Dimensionality Dependence of the Metal-Insulator Transition in the Anderson Model of Localization

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The metal-insulator transition is investigated by means of the transfer-matrix method to describe the critical behavior close to the lower critical dimension 2. We study several *bifractal systems* with fractal dimensions between 2 and 3. Together with 3D and 4D results, these data give a coherent description of the dimensionality dependence of the critical disorder and the critical exponent in terms of the *spectral* dimension of the samples. We also show that the upper critical dimension is probably infinite, certainly larger than 4.

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The question of localization of electronic states in disordered systems has been a central topic of research since the original formulation of the problem by Anderson [1]. The extensive amount of work was reviewed recently [2]. We limit our discussion here to the widely used Anderson model in the case without magnetic field. For one-dimensional (1D) systems it was rigorously shown [3] that infinitesimally small disorder is sufficient for localizing the electronic states irrespective of their energy. In higher dimensions no rigorous treatment is available so far. But there is now general agreement that all electronic states are localized in 2D [2]. Numerical simulations in 3D demonstrated the existence of a metal-insulator transition (MIT) separating extended and localized states in the energy-disorder diagram [4]. The results agree with the scaling hypothesis of localization [5] and with conclusions from the nonlinear σ model in terms of the ε expansion for $d = 2 + \varepsilon$ dimensions [6]. These analytical investigations suggest that $d = 2$ is the lower critical dimension of the model, so that the states in a 2D system are marginally localized for small disorder.

Naturally, the extensive numerical simulations were performed on square and simple cubic lattices in 2D and 3D, respectively. However, not only was the validity of the ε expansion itself questioned [6,7], but it was also a problem that the expansion parameter ε is not small any more for 3D systems which are paradigmatic for the MIT. This prompted us to look for appropriate systems with ε between 0 and 1, i.e., systems with a fractal dimension between 2 and 3. It is the purpose of the present Letter to present results for five such systems. They allow a reasonable extrapolation for $\varepsilon \to 0$ or $d \to 2$: We obtain for the critical disorder

$$W_c(\varepsilon) = \varepsilon W_c(\varepsilon = 1) = 16.5\varepsilon \qquad (1)$$

and for the critical exponent

$$\nu = \alpha/\varepsilon + 0.5\,, \qquad (2)$$

and a fit yields the constant $\alpha \approx 0.8$.

Our investigation also shows that the *spectral* dimension d_s rather than the *fractal* dimension d_f is characteristic for the behavior of the MIT. d_f describes how the mass of a system (i.e., the number of sites in our model) scales with the system size. Thus it does not depend on the coordination number or the connectivity of the underlying (fractal) lattice, which are significant for the localization of the electronic states. In contrast, the relation to nearest neighbors is taken into account by d_s, which controls not only the spectrum of low-energy vibrations (hence the name spectral dimension) but also the long-time behavior of a random walker [8] and thus the diffusion on the lattice. This led to the suggestion that d_s plays the decisive role for localization in the Anderson model [9,10]. By studying systems with the same d_f but different d_s as well as different systems with the same d_s we confirm the relevance of d_s for the MIT, i.e., that $\varepsilon = d_s - 2$ should be used in Eqs. (1) and (2). The significance of d_s also explains why an analysis [11] of strongly anisotropic 3D systems could not describe the transition between 3D and 2D behavior: In those systems one has always $d_s = 3$.

With respect to larger dimensions an interesting problem concerns the upper critical dimension d_u of the model, for which the model can be described by mean field theory. No such theory is known, but several speculations suggested $d_u = 4$, 6, 8, or infinity [12]. For the Bethe lattice a critical exponent $\nu_B = \frac{1}{2}$ was obtained. Therefore, one expects $\nu = \frac{1}{2}$ in mean field theory. Our subsequent investigation, which includes the mentioned fractal systems and 3D and 4D lattices, demonstrates that

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in 4D $\nu > \nu_B$, which means $d_u > 4$. The extrapolation (2) even suggests that $\nu > \nu_B$ for any dimension, i.e., d_u is probably infinite.

Our investigation is based on the Anderson model commonly used in the study of localization. In site representation the Hamiltonian

$$H = \sum_{i=1}^{N} |i\rangle \epsilon_i \langle i| + \sum_{ij}^{\text{n.n.}} |i\rangle V \langle j| \qquad (3)$$

comprises the random site energies ϵ_i chosen from a box distribution of width W and the transfer energies V between nearest neighbors. We set $V = 1$ to fix the energy scale.

The transfer matrix method allows us to determine the localization length λ_M of electronic states in quasi-1D systems with cross section M^{d-1} and length $L \gg M$ recursively from the Lyapunov exponents of the product of transfer matrixes describing the evolution of electronic states according to the Hamiltonian (3) along the quasi-1D system [2,4]. The hypothesis that these raw data for different W fall onto a common scaling curve f, i.e., $\lambda_M/M = f(\lambda_\infty/M)$ has to be corroborated by a finite-size scaling procedure. At W_c the resulting scaling parameter $\lambda_\infty(W)$ diverges with the critical exponent ν.

This approach was used extensively for square and simple cubic systems [2,4]. Here we apply it to lattices with d_f between 2 and 3. A MIT at finite disorder is expected only in a system in which the relevant dimension exceeds 2, i.e., $d_s > 2$. But most fractal systems fulfill [13] $d_s < 2$, even if $d_f > 2$. Therefore, we investigate so-called bifractals [13] combining a fractal and a Euclidean structure. Figure 1 shows the construction of such bifractals as regular stacks of identical fractals. Bifractals I and II, which are derived from the Sierpinski gasket, are exact bifractals since their generation scheme is completely predetermined and scale invariance is exactly obeyed. For a bifractal d_f is given by the sum of the dimensions of the fractal and the Euclidean part yielding $d_f^{\mathrm{I}} = d_f^{\mathrm{II}} = \ln 3/\ln 2 + 1 \approx 2.585$. We also use three statistical bifractals (III, IV, V) for which the fractal part is derived from the η model of dielectric breakdown [14]. For $\eta = 1$ this is equivalent to diffusion limited aggregation and scale invariance is fulfilled only in a statistical sense. The advantage is that d_f can be varied by adjusting η. Thus we constructed bifractals with $d_f^{\mathrm{III}} = 2.8$, $d_f^{\mathrm{IV}} = 2.6$ (see Fig. 1), and $d_f^{\mathrm{V}} = 2.4$.

For a Euclidean system d_s equals the Euclidean dimension. For bifractals d_s is obtained as the sum of the dimensions of the constituents. $d_s^{\mathrm{I}} = 2\ln 3/\ln 5 + 1 \approx 2.365$ follows from an exact determination of the density of states of low-frequency vibrations of the fractal lattice [10]. For the other bifractals such a derivation is not possible. Therefore, we simulated a random walker on the fractals and determined the scaling with time t of the mean-square displacement $\langle r^2 \rangle$. On fractal lattices the diffusion may be anomalous, i.e., $\langle r^2(t) \rangle \propto t^a$ with $a < 1$, while for Euclidean systems we have normal diffusion ($a = 1$). The exponent a relates d_s and d_f by [15] $d_s = a d_f$, i.e., $d_s < d_f$ for the fractal lattices with anomalous diffusion. Our simulations yielded, $d_s = 2.33$, 2.41, 2.54, 2.32, and 2.22 for I, ..., V. Thus all have $d_s > 2$ so that a MIT is expected. The numerical d_s^{I} is in reasonable agreement with the exact value. Within the numerical accuracy $d_s^{\mathrm{I}} = d_s^{\mathrm{IV}}$. On the other hand, d_s distinguishes I and II for which $d_f^{\mathrm{I}} = d_f^{\mathrm{II}}$.

The particular geometry of the bifractals allows us to apply the transfer matrix method in a straightforward way, i.e., we determine the localization length λ_M for the quasi-1D systems with cross section $M^{d_f - 1}$ and length $L \gg M$. Typical results are presented in Fig. 2. Because of the generation scheme of the Sierpinski gasket only a few cross sections with 9, 27, 81, and 243 sites can be used. The smallest system with three sites is too small; larger systems need too much computer power. For the statistical bifractals we use odd values of M between 5 and 17 (25, 35); the cross sections then contain

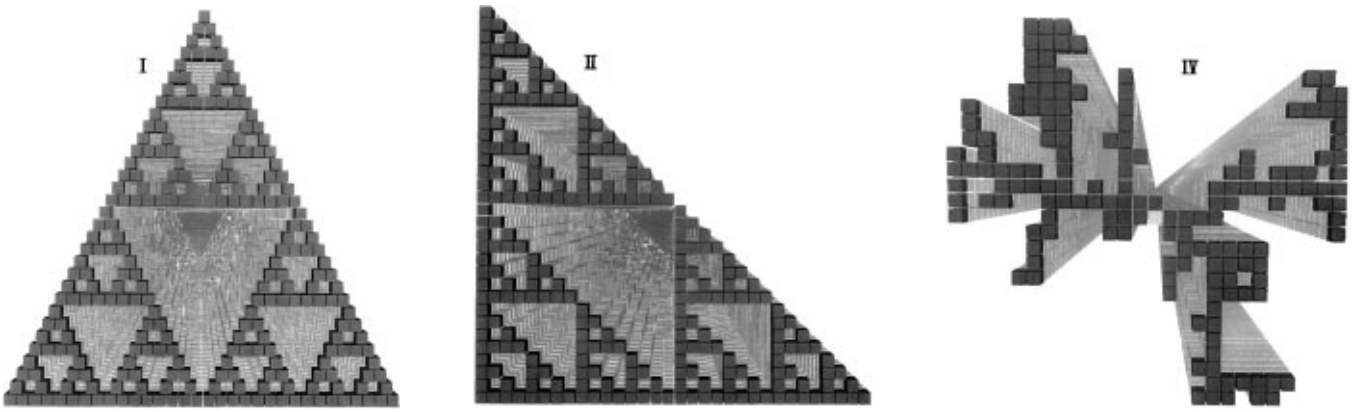

FIG. 1. Bifractals I, II, IV. Each site is indicated by a small cube. Cubes which have (partly) a common side represent nearest neighbor sites in the Anderson Hamiltonian (3). Thus in II every site has a neighbor above itself, while in I only every other site has a neighbor above itself. The average number of nearest neighbors is 4 in I and 5 in II.

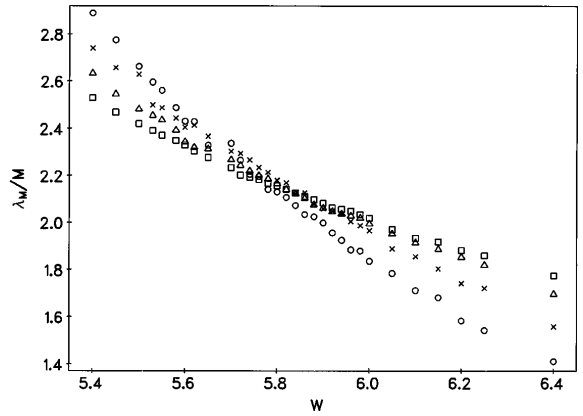

FIG. 2. Raw data for the localization length λ_M of bifractal I at energy $E = 0$ for different values of the disorder W. The symbols distinguish $M = 4$ (□), 8 (△), 16 (×), and 32 (○).

between 17 and 148 (13 and 161, 10 and 125) sites for bifractal III (IV, V). These raw data are sufficient to perform the finite-size scaling of $\lambda_M/M = f(\lambda_\infty/M)$ successfully. Scaling curves for I, II, and IV are shown in Fig. 3. The upper branches correspond to the metallic side, the lower branches to the insulating side of the MIT. It is important to note that I and IV with the same d_s yield the same scaling curve in contrast to II with larger d_s. This corroborates the significance of d_s rather than d_f.

The values of the scaling parameter λ_∞, comprised of the inset of Fig. 3, are characteristic for a second order phase transition. We note that these data can be identified with the inverse of the dc conductivity on the metallic side (small W) and with the localization length of the infinite system on the insulating side (large W) [2,4]. The critical disorder W_c at which λ_∞ diverges can be inferred from Fig. 3 as well as its inset. The results [16] are presented in the inset of Fig. 4, together with the 3D value [17] and our 4D result [18]. The data obey Eq. (1), which was already guessed from an investigation of a 4D system only [19]. We emphasize that Eq. (1) implies the absence of a MIT for $d = 2$, because ε and thus W_c vanish [20]. This agrees with the scaling hypothesis [5]. We note that the data points $W_c(d_f)$ scatter much more in the plot than $W_c(d_s)$, again confirming the relevance of d_s rather than d_f.

The phase transition between metallic and insulating behavior is characterized by the divergence $\lambda_\infty(W) \propto |W - W_c|^{-\nu}$. The critical exponent ν can be obtained from fitting this formula to the data in the inset of Fig. 3, but these data are rather inaccurate close to W_c, because the finite-size scaling procedure cannot be so precise near W_c. Therefore, we determine ν directly from the raw data [21]. The results in Fig. 4 show a sharp increase for $d_s \to 2$, for 4D we find $\nu = 1$. Thus all data fulfill the lower bound [22] $\nu > 2/d$. The nonlinear σ model yields $\nu = 1/\varepsilon$ to first order in the ε expansion [6] in reasonable agreement with our numerical data up to $\varepsilon = 0.5$. It is obvious from Fig. 4 that ν will reach the Bethe lattice limit $\nu_B = \frac{1}{2}$ only for very large d. Thus we can exclude the possibility that the upper critical dimension equals 4. Figure 4 rather suggests that it is infinite. This prompted us to combine ν_B and the dependence on ε from the ε expansion into Eq. (2). It enables a good fit to the data (see Fig. 4). We note that the agreement with the data can be improved only insignificantly, if we fit $\nu = \alpha/\varepsilon + \beta$. A statistical analysis [23] of the local Green's function gives additional support for our numerical result (2).

In conclusion, we exploited the idea to use bifractal systems for the analysis of the MIT in the Anderson model of localization so that dimensions between 2 and 3 become accessible to the numerical analysis, taking the spectral dimension as the relevant dimension. Because of their particular geometry, bifractals are ideally suited for this purpose. Applying the transfer matrix method with

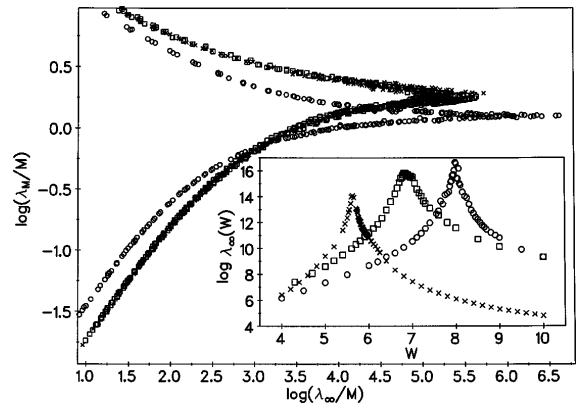

FIG. 3. Scaling curve (×) for bifractal I, obtained from the data in Fig. 2 by determining the scaling parameter $\lambda_\infty(W)$ by mean least squares fitting [4]. Data for 63 values of W between 3 and 10 (usually in steps of 0.2, but around $W = 6$ in steps of 0.02) are included. Data for II (○) and IV (□) are also shown. Inset: Scaling parameter $\lambda_\infty(W)$.

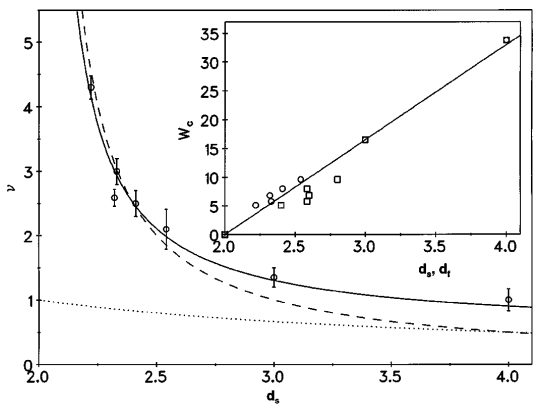

FIG. 4. Critical exponent ν from the present investigation (○), the fit of Eq. (2) by nonlinear regression (full line), the ε expansion in the nonlinear σ model to first order [6] (broken line), and the lower bound [22] (dotted line). Inset: Dependence of the critical disorder W_c at $E = 0$ on d_s (○) and d_f (□). The full line represents Eq. (1).

subsequent finite size scaling to five different bifractals, we have been able to derive the dimensionality dependence of the critical disorder and the critical exponent. A good agreement of the fit of Eq. (2) with the numerical results shows that the lower critical dimension is 2 and the upper critical dimension is probably infinite. In order to get a more comprehensive understanding of the dimensionality dependence of the MIT, it would be interesting to perform various other investigations of the MIT in the Anderson model of localization also on such bifractals as used in the present study. This concerns, for example, the level spacing statistics [24], i.e., the distribution of the energy levels of the Anderson Hamiltonian as well as the multifractal analysis [25] of the spatial distribution of the probability density of the wave functions. Respective calculations are in progress.

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