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Numerische Simulation auf massiv parallelen Rechnern

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Energy level statistics at the metal-insulator transition in the Anderson model of localization with anisotropic hopping

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Abstract

Recently, a metal-insulator transition (MIT) was found in the anisotropic Anderson model of localization by transfer-matrix methods (TMM) [1, 2, 3]. This MIT has been also investigated by multifractal analysis (MFA) [4] and the same critical disorders W_c have been obtained within the accuracy of the data. We now employ energy level statistics (ELS) to further characterize the MIT. We find a crossover of the nearest-neighbor level spacing distribution $P(s)$ from GOE statistics at small disorder indicating metallic behavior to the Poisson distribution at large disorder characteristic for localized states. An analysis of the system size dependence of the spectral rigidity $\Delta_3(L)$ confirms the values of W_c found in Ref. [3, 4].

1 Introduction

Recent TMM studies [1, 2, 3] of the anisotropic Anderson model show that an MIT exists even for strong hopping anisotropy γ. The values of the critical disorder in the band center were found to follow a power law $W_c \propto (1-\gamma)^\beta$ independent of the orientation of the quasi-1D bar. β was argued to be independent of the strength of the anisotropy. This is supported by multifractal analysis of the eigenfunctions [4], where the system size dependence of the singularity spectra is used to determine W_c. In order to check this further, we employ energy level statistics as another independent method. ELS is based on random matrix theory [6] and was successfully used to investigate the MIT in the isotropic case [5, 7, 8]. Directly at the MIT, the ELS was argued to be given by a universal distribution $P_c(s)$, which should correspond to a "critical ensemble" [5] distinct from the case of a Gaussian orthogonal ensemble (GOE) and also from the Poissonian case. However, recent results [9] show that $P_c(s)$ depends on the boundary conditions and the shape of the samples considered.

In this work, we show that the MIT in the anisotropic systems can be characterized conveniently by ELS and we find that the critical disorders W_c are in good agreement with the results of Refs. [3, 4]. We further find that $P(s)$ at the MIT in the anisotropic systems depends on the anisotropy γ. Thus an estimation of W_c by use of the "critical ensemble" is incorrect.

2 The anisotropic Anderson model of localization

The Anderson Hamiltonian is given as [10]

$$H = \sum_i \epsilon_i |i\rangle\langle i| + \sum_{i\neq j} t_{ij} |i\rangle\langle j| \quad . \tag{1}$$

We use a simple cubic lattice of size N^3 with orthonormal states $|i\rangle$ at site $i = (x, y, z)$. The potential site energies ϵ_i are random numbers, uniformly distributed in the interval $[-W/2, +W/2]$. The transfer integrals t_{ij} are restricted to nearest neighbors. They depend only on the spatial direction, thus $t_{ij} = t_x$, t_y or t_z. We study the two cases of: (i) *weakly coupled planes* with $t_x = t_y = 1$, $t_z = 1 - \gamma$ and (ii) *weakly coupled chains* with $t_x = t_y = 1 - \gamma$, $t_z = 1$. The anisotropy parameter γ ranges from $\gamma = 0$, the isotropic case, to $\gamma = 1$ where the planes/chains are completely uncoupled.

We use the Lanczos algorithm [11] to compute the spectrum of H. It is well suited for the diagonalization of our sparse matrices [12] and allows us to compute all eigenvalues of H for system sizes of $N = 48$ on a parallel machine within 60 hours. We use 50% of the eigenvalues around the band center $E = 0$ and average over up to 400 realizations of the random potential, such that at least 2×10^5 eigenvalues are used for each set of parameters $\{W, \gamma, N\}$. Due to the large computational effort, we restrict the systematic investigations to sizes up to $N = 30$. For comparison with predictions of random matrix theory, we unfold the spectra by fitting cubic splines [7] to the integrated density of states. This sets the mean-level spacing to one. We then characterize the local spectral fluctuations by means of the nearest neighbor level spacing distribution $P(s)$ and the Δ_3 statistics. The latter measures the rigidity of the spectra [6].

3 Results

Extended states in a metal contribute to charge transport even at $T = 0$. The overlap of the extended states results in level repulsion and their spectral properties are characterized by the GOE. On the other hand, *localized* states cannot contribute to charge transfer at $T = 0$, resulting in insulating behavior. The energy levels are uncorrelated, consequently the probability that energy levels are close together is very high and the ELS is given by the Poissonian statistics. Thus a change from the GOE behavior to Poissonian may indicate the existence of an MIT.

As expected from the isotropic case, we find $P(s)$ to be close to the GOE statistics at small disorder and close to Poisson statistics at large disorder as shown in Fig. 1 for an already quite strong anisotropy. For stronger anisotropy γ, the transition occurs at smaller values of the disorder

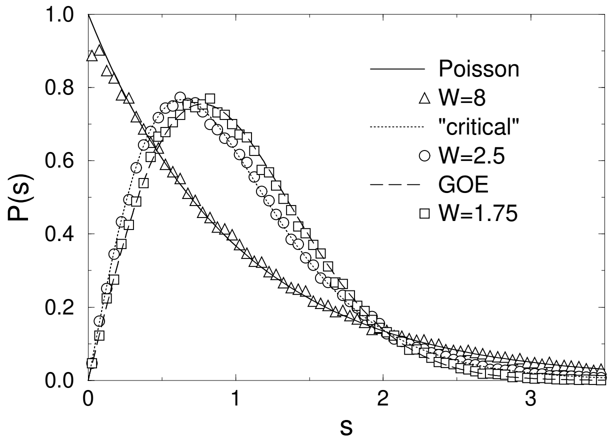

Figure 1: $P(s)$ for weakly coupled chains with $N = 24$ and $\gamma = 0.9$.

parameter W.

In an infinite system, there is a sharp transition from extended to localized behavior at the MIT. However, in any finite system, the characteristic lengths scales of the states close to the transition will exceed the system size. Thus for a given N, one finds characteristic deviations which result in a continuous change from GOE to Poissonian statistics as W is varied across the MIT. Only directly at W_c the statistical properties are independent of N, because of the scale invariance of the multifractal wave functions at the MIT [13, 4]. In order to identify the extended, critical and localized regimes and to determine the critical disorder W_c properly, we therefore examine the system size dependence of the ELS.

As an example we show in Fig. 2 the Δ_3 statistics for weakly coupled planes at $\gamma = 0.9$ for 4 system sizes N ranging from 13 to 30. For $W = 6$, we find that upon increasing N that there is a clear trend towards the GOE prediction. On the other hand, the data for $W = 12$ tend towards the Poissonian result. At $W = 9$, the Δ_3 statistics is independent of N within the accuracy of our calculation. Thus the critical disorder for the present example is $W_c \approx 9$. In addition to

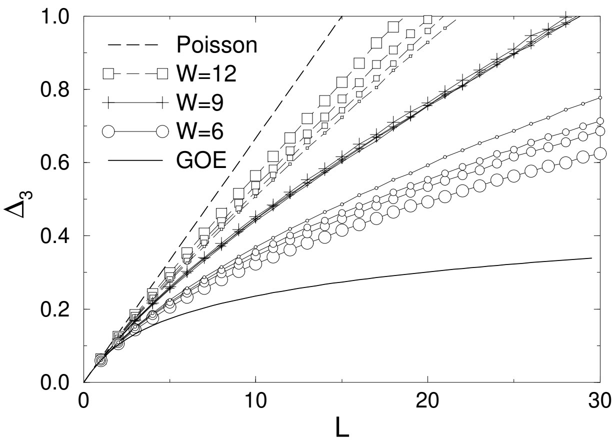

Figure 2: $\Delta_3(L)$ for weakly coupled planes with $\gamma = 0.9$ for $N = 13, 17, 21, 30$. Larger N corresponds to larger symbol size.

this finite-size dependence, we have also used finite size scaling analysis for quantities such as $\alpha = \int_0^{30} \Delta_3(L)dL$. We have constructed scaling functions, which further support the values of W_c obtained above and confirm the one-parameter scaling hypothesis and thus the existence of the MIT in these anisotropic systems. Details will be published elsewhere [14].

The critical disorders obtained by this analysis agree reasonably well with the results from TMM [3] and MFA [4]. W_c decreases with increasing anisotropy with a power law $W_c = 16.3(1-\gamma)^\beta$, where $\beta = 0.25$ for weakly coupled planes and $\beta \approx 0.6$ for weakly coupled chains, respectively.

For a given anisotropy and system size, we can also identify a disorder W' at which $P(s)$ agrees with the so called "critical statistics", characteristic for the MIT of the isotropic system (cp. Fig. 1). However, this disorder is much smaller than W_c for strong anisotropies. And, of course, the value of W' changes when we change the system size. Thus, $P_c(s)$ is not characteristic for the MIT in anisotropic systems. We find that upon increasing the anisotropy that the statistical properties at the MIT drift slowly from the "critical statistics" $P_c(s)$ of the isotropic case [5] towards Poisson statistics. In that sense, the states at W_c seem to be less extended in the anisotropic system compared to the isotropic case. This coincides with the results of the MFA [4].

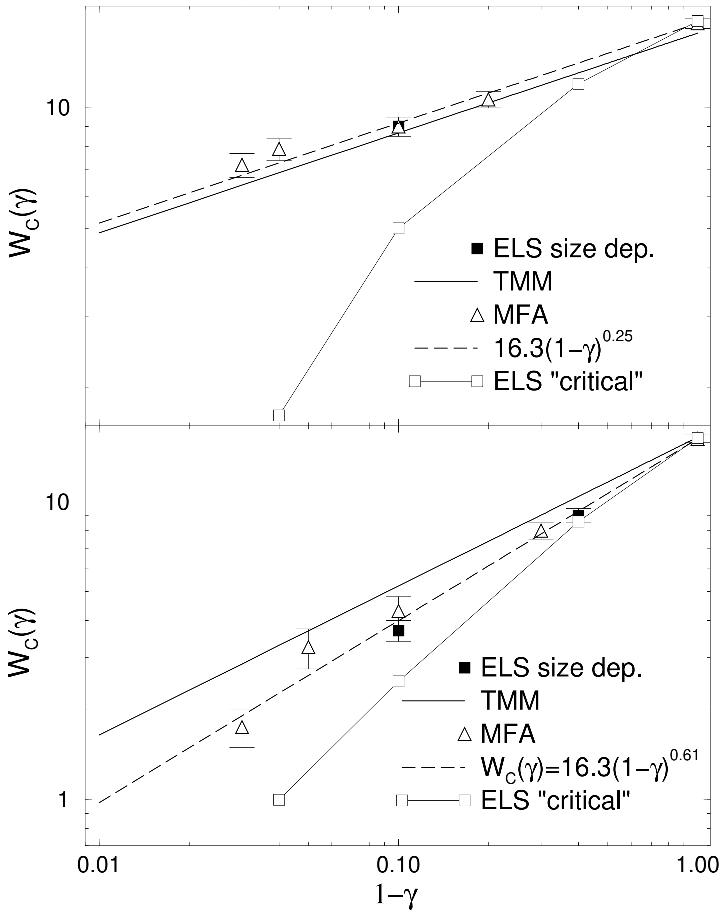

Figure 3: $W_c(\gamma)$ for weakly coupled planes (above) and chains (below) as obtained with various methods. The thick solid line is the TMM result of Ref. [3]. The open squares are the disorder values, where the "critical statistics" is found for system size $N = 21$.

4 Conclusions

We find that a metal to insulator transition exists in the anisotropic Anderson model. The critical disorders obtained from the ELS coincides reasonably well with the results from TMM [3] and MFA [4]. The system-size independent $P(s)$ and $\Delta_3(L)$ at the MIT depend on the specific values chosen for the microscopic hopping elements t_x, t_y, and t_z. They are different for each γ and the two anisotropy realizations, namely, weakly-coupled planes and chains. Furthermore, the ELS at the MIT is also different from the ELS of the isotropic case. Thus we find that $P(s)$ at the MIT is not universal,i.e., not independent of the microscopic parameters of the model.

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