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Level statistics for electronic states in a disordered fractal

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Abstract. We present results for the density of states and the statistics of the energy levels in a random tight binding matrix ensemble defined on a disordered two-dimensional Sierpinski gasket. In the absence of disorder the nearest level spacing distribution function $P(S)$ is shown to follow the inverse power law $P(S) \propto S^{-D_0-1}$, which defines the fractal dimension $D_0 = 0.56 \pm 0.01$ of the corresponding spectrum. In the random case $P(S)$ approaches, instead, the Poisson law e^{-S}, which is consistent with localization of the corresponding eigenstates. In the presence of a random magnetic flux our results also scale towards the Poisson statistics.

Energy level statistical methods have been originally developed to describe the spectra in complex and chaotic systems [1–3]. They have also been recently introduced in order to understand the electronic localization properties of disordered materials [4–10]. It has become clear that for diffusing electrons, where the corresponding wavefunctions are extended having a constant amplitude on average, the energy levels are correlated displaying level repulsion at short distances. The opposite occurs for localized electrons since the wavefunction amplitudes decay exponentially in space and the corresponding energy levels are uncorrelated or randomly distributed. Moreover, level statistics can be a powerful tool to locate the Anderson metal–insulator transition at the point in the spectrum (mobility edge) where the statistics changes and also to identify the related critical behaviour [7–14].

In a quantum disordered system apart from averages for the measurable physical quantities their fluctuations must also be computed. Such calculations can conveniently proceed from energy level statistical studies via the diagonalization of random Hamiltonian matrices within an appropriate statistical ensemble. Usually non-interacting electrons are considered in the dimensionality d-dependent tight binding approximation. In the metallic phase where the states are extended the level statistics resembles that found in the Wigner–Dyson (WD) Gaussian random matrix ensembles [1–3], which are classified according to symmetry into three universality classes corresponding to the Gaussian orthogonal ensemble (GOE), the Gaussian unitary ensemble (GUE) and the Gaussian symplectic ensemble (GSE). The simplest level fluctuation measure which can be introduced is the nearest-level spacing distribution function $P(S)$ and level repulsion causes a power-law behaviour $P(S) \propto S^{\beta}$ for $S \to 0$, where $\beta = 1, 2, 4$ for GOE, GUE and GSE, respectively. The full result for the GOE is the well known Wigner surmise $P(S) = (\pi S/2)\exp(-\pi S^2/4)$, defined so that the mean level spacing is $\Delta = \langle S \rangle = 1$. The agreement for the level statistics between the tight binding random matrix ensembles and the WD ensembles holds in any d as long as

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the disordered system is well in its disordered metallic phase. The level repulsion arises in this case because of the extended nature of the wavefunctions which overlap with each other. In the localized regime, however, the states are non-overlapping in space and imply uncorrelated spectra with levels obeying normal Poisson statistics with $P(S) = \exp(-S)$. The problem of level statistics at the mobility has been considered in many recent studies and a new universal $P(S)$ which also shows the WD behaviour proportional to S^{β} for $S \to 0$ has been obtained [6–10]. Asymptotic power laws for the behaviour at large S have also been proposed [11-14].

In this paper we study, via level statistics, the localization induced by randomness in a Sierpinski gasket lattice [15]. This deterministic self-similar structure is built in a Euclidean dimension $d = 2$ and has a non-integer fractal dimensionality $d_{\mathrm{f}} = \ln 3/\ln 2 \approx 1.58$. In the absence of disorder scaling computations reveal exotic localization properties induced by the long-range correlated fractal lattice potential [16, 17]. We show that these localization effects are also manifested in the spectrum with a self-similar density of states characterized by a fractal dimension D_0 and an inverse power-law level spacing distribution $P(S) \propto S^{-D_0-1}$, denoting a kind of level clustering instead of level repulsion. In the presence of a random site potential (finite W) we show that the statistics becomes Poisson, in agreement with the scaling theory of localization [18], which predicts a metal–insulator transition only for $d > 2$ in the absence of spin dependence or an added magnetic field. In order to check whether extended states might exist in the presence of a random magnetic field, which breaks the time-reversal invariance so that the GUE becomes the appropriate metallic limit, we have also introduced a random phase model. This corresponds to the presence of random magnetic flux and its $d = 2$ analogue has attracted much attention recently in connection with the half-filled quantum Hall effect and also high-T_{c} superconductivity [19, 20]. Our results for this case are also consistent with localization of the states.

We find the eigensolutions for an ensemble of tight binding electronic Hamiltonians on the Sierpinski gasket

$$\mathcal{H} = \sum_{j} \epsilon_j c_j^{+} c_j + \sum_{(j,j')} V_{j,j'} c_j^{+} c_{j'} \tag{1}$$

where c_j^{+} creates an electron on site j and j labels all the sites $|j\rangle$ of the fractal lattice which define an orthogonalized basis set. The second sum is taken over all nearest-neighbour lattice pairs (j, j') and the hopping parameter is $V_{j,j'} = -1$. The spin-independent random on-site potential ϵ_j denotes the diagonal disorder and is taken as a random variable chosen from a uniform probability distribution of width W, which denotes the strength of disorder. We have also adopted the boundary conditions of [16], which identify the corners of the two identical triangles on the largest scale (see figure 1) and the lattice is generated by inserting sites onto each of the triangles. In this representation every site has exactly four nearest neighbours and the corresponding spectrum lies in $[-4, 4]$. If we denote by n the number of insertions the corresponding system has 3^{n+1} sites and the Hamiltonian of equation (1) is considered for finite n's.

In the absence of diagonal disorder $W = 0$ the self-similarity of the gasket leads to a natural decimation renormalization group procedure [16, 17]. The energy levels and the wavefunctions can be directly computed by using the recursive relation for the energy

$$E' = -E(E + 3) \tag{2}$$

which for each state with energy E'_{n-1} of the level $n-1$ gives two states at the level n with

energies

$$E_{n,\pm} = \frac{-3 \pm (9 - 4E'_{n-1})^{1/2}}{2} \tag{3}$$

with E other than 1 and ± 2 which have to be treated separately. The main result from these computations is that the spectral measure is composed of two kinds of energies. The first kind consists of a pure point spectral measure corresponding to strongly localized (molecular) states and the other defines a singular continuous spectrum with critical states (see, however, [21]).

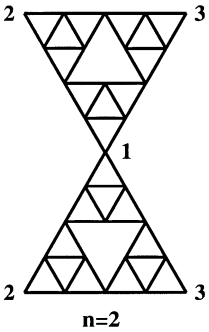

Figure 1. The Sierpinski gasket lattice at the generation $n = 2$. The lower (upward pointing) triangle is a prototype of a basic structure from which sites can be eliminated by decimation. The adopted boundary conditions are denoted by the numbers 1, 2, 3 for the two largest triangles.

We have used the above decimation procedure when $W = 0$ to generate all the levels E_i, $i = 1, 2, \ldots, 3^{n+1}$, for up to $n = 11$. Our results for the integrated density of states $N(E) = \int_{-\infty}^{E} \rho(E')\,\mathrm{d}E'$ are plotted in figure 2(a). We observe a 'devil's staircase' picture with plateaux and jumps corresponding to gaps and degeneracies, respectively. There is no need to distinguish between the two kinds of states although it should be mentioned that the strongly localized states have non-zero amplitudes only on a finite number of sites (molecular states) [17] and the rest are critical states (1/3 of the total number), which consist of the non-degenerate uniform $E = -4$ level and the $E = +1$ plus all its 'descendants' via equation (3) forming the edges of the gap intervals. In order to consider level fluctuations we have computed the integrated level spacing distribution $N(S) = \int_{S}^{\infty} P(S')\,\mathrm{d}S'$ for the same system, whose derivative gives $-P(S)$. Our results, after sorting out all the levels with increasing magnitude and normalizing $N(S)$ so that $N(0) = 1$, are displayed in figure 2(b). It is clearly seen that $N(S)$ obeys the inverse power law $N(S) \propto S^{-D_0}$ with the exponent determined by a least-squares fit, which gives $D_0 = 0.56 \pm 0.01$. Thus the level spacing distribution behaves as

$$P(S) \propto S^{-D_0-1}. \tag{4}$$

In the presence of disorder (finite W) a statistical random matrix ensemble is created and for each random matrix we numerically find all the eigenvalues by exact diagonalization. The plots for the ensemble averaged density of levels $\rho(E)$ and the corresponding $P(S)$ distributions are shown in figures 3–5. We observe that the strong degeneracies in the density of states which exist in the $W = 0$ case now disappear. However, for small W remnants of the dominant spectral gaps are still present in the spectrum (see figure 3(a)) which vanish only for larger W values (figures 4(a) and 5(a)). In order to compute

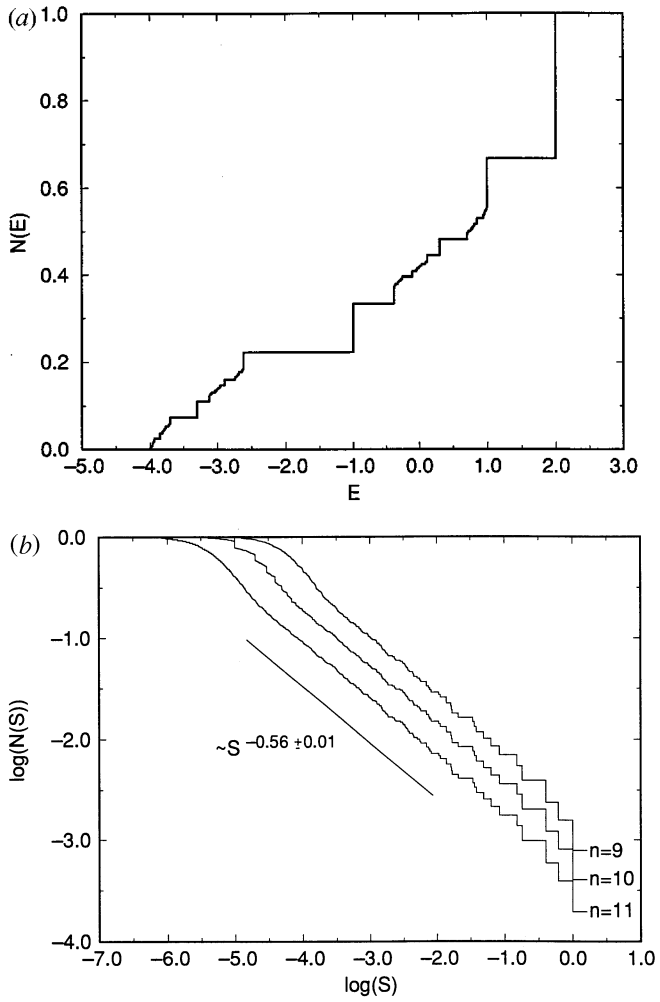

Figure 2. (*a*) The computed integrated density of states for the Sierpinski gasket at the $n = 10$ generation in the absence of a random potential ($W = 0$), which contains 3^{11} states by including level degeneracies. The plateaux correspond to gaps and the vertical lines to degenerate states in the band. (*b*) The corresponding integrated level spacing distribution function for three successive generations $n = 9$, 10, 11, together with the inverse power-law best fit S^{-D_0}. The obtained results imply for the level spacing distribution the inverse power law $P(S) \propto S^{-1.56}$.

the $P(S)$ it was essential to unfold the energy levels by considering the distribution of $x_{i+1} - x_i = \langle N(E_{i+1})\rangle - \langle N(E_i)\rangle$, instead of $E_{i+1} - E_i$, where $\langle N(E)\rangle$ is the averaged integrated density of states. There was no need to unfold the spectrum for the non-random $W = 0$ case since the spectral fluctuations there remain self-similar in all scales and unfolding does not change the obtained power law of equation (4). In the random case we firstly compute $\langle N(E)\rangle$ in a few points within the adopted energy range and then to more (about 10 000 points) by cubic interpolation to obtain the set of unfolded levels $x_i = \langle N(E_i)\rangle$. The $P(S)$ function computed for $S_i = x_{i+1} - x_i$ satisfies the constant density requirement with $\Delta = \langle S\rangle = 1$. The calculated $P(S)$ using the unfolded levels for finite W and different system sizes scales towards the Poisson distribution in all the cases considered

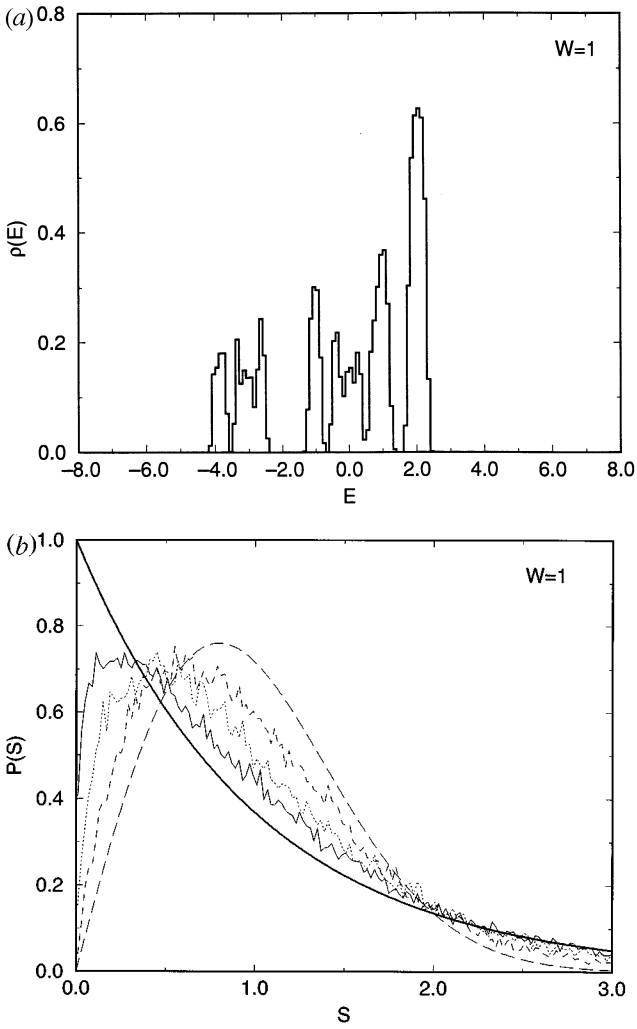

Figure 3. (*a*) The computed enemble averaged density of states for the Sierpinski gasket with added diagonal disorder ($W = 1$) at the $n = 6$ generation, which contains 3^7 levels and for 100 random runs, that is with a total number of 100×3^7 levels. The gaps which exist in the $W = 0$ case have not completely closed in this case. (*b*) The level spacing distribution function for disorder strength $W = 1$ using the unfolded data in the energy window $[-1, 1]$ for gaskets of different sizes corresponding to the generations $n = 4$ (broken curve), $n = 5$ (dotted curve) and $n = 6$ (continuous thin curve). The statistical ensemble consists of 900, 300 and 100 random matrices in each case, with 67 678, 67 727 and 67 612 levels in the chosen window, respectively. The GOE Wigner surmise is also shown for comparison (wide broken curve) which should be approached for infinite size in the metal and the continuous thick curve is the Poisson law approached in the localized case.

(figures 3(*b*), 4(*b*) and 5(*b*)). From these results we can reach the conclusion of localization for the corresponding wavefunctions in the random gasket.

We have also considered a model which breaks the time-reversal symmetry due to a

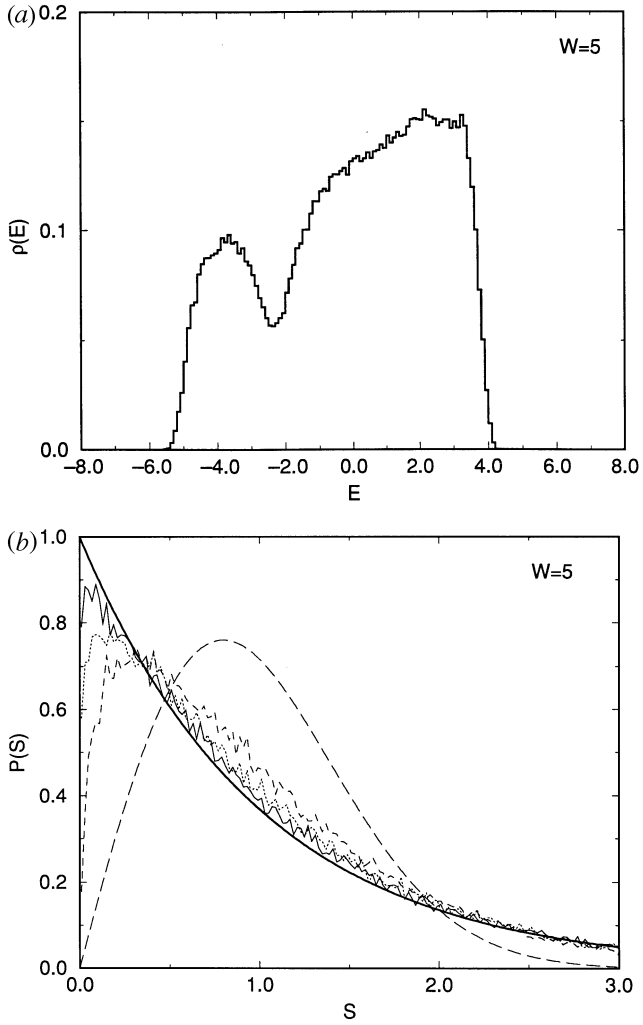

Figure 4. (*a*) The same as in figure 2(*a*) but for disorder $W = 5$. No gaps are seen in this case. (*b*) The same as in figure 2(*b*) but for $W = 5$ and within the the energy window $[-2, 2]$. The levels which fall in the window are 109 434, 109 225 and 109 595 for each size $n = 4$, 5 and 6, respectively.

random magnetic field. The corresponding Hamiltonian is

$$\mathcal{H} = \sum_{(j,j')} \mathrm{e}^{2\pi i \phi_{j,j'}} c_j^+ c_{j'} \tag{5}$$

where the sum is taken over all nearest-neighbour lattice pairs (j, j') on the Sierpinski gasket and the phase $\phi_{j,j'}$ is a random variable uniformly distributed between 0 and 1. The corresponding WD limit in this case is the GUE and should be reached only if extended states are present in the system. The random matrices of equation (5) are complex Hermitian and for the numerical diagonalization we have also used the Lanczos method [8]. Our results for the density of states are displayed in figure 6(*a*) and we observe no spectral singularities but a broad minimum around the band centre, which is similar to what was found in the two-dimensional case [20]. In order to compute the $P(S)$ function the levels are collected

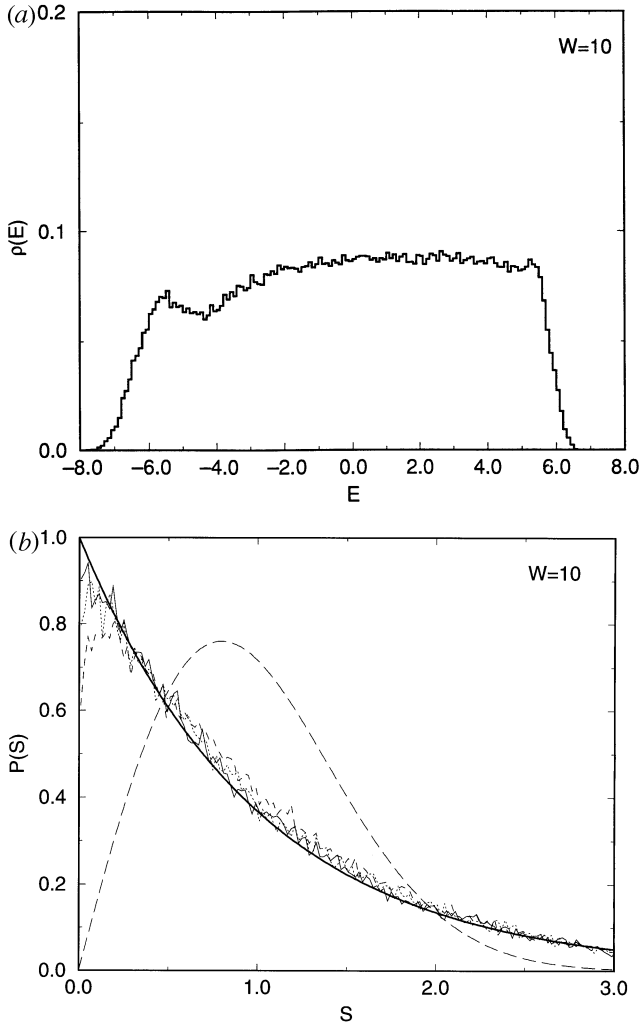

Figure 5. (*a*) The same as in figure 2(*a*) for $W = 10$. No gaps are seen in this case. (*b*) The same as in figure 2(*b*) for $W = 10$ and the energy window $[-2, 2]$. The levels in the window are 75 551, 75 739 and 75 431 for $n = 4$, 5 and 6, respectively.

in a specific narrow energy window around the band centre for $n = 4$, 5 and 6 for many random runs. Our purpose is to exclude the possibility of extended states near the band centre, since it is very unlikely that such states can exist in other parts of the band. Our results are shown in figure 6(*b*) for levels near the band centre. We observe that the $P(S)$ function moves slowly towards the Poisson limit when the system size increases so that the corresponding states should be localized, although with larger localization lengths than in the random model of equation (1).

In summary, we have considered the density of states and the energy level fluctuations for two tight binding models with and without time-reversal symmetry defined on a deterministic fractal system. Localization of the wavefunctions is probed in the space of non-integer d by powerful level statistical techniques. The most important results are as follows. (1) The level statistics in a non-random fractal is characterized by an inverse power-

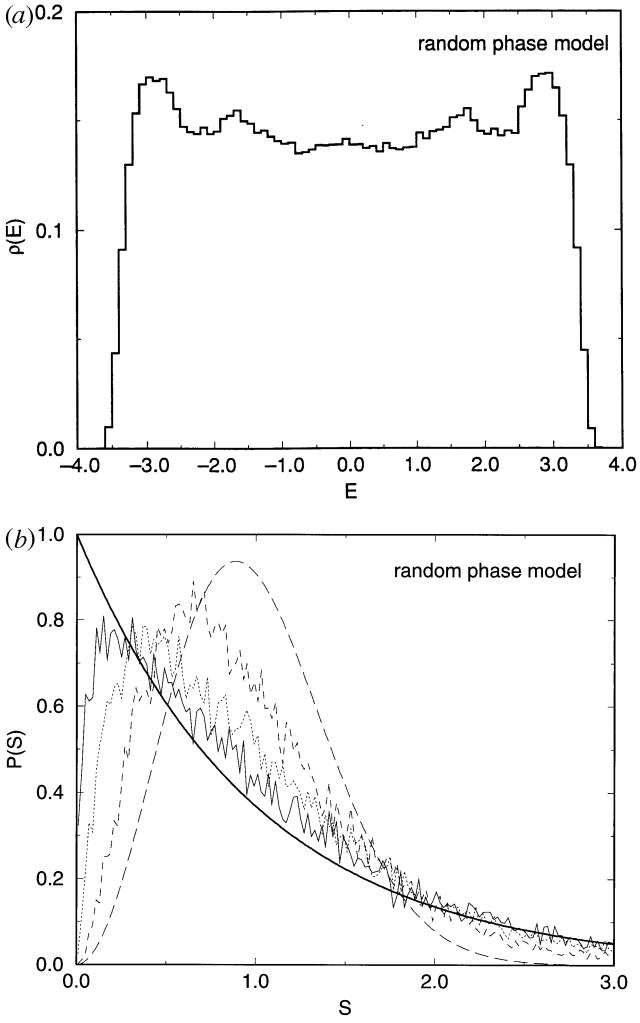

Figure 6. (*a*) The computed averaged density of states for the random phase model at the $n = 5$ generation containing 3^6 levels for 300 random runs. (*b*) The level spacing distribution function for the unfolded data in the random phase model with system sizes $n = 4$, 5, 6 and 800 runs for each size. The adopted windows are $[-0.45, 0.45]$, $[-0.15, 0.15]$ and $[-0.05, 0.05]$ for $n = 4$, 5 and 6 with 24 158, 24 327 and 24 519 levels in each case, respectively. The wide broken curve is the GUE Wigner surmise $P(S) = (32/\pi^2)S^2 \exp(-(4/\pi)S^2)$, which corresponds to the metal (shown for comparison), and the continuous curve is the Poisson law which should be approached for infinite size.

law distribution of the nearest level spacings in which enters the fractal dimension D_0 of the density of states. (2) From the scaling analysis of the $P(S)$ distribution we can conclude that the states localize for any non-zero amount of disorder. (3) A random phase model, which corresponds to an added random magnetic field, is also consistent with localization of the states. The kind of inverse power-law level statistics obtained for the non-random fractal is familiar from quasi-periodic $d = 1$ systems [22]. Our results could contribute towards a better understanding of localization in such materials, which lie between crystalline and random, and can be used in order to check various dimensionality dependent results.

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