Now with the above definition, we consider a energy spectral measure $\mu(E)$ which has the following scaling behaviour at energy E:

$$\Delta\mu(E) = \mu(E+\delta) - \mu(E-\delta) \propto \delta^{\alpha(E)} \tag{10}$$

which means that the integral

$$J_\mu(\alpha', E) = \int_0^1 \frac{[\mu(E+\delta) - \mu(E-\delta)]}{\delta^{\alpha'+1}}\, \mathrm{d}\delta \tag{11}$$

converges for $\alpha' < \alpha(E)$ and diverges if $\alpha' > \alpha(E)$. $\alpha(E) = 1$ for an absolutely continuous measure, whereas $\alpha(E) = 0$ for a pure point spectrum. The converse is not true: for instance, $\Delta\mu(E)$ may behave like $\delta \ln \delta$ which implies $\alpha(E) = 1$ but μ is not absolutely continuous. Let us remark that $\alpha(E) \leqslant 1$ with probability one with respect to μ. This means that values of E with $\alpha > 1$ may occur but they are exceptional in the spectrum and irrelevant for the time evolution of observables (see below). The purpose of this paper is to show how information about the scaling exponent $\alpha(E)$ can be extracted from the behaviour of $P(E, \epsilon)$.

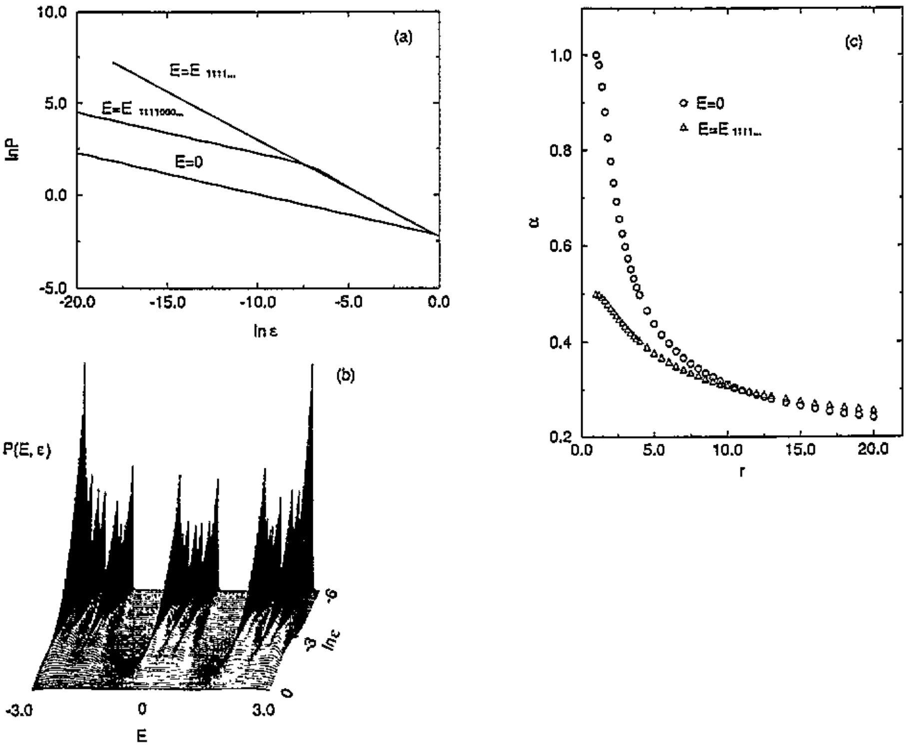

Figure 1. Scaling behaviour of the DOS (density of states) measure of the Fibonacci chain for the off diagonal model: (a) $\ln P(E, \epsilon)$ against $\ln \epsilon$ at eigenenergies $E = 0$, $E = E_{1111...} = 2.833\,956\,43...$ and $E = E_{11110000...} = 2.833\,023\,89...$ for $t_A = 1$, $t_B = 2$; (b) plot of $P(E, \epsilon)$ for $t_A = 1$, $t_B = 2$; (c) relation between the scaling of the measure and the quasiperiodicity strength $r = t_B/t_A$, $t_A = 1$.

From (5) and (7), an integration by parts leads to

$$P(E, \epsilon) = \frac{\epsilon}{\pi} \int_{-\infty}^{+\infty} \frac{2(E'-E)\mu(E')}{[(E'-E)^2 + \epsilon^2]^2}\, \mathrm{d}E'. \tag{12}$$

Let $\xi = (E' - E)/\epsilon$; (12) gives

$$P(E,\epsilon) = \frac{1}{\pi}\int_0^\infty \frac{2\xi[\mu(E+\epsilon\xi) - \mu(E-\epsilon\xi)]}{\epsilon(1+\xi^2)^2}\,d\xi. \tag{13}$$

We consider the following integral:

$$I_\mu(\alpha', E) = \int_0^1 \frac{P(E,\epsilon)}{\epsilon^{\alpha'}}\,d\epsilon. \tag{14}$$

Using (13) and letting $\delta = \epsilon\xi$, we have

$$I_\mu(\alpha', E) = \frac{1}{\pi}\int_0^\infty \frac{[\mu(E+\delta) - \mu(E-\delta)]}{\delta^{1+\alpha'}}\,d\delta \int_\delta^\infty \frac{2\xi^{1+\alpha'}}{(1+\xi^2)^2}\,d\xi. \tag{15}$$

Note that

$$\int_\delta^\infty \frac{2\xi^{1+\alpha'}}{(1+\xi^2)^2}\,d\xi \leqslant \int_0^\infty \frac{2\xi^{1+\alpha'}}{(1+\xi^2)^2}\,d\xi = \frac{\alpha'\pi}{2\sin(\alpha'\pi/2)} \qquad 0 < \alpha' < 2 \tag{16}$$

and

$$\int_0^\infty \frac{[\mu(E+\delta) - \mu(E-\delta)]}{\delta^{1+\alpha'}}\,d\delta \leqslant \int_0^1 \frac{[\mu(E+\delta) - \mu(E-\delta)]}{\delta^{1+\alpha'}}\,d\delta + \frac{1}{\alpha'} \qquad \alpha' > 0. \tag{17}$$

To get (17), we have used the obvious relation $\mu(E+\delta) - \mu(E-\delta) \leqslant 1$ and

$$\int_1^\infty \frac{[\mu(E+\delta) - \mu(E-\delta)]}{\delta^{1+\alpha'}}\,d\delta \leqslant \int_1^\infty \frac{1}{\delta^{1+\alpha'}}\,d\delta. \tag{18}$$

From (11), (14), (15) and (17), one can see that $I_\mu(E,\alpha')$ is convergent (divergent) if $J_\mu(E,\alpha')$ converges (diverges), and vice versa. This indicates that

$$P(E,\epsilon) \propto \epsilon^{\beta(E)} \tag{19}$$

such that

$$\beta(E) = \alpha(E) - 1. \tag{20}$$

The above analysis shows that a singular continuous measure with the scaling properties described in (10) leads to a scaling behaviour of the imaginary part of the Green function. Since the reciprocal case is also true, one can use the imaginary part of the Green function to investigate the singularities of the spectral measure. If one plots $P(E,\epsilon)$ in the (E,ϵ) plane, one gets at once the information about the spectral singularity distribution in the energy space. Let us stress here that, in our analysis, we only focus on the correspondence between the exponents $\alpha(E)$ and $\beta(E)$. We may find cases where $\beta(E) = 0$, which means $\alpha(E) = 1$. This does not mean automatically that the spectrum is absolutely continuous, as will be discussed later. In the following, we exemplify this approach in the case of the well known Fibonacci chain.

As a 1D model of quasicrystals, tight-binding Hamiltonians on Fibonacci chains have attracted much attention [4–10]. It has been shown that the spectral measure is a multifractal with a continuous scaling distribution function $f(\alpha)$ in the range $[\alpha_{\min}, \alpha_{\max}]$ [5]. We now study the off-diagonal Fibonacci model. The Hamiltonian parameters in (3) are chosen to be $v_i = 0$, $t_{ij} = t_A$ or t_B for nearest-neighbour hopping and 0 for others. t_A and t_B are two different values corresponding to the tiles A and B in the Fibonacci sequence which is generated by the inflation rule $(A, B) \to (AB, A)$. The spectrum of this model has a trifurcating structure [5–7]. So the eigenenergies can be noted by codes $[C_n]$,where n numbers the eigenenergies [5]. A given $[C_n]$ is a semi-infinite ordered sequence composed of three kinds of number 0, 1 and -1, which represent respectively the middle-, the upper-

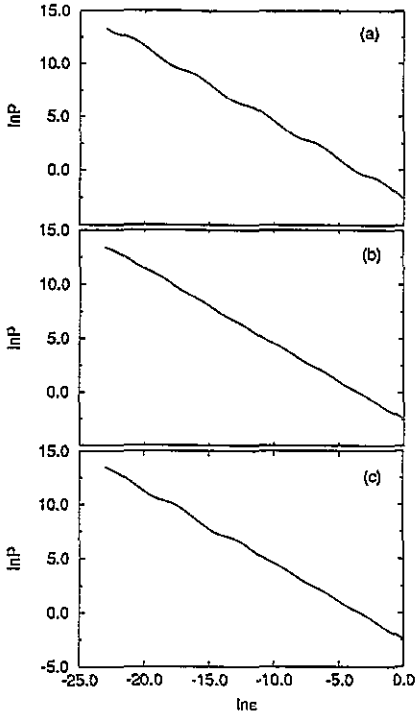

Figure 2. Scaling behaviour of the DOS measure of the Fibonacci chain for the off-diagonal model with $t_A = 1, t_B = r_c \simeq 10.6$: (a) $E = 0$; (b) $E = E_{1111...} = 11.17942667...$; (c) $E = E_{11110000...} = 11.17942509...$.

and the lower-eigenenergy clusters. For instance, the eigenvalue $E = 0$ (which belongs to the spectrum) is denoted [0000...], the upper and lower edges of the spectrum being represented by [1111...] and $[-1-1-1-1...]$, respectively.

3. Spectral measure of the density of states

We first present numerical results for the DOS measure. The average Green function associated with the DOS measure can be exactly calculated using a renormalization group method [9]. In figure 1(a), the scaling β at three eigenenergies is presented (for $t_A = 1, t_B = 2$). Comparing with the scaling of the measure at those energies [5], we find $\beta(E) = \alpha(E) - 1$, as expected. A crossover is found for $E_{11110000...}$, which corresponds to a transition from an edgelike behaviour to an (asymptotic) centre-like behaviour. To see the scaling distribution in the energy space, we plot $P(E, \epsilon)$ versus (E, ϵ) in figure 1(b). From figure 1(b), one can see that the minimum value of β (which is associated with the minimum scaling α) is located at the edge of the spectrum, while β_{max} (α_{max}) is at the centre. The scaling varies with energy, indicating that the measure is multifractal (with a scaling distribution from $\alpha_{min} = \alpha(E_{1111...})$ to $\alpha_{max} = \alpha(E = 0)$).

It is interesting to investigate the relation between the scaling properties of the measure and the quasiperiodicity strength. We assume $t_A = 1$ and $t_B = r$. The relation between r and $\alpha(E = 0)$ and $\alpha(E_{1111...})$ is given in figure 1(c). An interesting result is that there exists a critical point r_c, where $\alpha(E = 0) = \alpha(E_{1111...})$. This result is a direct consequence of the known analytical form of α_{min} and α_{max} as functions of r [5], but does not seem to have been

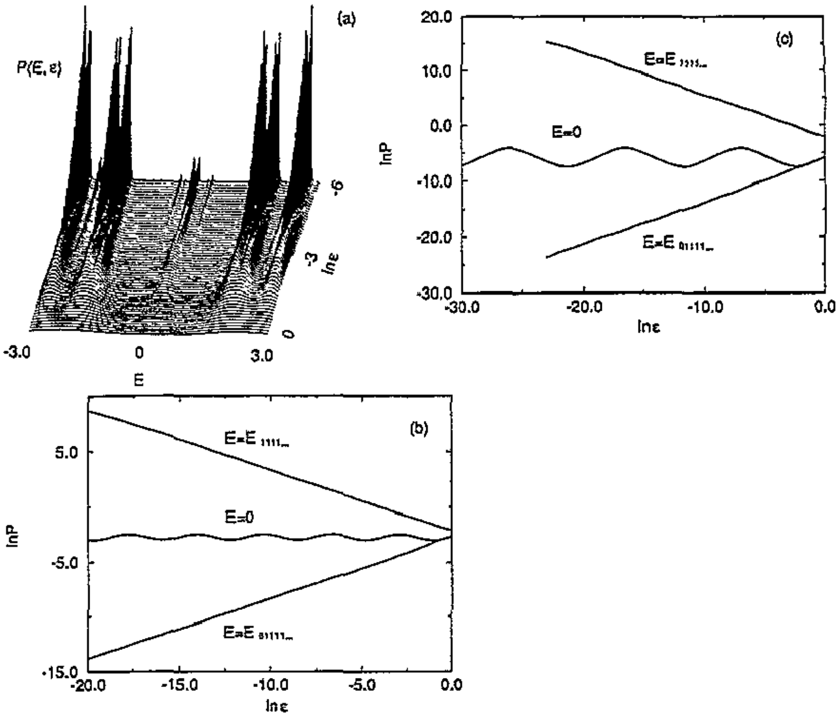

Figure 3. Scaling behaviour of the LDOS measure at the site corresponding to the transformation T_a: (a) plot of $P(E,\epsilon)$ for $t_A = 1, t_B = 2$; (b) ln $P(E,\epsilon)$ against ln ϵ at eigenenergies $E = 0$, $E = E_{1111...} = 2.833\,956\,43...$ and $E = E_{01111...} = 0.479\,162\,81...$ for $t_A = 1, t_B = 2$; (c) ln $P(E,\epsilon)$ against ln ϵ at eigenenergies $E = 0, E = E_{1111...} = 11.179\,426\,67...$ and $E = E_{01111...} = 0.097\,757\,44...$ for $t_A = 1, t_B = r_c = 10.6$.

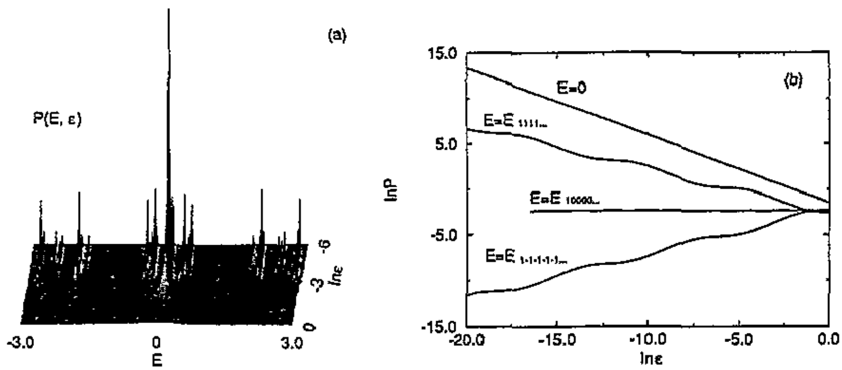

Figure 4. Scaling behaviour of the LDOS measure at the site corresponding to the transformation T_c with $t_A = 1, t_B = 2$; (a) plot of $P(E,\epsilon)$; (b) ln $P(E,\epsilon)$ against ln ϵ at eigenenergies $E = 0$, $E = E_{1111...} = 2.833\,956\,43...$, $E = E_{10000...} = 2.416\,449\,19...$ and $E = E_{1-1-1-1-1...} = 1.642\,391\,60...$.

noticed previously. For $r < r_c$, $\alpha(E = 0) > \alpha(E_{1111...})$, while $\alpha(E = 0) < \alpha(E_{1111...})$ in the region $r > r_c$. According to the above discussion, at $r = r_c$ ($= 10.592\,337\,60...$) the spectral measure seems to be a homogeneous fractal measure (with a single scaling exponent) while it is multifractal for any other value. In figure 2, scalings at energies $E = 0$, $E_{1111...}$ and $E_{1111000...}$ for $r \simeq r_c$ are illustrated. As expected, the slopes are identical and the crossover at $E = E_{1111000...}$ is masked in figure 2(c). This single scaling is independent of the energy as we numerically checked for several other energies.

4. Spectral measure of the local density of states

As opposed to a periodic system, a quasiperiodic tiling has no translational symmetry. Different sites have different environments, with different local electronic properties. Studies of the single-electron motion in a quasiperiodic lattice showed that different initial electron locations lead to different quantum diffusion behaviours [10–14]. A recent work shows that quantum diffusion [13], or even the probability for an electron to remain at a site [14], are constrained by the LDOS measure scaling. In the following, we study the LDOS measure scaling properties in this system. Owing to self-similarity of the Fibonacci chain, one can use the three basic renormalization group trasformations T_a, T_b, and T_c to exactly calculate the local Green functions (LGFs) of the chain as described in detail elsewhere [9]. T_a, T_b and T_c are decimation operations represented by (BAA, BA) $\to$ (A′, B′), (AAB, AB) $\to$ (A′, B′) and (ABABA, ABA) $\to$ (A′, B′), respectively.

In figure 3(a) we display $P(E, \epsilon)$ at the site whose LGF is calculated by successive iterations of the transformation T_a. Similar to the average DOS, the minimum scaling exponent β_{min} (α_{min}) appears at the edge of the spectrum. However the scaling distribution in the energy space is quite different from that in the DOS measure (see figure 1(b)). From figure 3(b), one can see that, at $E_{1111...}$, the scaling exponent β is different from the value it takes in the average DOS. In addition, in figure 3(a), there are small peaks around the edges of the first centre cluster, which indicates large scaling exponent β (large α) at these energies. figure 3(b) shows the scaling behaviour at energies $E = 0$, $E_{1111...}$ and $E_{01111...}$. It is quite interesting that $\alpha(E = 0) = 1$, which is the value for a continuous measure, but here with subdominant periodic oscillations. Furthermore $\alpha(E_{01111...}) \simeq 1.558$. We have verified numerically that $\alpha(E = 0) = 1$ and $\alpha(E_{01111...}) > 1$, independently of the strength r. Figure 3(c) shows the scalings at the same 'coded' energies for $t_A = 1, t_B = 10.6 \simeq r_c$ which corresponds to the above critical point of the DOS measure. Figure 3(c) indicates clearly that for a singular continuous measure, the LDOS measure can be multifractal even for a homogeneous fractal DOS measure.

Figure 4 is devoted to the site whose LGF can be obtained by the successive transformation T_c. Figure 4(a) has a quite different scaling distribution from figure 1(b) and figure 3(a). In figure 4(a), β_{min} (α_{min}) arises at the centre $E = 0$, while large β (large α) values arise around cluster edge regions. Scalings for several energies are given in figure 4(b). One can see that the position where $\alpha = 1$ shifts from $E = 0$ to the 'edge centre' $E = E_{10000...}$. At $E = E_{1-1-1-1-1...}$, $\alpha(E) = 1.487$. Similarly we find that $\alpha(E_{10000...}) = 1, \alpha(E_{1-1-1-1-1...}) > 1$ independently of r. The scaling distributions for other sites have been investigated. It shows that the LDOS scaling distribution versus energy varies with the position of the site.

From the above discussion, we have thus illustrated the fact that for a singular continuous measure, the scaling properties of the LDOS measure are quite different from those of the DOS measure. The differences are not only in the scaling distribution in energy space, but also in the values the scaling exponent can take. For the LDOS measure, we have found energies where the scaling can be equal to or larger than unity. At first sight, this point could be seen as surprising with respect to the electron motion in Fibonacci chains. The electron motion can be described by the quantum diffusion distance $d(t)$ at time t, which is defined by $d^2(t) = \sum_n \langle\psi_n(t)\left|(n - n_0)^2\right|\psi_n(t)\rangle$, where n is the position of the site, and $\psi_n(t)$ the nth site wavefunction at time t which is determined by the time dependent Schrödinger equation $i\dot{\psi}_n(t) = H_{n,n-1}\psi_{n-1}(t) + H_{n,n+1}\psi_{n+1}(t)$ with the initial condition $\psi_n(t) = \delta_{n,n_0}$. Numerical calculations show that for long time t, $d(t) \sim t^{\gamma}$ and that for different initial conditions (i.e. at $t = 0$, the electron is located at different sites) one can find different values of the exponent γ. A recent analytical analysis [13] proved that $\gamma \geqslant \alpha$ for any 1D system with a singular continuous measure, where α is the scaling exponent of the LDOS measure of the site where the electron is initially located. This is not in contradiction with our results stating that there are energies where $\alpha > 1$, which would then lead to electron motions faster than standard ballistic motion corresponding to $\gamma = 1$. It simply implies that these energies form a subset of measure zero in the spectrum, and are therfore irrelevant for the electronic motion.

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