Metal-insulator transition in three dimensional Anderson model: scaling of higher Lyapunov exponents

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Abstract

Numerical studies of the Anderson transition are based on finite-size scaling analysis of the smallest positive Lyapunov exponent. We prove numerically that the same scaling holds also for higher Lyapunov exponents. This scaling supports the hypothesis of the one-parameter scaling of the conductance distribution. From collected numerical data for quasi one dimensional systems up to system size $24^2 \times \infty$ we found the critical disorder $16.50 \leq W_c \leq 16.53$ and the critical exponent $1.50 \leq \nu \leq 1.54$. Finite-size effects and the role of irrelevant scaling parameters are discussed.

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The main problem of the theory of Anderson transition is to prove that there is only one relevant parameter which controls the behavior of all quantities of interest in the neighborhood of the critical point. An excellent example of such a quantity is the smallest positive Lyapunov exponent (LE) \( z_1 \) which follows the one-parametric scaling relation \(^1\)

\[
z_1(L, W) = f(L/\xi(W))^{1/\nu}.
\]

In (1), \( W \) is the disorder, \( L \) defines the width of the quasi-one dimensional system \( L \times L \times L_z \) and \( \xi(W) \) is the universal scaling parameter. In Q1D geometry, Lyapunov exponents \( z_i \) are defined through eigenvalues \( t_i \) of the transfer matrix \( T^\dagger T \) as \( z_i = 2\frac{L}{L_z} \log t_i \). In the limit \( L_z \gg L \), all \( z \)s are self-averaged quantities \(^2\). Relation (1) determines the disorder and the system size dependence of \( z_1 \) in the neighborhood of the critical point \( W_c \) and enables us to determine \( W_c \) and critical exponents for conductance (\( s, W < W_c \)) and for localization length (\( \nu, W > W_c \)) \(^1, 3, 4, 5, 6, 7\).

In the pioneering work \(^1\), critical parameters were found as \( W_c \approx 16.5 \pm 0.5 \) for the box distribution of the disorder energies, and \( s = \nu \approx 1.5 \pm 0.1 \). This result was later confirmed by more accurate numerical studies \(^4, 8, 5\), and also by analysis of the level statistics \(^9\). Calculations performed for different microscopic models confirmed the universality of exponent \( \nu \) within a given universality class \(^3\).

To complete the proof of the universality of the metal-insulator transition, the one parameter scaling should be found also for more realistic variables, such as the conductance \( g \) \(^10, 11\). This must be done for the cubic samples. Here, owing to the absence of self-averaging, it is necessary to test the universal scaling of the whole distribution \( P(g) \). It is unrealistic to perform such

\(^1\)Instead of \( z_1 \), the inverse quantity \( \Lambda = 2/z_1 \) is commonly used. The present discussion is identical for both quantities, but \( z \)'s seem to be more natural variables for our purposes.

\(^2\)
analysis with the numerical accuracy comparable to that achieved from Q1D studies. Therefore, previous studies of $P(g)$ concentrated only on estimation of the conductance distribution at the critical point [12, 13, 8, 5, 14] and in the metallic and localized regime [12].

The aim of this work is to support the idea of the one-parametric scaling of the conductance and of its distribution. Instead of the study $g$, we prove numerically that the higher Lyapunov exponents $z_2, z_3, \ldots$ follow the same scaling behavior as the first one in the Q1D systems. Common scaling proves that the spectrum of the transfer matrix in the Q1D limit is determined only by one parameter. Strong correlation of $z$s gives also the serious basis for the generalization of the random - matrix theory to the description of the critical region [16, 17, 18].

Although we deal only with Q1D geometry, it is reasonable to suppose that the observed correlation survives also for the cubic geometry. Then the relation between $g$ and $z$s, $g = \sum_i \cosh^{-2} z_i/2$, [19] assures that $g$ also follows the one-parametric scaling.

Collected numerical data also provide us with a very accurate estimation of the critical disorder $W_c$ and the critical exponent $\nu$. It is the first time that numerical data for system size $L > 16$ has been collected and analyzed. Our data for large $L$ enable us to check the finite-size corrections to scaling proposed in [3].

The scaling behavior of higher LEs was originally studied in the Henneke’s PhD Thesis [7]. Due to the insufficient accuracy of his data and small system size, no acceptable proof of the common scaling was found. The first indication of the common scaling was shown in [15] and generalized to the neighborhood of the critical point in [16, 17]. The common behavior of higher LEs, $z_i \sim i$ is well known in the metallic regime; it was already used in [1] to explain the physical meaning of the scaling parameter $\xi(W)$, and confirmed by random-matrix studies [19]. In the localized regime, $z$s follow the relation $z_i(W, L) = z_1(W, L) + \Delta_i$ with $W$ and $L$-
independent constants $\Delta_i$.

For the Q1D systems $L^2 \times L_z$ we calculated all LEs for cca 21 different values of disorder, $16 \leq W \leq 17$. $L$ grows from $L = 4$ up to 24. For the smallest $L$, the relative accuracy of the first LE $z_1(W, L)$, $\varepsilon_1 = \sqrt{\text{var}(z_1)} / z_1(W, L)$ was 0.05% while $\varepsilon_1$ was only 1% for $L = 21, 22$ and 24, being 0.5% for $L = 16, 18$. The accuracy of higher LE is much better; in particular, $\varepsilon_2 \approx \varepsilon_1/2$ and $\varepsilon_9 \approx 0.17\varepsilon_1$ for all system size.

The interval of the disorder is narrow enough to approximate the $W$ dependence of $z$’s by the linear fit

$$z_j(W, L) = z_j^{(0)}(L) + W z_j^{(1)}(L), \quad j = 1, 2, \ldots$$

Small differences between fits containing higher powers of $W$ and (2) appear only for $L > 18$ and even then they do not exceed the numerical inaccuracy of the raw data. The typical $W$-dependence of our data is presented in Fig. 1 for $z_2$.

The scaling behavior requires that

$$z_j(W, L) \approx z_{jc} + A \times (W - W_c) \times L^\alpha, \quad \alpha = 1/\nu,$$

Comparison of (2) with (3) offers the simplest way to estimate the critical exponent $\alpha$. In Fig. 2. we present the $L$-dependence of $z_j^{(1)}$ for the first six LEs and for $z_9$. It confirms that close to the critical point these LEs scale with the same exponent $\alpha$:

$$\alpha \approx 0.655 \pm 0.010$$

which determines $\nu = 1.526 \pm 0.023$. This estimation is in very good agreement with the result of MacKinnon [4] and differs slightly from [3, 5].
Figs. 1 and 2 also show also the important influence of the finite-size effects (FSE) in the present analysis. Evidently, the small \( L \) data are of no use in the analysis of higher LEs. We found that the numerical data for \( z_j \) could be used only when

\[
L > z_j. 
\]  

(5)

It is easy to understand. If \( z_j > L \) then the \( j \)th channel is rather "localized" than critical on this length scale. Therefore only a small part of the spectra which fulfills the relation (5) follows the scaling behavior. The rest of the spectrum depends on \( L \) even at the critical point. This conclusion is supported also by the analysis of the density \( \rho(z) \) of all LEs for the cubic samples [21]. At the critical point, the number of system-size independent LEs grows as \( \sim L \) when \( L \to \infty \) [16]. As \( z_1 \approx 3.4 \), the above mentioned effect does not influence the analysis of the first LE \( z_1 \). Nevertheless, other FSE must be taken into account in the scaling analysis of \( z_1 \) [3, 22].

More reliable estimation of the exponent \( \alpha \) [4] and of the critical disorder \( W_c \) is given by the position of the minimum of the function

\[
F(W_c, \alpha, \ldots) = \frac{1}{N} \sum_{W,L} \frac{1}{\sigma_j^2(W,L)} [z_j(W,L) - z_j^{\text{fit}}(W,L)]^2. 
\]  

(6)

In (6), \( N = \sum_{W,L} \) is the number of points, and \( \ldots \) stays for all other fitting parameters.

The natural choice of the fitting function \( z_j^{\text{fit}} \) in (3) is the rhs of (2). None FSE are explicitly included in (2). Nevertheless, it still enables us to test the sensitivity of the critical parameters to the size of the analyzed systems. To do so, we considered different sets of input data \( z_j(L,W) \) with the restriction \( L_{\text{min}} \leq L \leq L_{\text{max}} \) (\( L_{\text{min}} \leq 12 \)). Then, the \( L_{\text{min}} \)- and \( L_{\text{max}} \)-dependence of \( W_c \) and \( \alpha \) was analyzed. While the influence of the choice of \( L_{\text{max}} \) is, as supposed, negligible, both
$W_c$ and $z_{jc}$ increase with $L_{\text{min}}$. We found the $L_{\text{min}}$-independent results only for the two smallest LEs $z_1$ and $z_2$. For the higher LEs, critical parameters do not reach their limiting values even for $L_{\text{min}} = 12$. In difference to $W_c$, the estimation of the critical exponent $\alpha$ does not depend on the choice of interval of $L$. Obtained data are in good agreement with estimation (4) for all LEs under consideration.

The weak $L_{\text{min}}$ - sensitivity of the critical exponent agrees with an assumption that FSE influence primarily the $W$-independent part of $z_j$ [4]. Fig. 1. offers a simple interpretation of this result: to eliminate FSE one has to shift each line by the disorder-independent constant $B(L)$ which should be added to the rhs. of (2). The proper choice of $B(L)$, assures that all lines cross at the same point as it is proposed by the scaling theory. Finite size corrections to the line slope are only of the ”higher order”.

Slevin and Ohtsuki [3] fitted $z_1(W, L)$ (resp. its inverse $z_1^{-1}$) to the more general function

$$z_{\text{fit}}^1(L, W) = z_{jc} + \sum_{n=0}^{N_x} \sum_{m=0}^{N_y} A_{nm} x^n y^m$$

with $N_x = 3$, $N_y = 1$. In (7), $x = (w + b_1 w^2 + b_2 w^3)L^\alpha$, $w = W - W_c$ and $y = L^\beta$ with $\beta < 0$. Exponent $\beta$ represents the second critical (irrelevant) scaling exponent. We applied this function to our data with restriction (5) and with $b_1 = b_2 = 0$, $n + m \leq 1$. Then

$$z_{\text{fit}}^j(L, W) = z_{jc} + A \times (W - W_c)L^\alpha + BL^\beta. \quad (8)$$

We have checked that more sophisticated fits do not provide us with any reasonable improvement of the accuracy of critical parameters.

To test the quality of the fit (8), we again studied the sensitivity of our results to a change of the input data. Evidently, for large enough $L_{\text{min}}$ the role of the irrelevant scaling exponent is
negligible. The finite size effects become small and difficult to measure. Value of the irrelevant critical exponent $\beta$ obtained from fitting function (8) decreases to $\approx -20$ for large $L_{\text{min}}$.

For small values of $L_{\text{min}}$, however, the three-parametric fit (8) still does not provide us with the $L_{\text{min}}$-independent estimation of critical parameters. We averaged therefore the values of $W_c$ and $\alpha$ obtained from various choices of $L_{\text{min}}$.

Table 1. presents our results for the first five LEs obtained from fits (2) and (8). On the basis of the presented data we estimate

$$16.50 \leq W_c \leq 16.53 \quad \text{and} \quad 1.50 \leq \nu \leq 1.54$$

These values are in a very good agreement with \cite{4}.

Our results (9) differ from that obtained by many parametric fitting procedure in Ref. \cite{5} (Table 1.). None of the analyzed statistical ensemble provides us with such high value of $\nu$. This discrepancy is probably caused by different input data. Contrary to previous treatments \cite{4,5}, we collected data for large system size in order to simplify the fitting function. The main shortcoming of this strategy is a lower accuracy of our data for $z_1$. On the other hand, the fact that the results obtained from the many parametric fitting procedure depend on $L_{\text{min}}$ indicates that the fitting function (8) is still insufficient to reflect completely the corrections to scaling. The only way to obtain a more accurate estimation of the critical parameters is to collect more exact numerical data for large system size.

To conclude, we have collected numerical data for the quasi one dimensional Anderson model up to system size $L = 24$. Our data prove that higher Lyapunov exponents of the transfer matrix follow the one-parametric scaling law. The critical exponent $\nu$ coincides with that calculated from the scaling treatment of the smallest LE. The scaling holds only for Lyapunov exponents
which are smaller than the system size considered.

The common scaling enables us to express all relevant LEs as the unique function of the first one. Evidently, the same holds also for any function of zs. This indicates the validity of the scaling theory for the conductance. However, our analysis was restricted to the quasi-one dimensional systems. Rigorous proof of the one-parametric scaling of the conductance requires repeating the performed scaling analysis for the cubic samples, where no self-averaging of zs and of g takes place.

We show for the first time, that the numerical data for higher LE could be used for calculation of critical parameters of the metal-insulator transition. The numerical accuracy of higher LE is much better than that of $z_1$. The price we pay for it is a stronger influence of the finite-size effects which causes that the data obtained for small system size cannot be used for the scaling analysis. The best compromise between the accuracy and FSE offer data for the second LE $z_2$. We discussed the methods of elimination of the finite size effects and estimated the critical disorder and the critical exponent $\nu$ by relation (3).

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Table 1: Critical disorder $W_c$ and critical exponent $\nu$ as have been found from numerical data for the $j$th LE for the three-parametric and two-parametric fits (*) and their comparison with other results. Number of analyzed points is $\approx 21 \times (L_{\text{max}} - L_{\text{min}})$. The minimum of $F$ was found $\leq 1.05$ for all analyzed sets (with exception of $z_3$, where it was 1.09).

| $j$ | $L_{\text{min}}$ | $L_{\text{max}}$ | $W_c$ | $z_{jc}$ | $\alpha$ | $\nu$ | $\beta$ |
|-----|------------------|------------------|-------|----------|---------|-------|-------|
| 1   | 4-5              | 24               | 16.515| 3.46     | 0.644   | 1.55  | -3.5  |
| 1*  | 8-12             | 20-24            | 16.505| 3.451 (07)| 0.681 (15) | 1.470 (30) | -    |
| 2   | 5-10             | 24               | 16.527| 5.588 (02)| 0.654 (08) | 1.529 (18) | -3.2 (6) |
| 2*  | 10-12            | 22-24            | 16.500| 5.500 (07)| 0.659 (05) | 1.517 (11) | -    |
| 3   | 9                | 24               | 16.508| 7.167     | 0.647   | 1.545 | -6.0  |
| 4   | 8-10             | 24               | 16.504| 8.422 (05)| 0.663 (04) | 1.509 (9) | -3.7 (2) |
| 5   | 9-12             | 24               | 16.517| 9.560 (30)| 0.661 (06) | 1.513 (14) | -3.3 (8) |

*1 [4-12] 16.500 (50) 1.515 (33)
*1 [6] 16.448 (14) 1.59 (3)
*1 [4] 16.540 (10) 1.57 (2) -2.8 (5)
*1 [8] 16.514 (07) 1.58 (5) -
Figure 1: The $W$-dependence of the second LE $z_2$ for different system size.
Figure 2: The $L$-dependence of $z_j^{(1)}$ for the first six LE and for $z_0$ (counted from below). The slope determines critical exponents as $\alpha = 1/\nu$. Inset: values of $1/\nu$ found from presented fits.