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ELECTRONIC STATES IN MESOSCOPIC SYSTEMS

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Abstract Electronic states in disordered systems are studied within the Anderson model of localization. By means of the Green's function technique we derive the transmission coefficient for electronic states through mesoscopic samples. The transmission coefficient is shown to be not self-averaging due to strong spatial fluctuations of the amplitude of the eigenstates, which are obtained by direct diagonalization of the respective secular matrices. The wave functions display a multifractal behaviour, characterized by the set of generalized fractal dimensions and the singularity spectrum of the fractal measure.

INTRODUCTION

The observation[1] of unusually large statistical fluctuations of the conductance in mesoscopic samples of disordered metals has led to intensive research on the statistical behaviour of transport properties.[2] In small metallic samples the universal conductance fluctuations are well established experimentally as well as theoretically.[2] Even more pronounced fluctuations appear in the insulating regime where electronic states are localized and transport takes place via hopping processes. These fluctuations reflect the microscopic structure of the disordered sample and can be used as *fingerprints* to characterize a given sample.

Averaging, e. g., the transmission coefficient t over a large number of samples, however, does not yield a reasonable mean value because this quantity is not self-averaging. The fluctuations grow (and finally dominate the average) with increasing sample size as long as it remains smaller than the inelastic mean free path. In one-dimensional (1D) samples it can be shown[3] that the variance of t increases exponentially with the system size. Here we present results for t in 2D and 3D samples. We investigate the fluctuations and demonstrate that the logarithm of t self-averages.

It is reasonable to assume that the fluctuations of the transmission coefficient are a consequence of the behaviour of the wave functions, e. g., the spatial dependence of the amplitude of the eigenstates. Aoki[4] has originally suggested that the wave functions are fractal entities. We note that such a fractal picture is in accordance with the mentioned observation that fluctuations increase with increasing

sample size. However, it turned out[5,6] that the wave functions cannot be adequately described by simple fractals. Rather the more general concept of multifractality[7,8] has to be used. In the following we also present a multifractal analysis of the spatial fluctuations of individual eigenstates in 3D disordered samples.[9]

Although the Anderson model of localization has been usually discussed[2] in the context of conduction phenomena in amorphous semiconductors or dirty metals, the fluctuations studied here are by no means restricted to such materials. Large molecular aggregates are another interesting class of materials of mesoscopic extensions where fluctuations should drastically influence the transport properties of excited states, like the photoconductivity. Moreover, the excitation process itself should reflect these fluctuations, e.g., in the intensity of the absorption.

FLUCTUATIONS OF THE TRANSMISSION COEFFICIENT

Our investigation is based on the Anderson model which is commonly used to describe electronic states in disordered systems. In site-representation the Hamiltonian

$$H = \sum_{n} |n> \varepsilon_n <n| + V \sum_{n,m}^{n.n.} |n> <m| \qquad (1)$$

comprises the constant nearest neighbour transfer integral V $(=1)$ and random potential energies ε_n which are chosen according to either a uniform distribution of width W or a Gaussian distribution with variance $W/\sqrt{12}$, on the sites n of a simple cubic lattice. In the following we restrict ourselves to the energy $E = 0$.

For the present analysis it is of advantage to investigate small boxes of length L and cross-section MxM sites, because the Green's function G_{1L} which couples the electronic states on the first and the L-th slice of our system can be recursively calculated from the iteration of the selfenergy.[10] The transmission probability t through the sample then follows as $t = tr|G_{1L}|^2$. For very long samples the transmission probability will decay exponentially so that a localization length λ can be asymptotically defined by $\lambda^{-1} = - tr(t) / 2L$.

In 1D systems it can be shown that $tr(t)$ is self-averaging.[11] In Fig. 1 we present results for $tr(t)$ on 2D and 3D systems. In the investigated localized regime the calculated values are distributed according to a Gaussian distribution[12,13] but the standard deviation increases with the system size L as can be seen from Fig. 1. As the quantity $tr(t)$ is also proportional to L, self-averaging is assured.[13,14] On the other hand, the finite value of the standard deviation for vanishing $tr(t)$ corresponds to the above mentioned universal conductance fluctuations.

SPATIAL FLUCTUATIONS OF THE WAVE FUNCTION

In order to describe the spatial fluctuations of the wave functions we analyse mesoscopic systems of $N = 50^3$ sites with periodic boundary conditions described by the Anderson Hamiltonian. The respective secular matrix is tridiagonalized by means of the Lanczos algorithm,[15] and the tridiagonal matrix is diagonalized by standard techniques. In this way eigenfunctions $|\varphi_i> = \Sigma_n e_{in} |n>$ have been determined in the middle of the spectrum with an accuracy better than 10^{-6} for $\|H_i \varphi_i - E_i \varphi_i\|$. We analyse these wave functions by means of a standard box-counting procedure, determining the box probability of the wave function in N_L boxes of linear size L:

$$\mu_k(L) = \sum_{n=1}^{L^3} |e_{in}|^2 \quad ; \quad k = 1, \ldots, N_L \quad ; \quad N_L = N / L^3 \tag{2}$$

This measure and its q-th moments are averaged over all boxes and found to be proportional to some power $\tau(q)$ of the box size in the limit of small L:

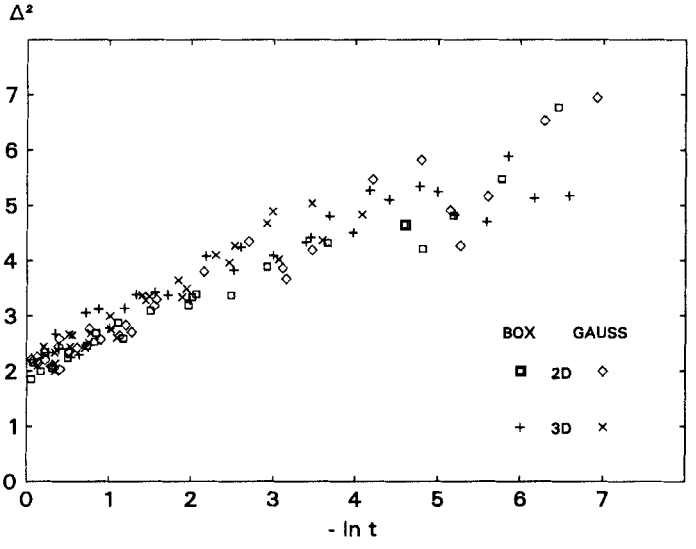

FIGURE 1 Standard deviation of the logarithm of the transmission coefficient, $t_n(t)$, as a function of $t_n(t)$ for disorder parameters W between 10 and 30, for width between $M = 20$ and 80 sites in 2D systems and cross section $MxM = 8x8$ up to 13x13 sites in 3D systems. The diagonal elements of the Anderson Hamiltonian are distributed according to a box distribution or a Gaussian distribution.

$$\chi_q(L) = < \sum_{k=1}^{N_L} \mu_k^q(L) > \sim L^{-\tau(q)} \qquad (3)$$

These mass exponents $\tau(q)$ allow to define generalized dimensions $D_q = \tau(q) / (1-q)$. The results are shown in Fig. 2 for different realizations of the random potential.

This figure clearly demonstrates the multifractal behaviour of the probability density of the wave function because the states can obviously not be described by a single dimension D. The physical meaning is that intertwined regions of the state scale in different ways according to the mass exponents $\tau(q)$. Each subset of the measure characterizes a fractal with its own generalized dimension D_q. Provided that the proportionality in Eq. 3 holds, a multifractal behaviour can be expected, with a set of different D_q. Alternatively, all generalized dimensions could be equal: $D_q = D$. This is usually the case for a homogeneous fractal. However, in the present model the wave functions are supported on every site (even an exponentially localized state vanishes nowhere exactly), so that the so-called similarity dimension equals the Euclidean dimension, $D_0 = D_E \equiv 3$, as can be clearly seen in Fig. 2. The assumption of a homogeneous fractal would therefore lead to integer dimensions for all q, namely: $D_q = 3$. This would be no fractal at all.

The information dimension D_1 is distinctly smaller than D_0 in all samples. The

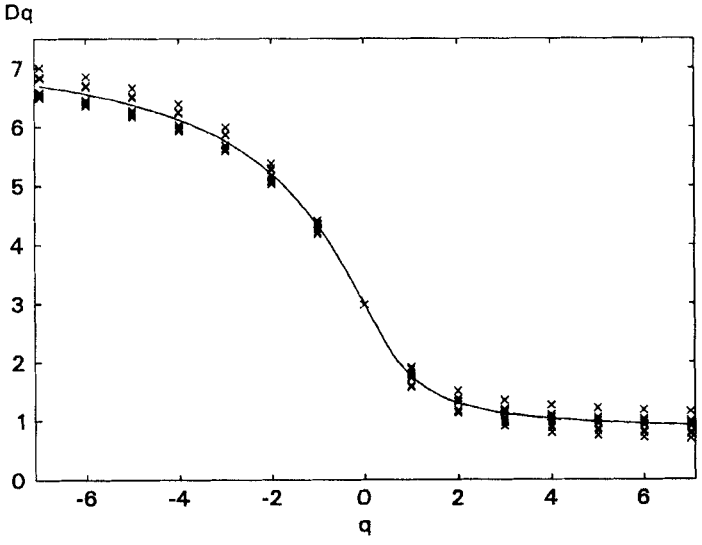

FIGURE 2 Generalized dimensions D_q of the q-th moment of the measure $\mu_k(L)$ for wave functions with $E_i \approx 0$ on 10 different samples of a simple cubic lattice of 50^3 sites for $W = 18$. Integer values of q are marked by symbols (×).

average value $D_1 \approx 1.7$ demonstrates that a subset with a fractal dimension $D_1 < 2$ contains a fraction of the measure which is arbitrarily close to the complete measure, i. e., it contains all the information. The correlation dimension D_2 describes the scaling of the participation number or, equivalently, the scaling of the density-density correlation function. Within the statistical errors the obtained value $D_2 = 1.3$ is in agreement with the results of previous investigations[16].

A more abstract characterization of multifractal sets is given by the singularity spectrum $f(\alpha)$, which can be derived from the singularity strength α that is given in the k-th box by $\mu_k(L) \sim L^{\alpha(k)}$. The number of boxes $N(\alpha)$ in which the strength α can be found is a subset that scales with the box size: $N(\alpha) \sim L^{-f(\alpha)}$. The fractal dimension f reflects the scaling of the singularity strength of the wave function. Representative results are compiled in Fig. 3 displaying a singularity spectrum that is typical for multifractal entities. For a homogeneous fractal the complete curve would contract to a single point. For the actual calculation of Fig. 3 the parametric representation[17] of f and α in terms of q has been employed. Besides the above mentioned cases $q = 1$ and $q = 2$ the extreme values of q are of special interest. The limit $q \to +\infty$ ($q \to -\infty$) corresponding to the minimal (maximal) generalized dimension in Fig. 2 yields the minimal (maximal) value of α, which characterizes the singularity that is associated with the subset containing the largest (smallest) measure.

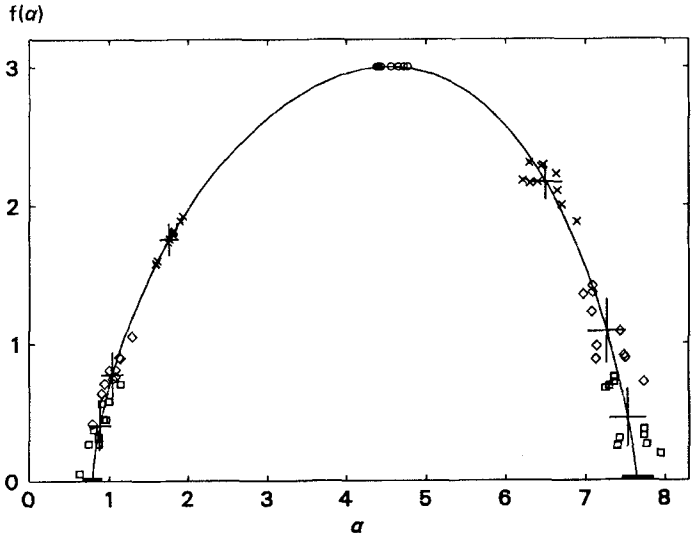

FIGURE 3 Singularity spectrum $f(\alpha)$ for the same wave functions as in Fig. 2. Integer values of the implicit parameter q are marked by symbols for $q = 0$ (o), ± 1 (×), ± 2 (◇), ± 3 (□). The crosses (+) denote the respective averages and error bars for α and f. The solid bars denote the range of α-values for $q \to \pm\infty$.

SUMMARY AND CONCLUSIONS

We have demonstrated the multifractal behaviour of the spatial fluctuations of the eigenfunctions of the Anderson Hamiltonian. Therefore fluctuations on all length scales are an inherent property of disordered systems. Moreover, multifractality means that intertwined regions scale in different ways according to the generalized fractal dimensions. It is therefore not surprising that physical quantities like the transmission coefficient display strong fluctuations as shown in Fig. 1. If these fluctuations were primarily of statistical origin one could expect to obtain reasonable expectation values by averaging over a large number of samples or over larger samples. The main conclusion of the present analysis is, however, that the fluctuations are a result of the multifractal character of the wave function. As a consequence, larger and larger fluctuations are encountered upon increasing the system size, because larger scales are taken into account in this way. Accordingly, self-averaging cannot be expected, and the fluctuations have to be taken into account as an inherent property of disordered mesoscopic systems up to the inelastic mean free path, which constitutes a natural limit for the length scale of these fluctuations. The quantitative investigation of the influence of these fluctuations on the spectroscopic properties as well as the transport behaviour of excited states of large molecular aggregates will be an interesting topic of future research.

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