Multifractal Wave Functions at the Anderson Transition

Michael Schreiber and Heiko Grussbach
Institut für Physikalische Chemie, Johannes-Gutenberg-Universität Mainz, Jakob-Welder-Weg 11, 6500 Mainz, Federal Republic of Germany
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Electronic wave functions in disordered systems are studied within the Anderson model of localization. At the critical disorder in 3D we diagonalize very large (103 823×103 823) secular matrices by means of the Lanczos algorithm. On all length scales the obtained strong spatial fluctuations of the amplitude of the eigenstates display a multifractal character, reflected in the set of generalized fractal dimensions and the singularity spectrum of the fractal measure. An analysis of 1D systems shows multifractality too, in contrast to previous claims.

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Within the problem of localization in disordered systems the behavior of the electronic wave functions is of crucial importance for a variety of phenomena, like the transport properties of amorphous semiconductors or the excitation dynamics in molecular crystals. The qualitative properties of such systems can be obtained already from a simple tight-binding model like the Anderson Hamiltonian which describes a regular lattice with site-diagonal disorder. This model is known [1] to yield extended states for weak disorder in three dimensions (3D) as well as in 2D samples with strong magnetic field. For strong disorder, on the other hand, the electronic states are localized and believed to decay exponentially in space. This was proven in 1D systems [2] and has been explicitly assumed in the scaling hypothesis of localization [3] and corroborated in a variety of numerical investigations [4].

However, this exponential decay relates to the asymptotic properties of the envelope of the wave function while the short-range behavior is characterized by strong fluctuations. Approaching the mobility edge, which separates the localized from the extended states in the energy-disorder diagram, this exponential decay constant diverges so that the wave functions can be expected to feature fluctuations on all length scales.

Even arbitrarily close to the mobility edge a state should occupy only an infinitesimal fraction of space if it is to be labeled a localized state. On the other side of the mobility edge the states should extend throughout the sample. Both characteristics can be accommodated at the mobility edge if one assumes a fractal wave function with a filamentary structure like a net over the whole sample, as suggested originally by Aoki [5]. This idea was numerically exploited by several authors, determining a fractal dimension from the density-density correlation function [6], the participation number [7-10], or the amplitude of the wave function [11]. A fractal behavior could thus be established not only at the mobility edge but more generally for short-range fluctuations of the wave functions in disordered systems up to length scales of the order of the localization length or the coherence length of the localized and the extended states, respectively. However, particularly in 3D systems the results were rather limited due to the small system size that could be treated numerically [6,7].

The observation of anomalous scaling properties [12] as well as the fractal behavior of different characteristics of the eigenstates as mentioned above show that the wave functions cannot be adequately treated as a simple fractal. Rather, the more general concept of multifractality [13-15] has to be employed, yielding a set of generalized dimensions. A few of these dimensions have been computed in 2D as well as in 3D systems [16-18], suggesting the multifractal picture. In the following we present a comprehensive analysis of the spatial fluctuations of individual eigenstates at the mobility edge in 3D samples [19]. Because of our efficient implementation of the Lanczos algorithm on a vectorizing computer we are able to investigate much larger samples than previously studied, clearly displaying the multifractal properties. As an analysis of the same model for 1D systems disproved self-similar fluctuations of the wave function [20], we have also investigated very long 1D chains and found multifractal properties, too, for very low disorder, in agreement with previous doubts [21] cast on Ref. [20].

Our investigation is based on the Anderson Hamiltonian

$$H=\sum_n |n\rangle\varepsilon_n\langle n| + V\sum_{n,m}^{\mathrm{nn}} |n\rangle\langle m| \,, \tag{1}$$

with constant nearest-neighbor transfer integral V and random potential ε_n governed by a uniform distribution of width W. At the band center ($E=0$) this model shows a transition between localized and extended states at the critical disorder $W_c=16.5V$ for 3D samples [1,4]. We restrict the subsequent 3D analysis to this disorder.

The respective secular matrix for a system of $N=47^3$ sites is tridiagonalized by means of the Lanczos algorithm [9], and the tridiagonal matrix diagonalized by standard techniques in a straightforward way. As we are interested in eigenvalues E_i in the middle of the spectrum the well-known occurrence of ghost solutions in the Lanczos recursion [9] presents a nontrivial complication. In the present case, the size of the tridiagonal matrix had to be increased up to 178000 to obtain the requested eigenstates $|\varphi_i\rangle = \sum_n e_{in}|n\rangle$ with an accuracy better than 10^{-6} for $||H\varphi_i - E_i\varphi_i||$.

The multifractal analysis is based on the standard box-counting procedure, dividing the system into N_L boxes of linear size L and determining the box probability of the wave function in the kth box,

$$\mu_k(L) = \sum_{n=1}^{L\times L} |e_{in}|^2, \quad k=1,\ldots,N_L, \tag{2}$$

as a suitable measure. If the qth moments of this measure counted in all boxes are proportional to some power $\tau(q)$ of the box size,

$$\chi_q(L) = \left\langle \sum_k \mu_k^q(L) \right\rangle \sim L^{-\tau(q)}, \tag{3}$$

multifractal behavior may be derived. A simple homogeneous fractal would be completely characterized by two of the moments; the respective $\tau(q)$ curve would be a straight line. Therefore the $\tau(q)$ curve presented in Fig. 1 is typical for a multifractal entity because of its nonlinearity. The physical meaning is that the measure distinguishes intertwined regions of the state which scale in different ways according to the mass exponents $\tau(q)$. Thus each subset of the measure characterizes a fractal

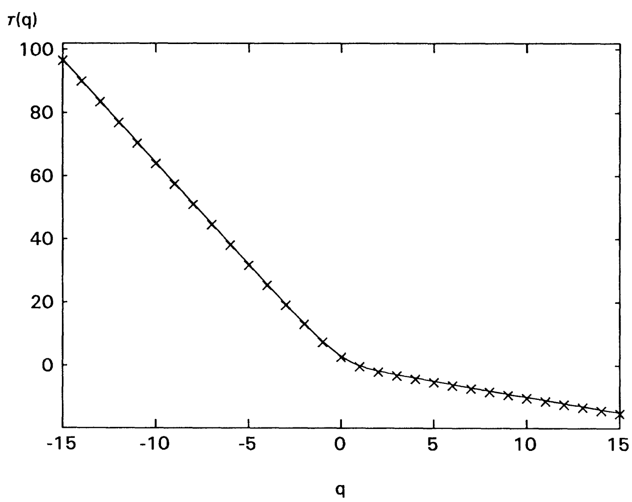

FIG. 1. Mass exponents $\tau(q)$ of the measure $\mu_k(L)$ for an Anderson-localized wave function at $W_c = 16.5V$ in a 3D sample of $N=47^3$ sites. Integer values of q are marked by symbols. The values of τ are obtained from Eq. (3) by fitting a straight line to the dependence of $\ln\chi$ vs $\ln L$. The accuracy of the least-squares fit, which has been controlled by computing the linear correlation coefficient, could be significantly improved by averaging over all possible choices of the origin of the box partitioning. This procedure also avoids the restriction that $N_L = N/L^3$ has to be an integer. In practice we have varied L between 2 and 46 and also included slightly noncubic boxes. The discrete lattice of course limits the possible range of the (multi)fractal behavior to scales above the lattice constant.

with its own fractal dimension, and no self-similarity of the complete state follows.

The generalized fractal dimensions D_q are then obtained from

$$-\tau(q) = (q-1)D_q = \lim_{L\to 0} \ln\chi_q(L)/\ln L. \tag{4}$$

For the computation of D_1 from Eq. (4) one has to employ a series expansion of μ_k^q around $q=1$. The important features of D_q shown in Fig. 2 are the following: The similarity dimension D_0 equals the Euclidean dimension, because the wave function is nowhere exactly zero, so that all boxes constructed above contribute to the box counting. This means that the support of the measure is given by the total volume instead of some fraction of it, and accordingly $D_0 = 3$. On the other hand, the information dimension $D_1 = 2.17$ is distinctly smaller [22]. This fact demonstrates that a subset with the fractal dimension $D_1 < 3$ contains a fraction of the measure arbitrarily close to the complete measure, i.e., all the information.

The correlation dimension D_2 reflects the scaling of the density-density correlation function or, equivalently, of the participation number. Within the respective numerical errors our value $D_2 = 1.68$ is in agreement with the results of previous investigations concentrating on the fractality of these quantities [6,7].

The limiting values of D_q for $q \to \pm\infty$ describe the scaling of those subsets where the measure, and thus the wave function, is most concentrated or rarified, respectively. We obtain $D_{+\infty} = 1.05$ and $D_{-\infty} = 6.06$, but the latter value is not very accurate because it is determined by the smallest amplitudes of the wave function, which are most sensitive to numerical errors.

While the discussion of the generalized dimensions D_q is quite illustrative, the abstract analysis of multifractals is often concerned [15] with the singularity strength of

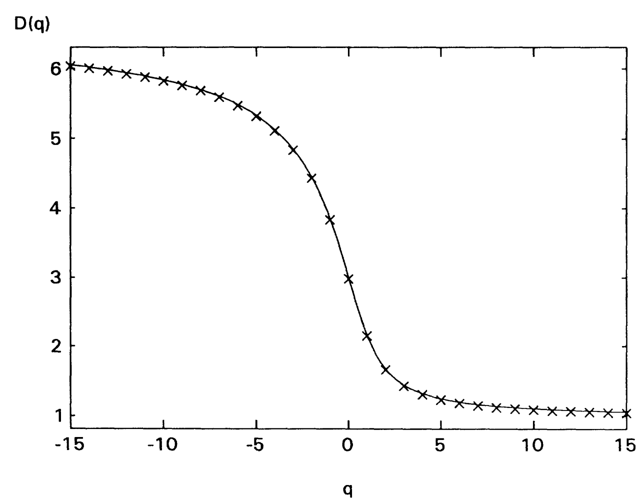

FIG. 2. Generalized dimensions D_q corresponding to $\tau(q)$ in Fig. 1.

the fractal, given by the Lipschitz-Hölder exponent α, and the corresponding singularity spectrum $f(\alpha)$. In the kth box the singularity strength α is given by

$$\mu_k(L) \sim L^{\alpha_k}. \tag{5}$$

The number of subsets $N(\alpha)$ in which this strength is observed is a fractal itself, with the Hausdorff dimension $f(\alpha)$:

$$N(\alpha) \sim L^{-f(\alpha)}. \tag{6}$$

The relation $f(\alpha)$ completely characterizes the multifractal. In principle, it can be obtained [13,15] from $\tau(q)$ by means of a Legendre transformation, which, however, strongly suffers from numerical inaccuracies [22]. Therefore we have employed a parametric representation [22] of f and α in terms of q, evaluating

$$f(q) = \lim_{L\to 0} \sum_k \mu_k(q,L) \ln\mu_k(q,L)/\ln L \tag{7}$$

and

$$\alpha(q) = \lim_{L\to 0} \sum_k \mu_k(q,L) \ln\mu_k(1,L)/\ln L \tag{8}$$

from the qth moment of the measure in the separate boxes,

$$\mu_k(q,L) = \mu_k^q(L) \Big/ \sum_k \mu_k^q(L). \tag{9}$$

The results are compiled in Fig. 3 displaying a singularity spectrum which is typical for multifractal entities.

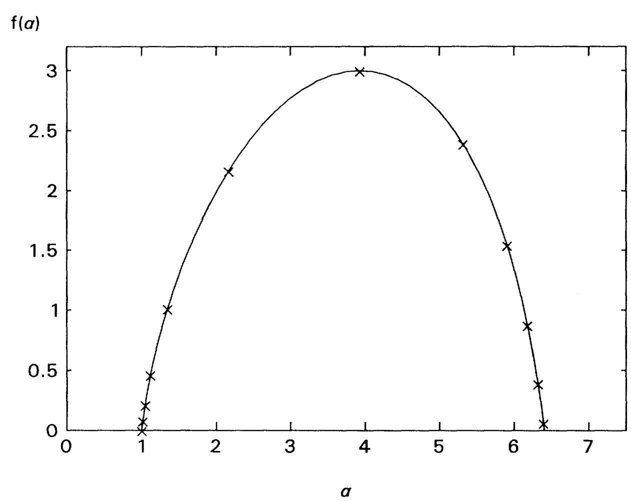

FIG. 3. Singularity spectrum $f(\alpha)$ for the same wave function as in Figs. 1 and 2. Integer values of the implicit parameter q are marked by symbols. The data are obtained by least-squares fits by Eqs. (7) and (8) for box sizes down to $L=2$, again averaging over all possible origins of the boxes and including slightly noncubic boxes. The accuracy, which is controlled by computing the linear correlation coefficient, becomes insufficient for the extreme values of q so that the expected infinite slope for $\alpha \to \alpha_{\max}$ and $\alpha \to \alpha_{\min}$ cannot be obtained.

The particular cases discussed above are contained in this plot in the following way: The maximum of the spectrum corresponds to $q=0$, yielding $f(\alpha_{\max})=3$, the dimension of the support of the measure. For $q=1$ we have $f(\alpha)=\alpha$. The limit $q\to+\infty$ ($q\to-\infty$) yields the minimal (maximal) value of α, projecting out the singularity associated with the box containing the largest (smallest) measure.

In conclusion, the computations of the mass exponents $\tau(q)$, the generalized dimensions D_q, the Lipschitz-Hölder exponents α, and the singularity spectrum $f(\alpha)$ consistently demonstrate the multifractal behavior of the spatial fluctuations of the investigated wave function at the critical disorder corresponding to the Anderson transition in 3D samples.

As these results contradict previous claims [20] with respect to 1D systems we have also diagonalized the secular matrix of Eq. (1) corresponding to a very large chain at low disorder. The derived $\tau(q)$ spectrum is shown in Fig. 4. We have tested that this feature is numerically and statistically significant by a detailed error analysis and by investigating several different wave functions. We note that for a good accuracy it is necessary to restrict the multifractal analysis in this case to box sizes below $L\sim 1600$. This is an obvious curtailment because this length is of the order of the localization length and it is unreasonable to expect the (multi)fractal behavior to persist on larger length scales than that of the exponential decay. The reason for the derivation in Ref. [20] is unclear; it may be due to the employed rescaling and averaging.

The multifractality observed here is in agreement with the characterization of the disorder fluctuations [20] that refer to different possible configurations of the disordered potential in Eq. (1). In contrast to Ref. [20] we do not

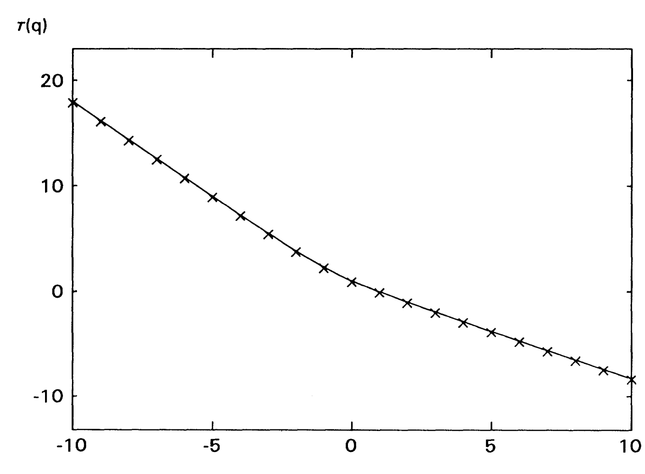

FIG. 4. Mass exponents $\tau(q)$ of the measure $\mu_k(L)$ for an Anderson-localized wave function at $W=0.25V$ in a 1D sample of $N=80000$ sites. Interger values of q are marked by symbols.

find that it is necessary to distinguish spatial fluctuations and disorder fluctuations. This is not surprising in view of the finite-size scaling studies [4] of the logarithm of the transmission probability, which explicitly use the property of self-averaging, i.e., the equivalence of averaging over disorder or spatial fluctuations.

In summary, we have demonstrated the multifractal behavior not only at the critical disorder separating localized and extended states in 3D systems, but also up to the localization length in the more general case of an undoubtedly localized wave function on a chain. We expect a respective behavior not only for localized states in 3D systems but also for extended states in disordered systems [19] up to the coherence length. It will therefore be an interesting problem to investigate whether the metal-insulator transition can be identified from such an analysis in some way, e.g., by a critical value of at least one of the generalized dimensions, as previously suggested for the simple fractals [6,7,23]. Even more important should be the consequences of the present analysis if one describes transport properties, which are expected [11] to be drastically influenced by the (multi)fractal behavior.

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