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LETTER TO THE EDITOR

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

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

Our contemporary understanding of the disorder-induced metal–insulator transition (MIT) is based on the scaling theory of localization [1]. It is believed that MIT is universal, independent on microscopic details of the model, and that its complete description requires only one relevant parameter, e.g. the conductance g of the system.

In spite of its success and elegance, the one-parametric scaling theory still requires thorough verification. The main problem is the absence of self-averaging of the conductance in a neighbourhood of the critical point [2, 3]. A complete scaling analysis requires therefore knowledge of the system-size dependence of the whole conductance distribution [4–6]. As no remarkable progress has been achieved in solving this problem yet, the existence of another relevant scaling parameter(s) can be neither confirmed nor excluded.

To avoid statistical fluctuations, numerical analysis of MIT concentrates on the quasi-one-dimensional (Q1D) systems. Here, the scaling behaviour of the smallest positive Lyapunov exponent (LE) z_1† was proposed as

$$z_1(L, W) = f(L/\xi(W)) \tag{1}$$

in [7] and proven numerically in [8]. In (1), W is the disorder, L defines the width of the Q1D system $L \times L \times L_z$ and $\xi(W)$ is the universal scaling parameter. In Q1D geometry, we define Lyapunov exponents z_i by the eigenvalues t_i of the transfer matrix T as $z_i = 2\frac{L}{L_z} \log t_i$. This definition of LEs differs from the standard one by the multiplicative factor $2L$ which guarantees that zs are functions of only one parameter. In the limit $L_z >> L$, all zs are self-averaged quantities [9]. The scaling parameter $\xi(W)$ diverges as $(W_c - W)^{-s}$ for $W \to W_z^-$ and as $(W - W_c)^{-\nu}$ for $W \to W_c^+$. Here, s and ν are critical exponents for the conductance and the localization length, respectively [10]. For the three-dimensional systems, $s = \nu$ [11].

† 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 are more natural variables for our purposes.

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The finite-size scaling (FSS) analysis of the numerical data for $z_1(L, W)$ enables us to determine the critical disorder W_c and the critical exponents [8,10,12–15]. In [8], the estimation of the critical parameters for the Anderson model with the box distribution of random energies were found to be $W_c \approx 16.5 \pm 0.5$ and $s = \nu \approx 1.5 \pm 0.1$. These results were later confirmed by the more accurate numerical studies [12,13], and also by the analysis of the level statistics [16]. The calculations performed for different microscopic models confirmed the universality of the exponent ν within a given universality class [14].

In this Letter we test the one-parametric scaling theory by the analysis of the scaling behaviour of higher LEs. We present numerical data for LEs $z_2, z_3, \ldots z_9$ and prove numerically that they follow the same scaling behaviour as z_1 in the Q1D systems. This proves that the lower part of the spectra of the transfer matrix in the Q1D limit is determined only by one scaling parameter. The collected numerical data also provides us with a very accurate estimation of the critical disorder W_c and the critical exponent ν. It is the first time that numerical data for system size $L > 16$ have been calculated and analysed. Our data for large L enable us also to check the finite-size corrections to the scaling proposed in [13].

The scaling behaviour of higher LEe has already been studied by Henneke in his PhD thesis [15]. Owing to insufficient accuracy of his data, no acceptable proof of the common scaling was found. More is known about the spectrum of LE. The linear dependence, $z_i \sim i$, is well known in the metallic regime; it was used in [8] to explain the physical meaning of the scaling parameter $\xi(W)$. Although the spectrum of LE is no more linear for stronger disorder [17], numerical data indicate that the ith LE, z_i, is still a simple function of index i. In particular, relation $z_i^2 \sim i$ was found at the critical point in 3D systems [18] and generalized to the neighbourhood of the critical point [19,20]. In the localized regime, zs follow the relation $z_i(W, L) = z_1(W, L) + \Delta_i$, where Δ_i depend neither on disorder W nor on the system size L [19].

To find the relation between zs (calculated numerically for very long Q1D models) and transport properties of real physical systems, the L_z dependences of all LEs were studied [21]. It was shown that although z_i itself depends on L_z, the qualitative form of the spectrum of LEs is the same for cubes and for bars. Of course, the statistical properties of the zs become important for L_z comparable to L. In the weak-disorder limit, the statistics of zs is understood and described by random-matrix theory (RMT) [22].

For Q1D systems $L^2 \times L_z$ we calculated all LEs for 21 different values of disorder $W = 16.00, 16.05, 16.10, 16.15, \ldots, 16.95, 17.00$. L increases from $L = 4$ up to 24. The relative accuracy $\varepsilon_1 = \sqrt{\mathrm{var} z_1}/z_1$ of the smallest $z_1(W, L)$, was 0.05% for $L \leqslant 12$, 0.5% for $L = 16$, 18 and 1% for $L = 21$, 22 and 24. The accuracy of the higher LE is much better; in particular, $\varepsilon_2 \approx \varepsilon_1/2$ and $\varepsilon_9 \approx 0.17\varepsilon_1$ for each system size.

The interval of the disorder is narrow enough to approximate the W dependence of the zs by the linear fit

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

The higher-order corrections to the linear fit (2) are negligible. Even in systems with $L > 18$ they do not exceed the numerical inaccuracy of the raw data. The typical W dependence of our data is presented in figure 1 for z_2.

Scaling theory provides us with the expansion of z_j in the neighbourhood of the critical point [23]

$$z_j(W, L) \approx z_{jc} + A \times (W - W_c) \times L^{\alpha} \qquad \alpha = 1/\nu. \tag{3}$$

Thanks to the linear W dependence of the zs (figure 1), we can neglect all higher order terms in the expansion (3). The comparison of (2) and (3) offers the simplest way to estimate the

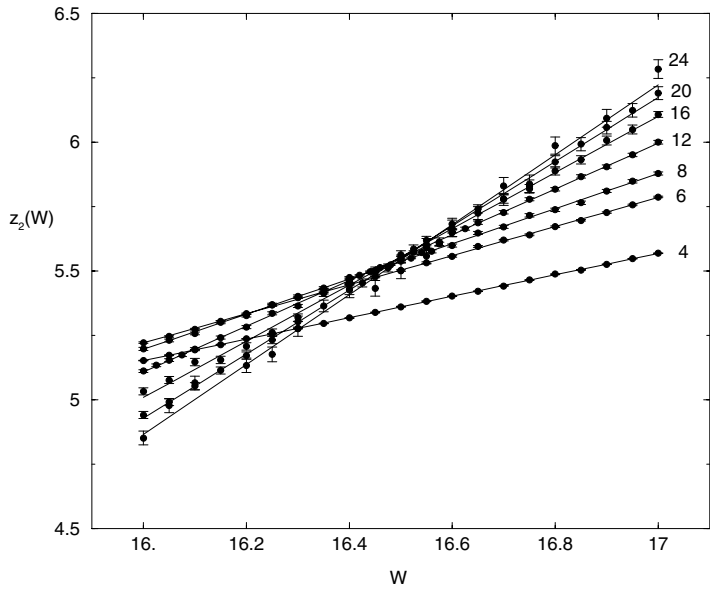

Figure 1. The W dependence of the second LE, z_2, for different system size.

critical exponent α. In figure 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 α:

$$\alpha \approx 0.655 \pm 0.010 \tag{4}$$

which determines $\nu = 1.526 \pm 0.023$. This estimation is in a very good agreement with the result of MacKinnon [12] and differs slightly from [4, 13] (see table 1). A more detailed method of the estimation of α will be discussed below.

Table 1. Critical disorder W_c and critical exponent ν as found from numerical data for the jth LE for the three-parametric (3) and two-parametric (8) fits (*) and their comparison with results of other authors. The number of analysed points is $\sim 21 \times (L_{max} - L_{min})$. The minimum of F was found to be $\leqslant 1.05$ for all analysed sets (with exception of z_3, where it was 1.09).

j	L_{min}	L_{max}	W_c	z_{jc}	α	ν	β
1	4–5	24	16.515	3.46	0.644	1.55	−3.5
1*	8–12	20–24	16.505 (10)	3.451 (07)	0.681 (15)	1.470 (30)	—
2	5–10	24	16.527 (02)	5.588 (02)	0.654 (08)	1.529 (18)	−3.2 (6)
2*	10–12	22–24	16.500 (07)	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 (02)	8.422 (05)	0.663 (04)	1.509 (9)	−3.7 (2)
5	9–12	24	16.517 (16)	9.560 (30)	0.661 (06)	1.513 (14)	−3.3 (8)
1 [12]	4	12	16.500 (50)			1.515 (33)	
1 [13]	6	12	16.448 (14)			1.59 (3)	
1 [4]	4	14	16.540 (10)			1.57 (2)	−2.8 (5)
1* [4]	8	14	16.514 (07)			1.58 (5)	—

Figures 1 and 2 show also the important influence of the finite-size effects (FSE) in the present analysis. We see that the small-L data are of no use in the analysis of higher LEs. We

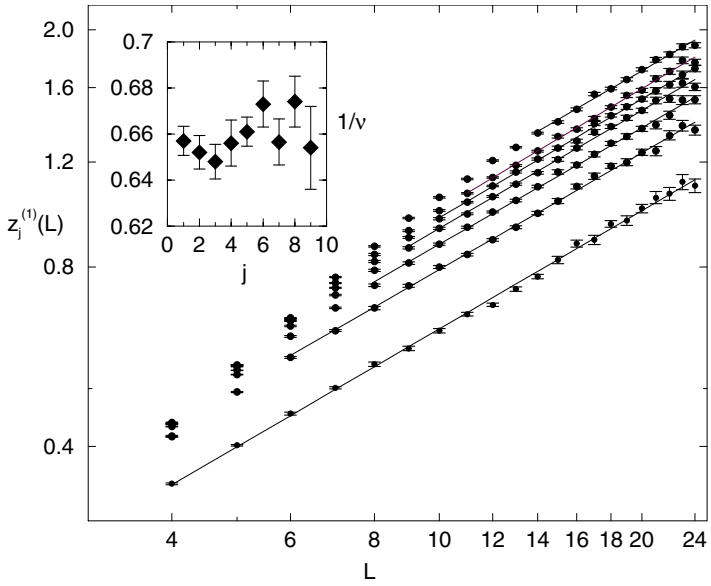

Figure 2. The L dependence of $z_j^{(1)}$ for the first six LEs and for z_9 (counted from below). The slope determines critical exponents as $\alpha = 1/\nu$. Inset: values of $1/\nu$ found from presented fits.

found that the numerical data for z_j could be used only when

$$L > z_j. \tag{5}$$

This is easy to understand. If $z_j > L$ then the jth channel is rather 'localized' than critical on this length scale. Therefore only a small part of the spectrum which fulfils relation (5) follows the scaling behaviour. The rest of the spectrum depends on L even at the critical point. This conclusion is supported also by analysis of the density $\rho(z)$ of all LEs for cubic samples [24]. At the critical point, the number of system-size independent LEs grows as $\sim L$ when $L \to \infty$ [20]. 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 [13, 25].

A more reliable estimation of the exponent α (4) and of the critical disorder W_c is given by the position of the minimum of the function

$$F(W_c, \alpha, \ldots) = \frac{1}{N} \sum_{W,L} \frac{1}{\sigma_j^2(W, L)} \big[z_j(W, L) - z_j^{\text{fit}}(W, L) \big]^2. \tag{6}$$

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

The natural choice of the fitting function z_j^{fit} in (6) is the RHS of equation (2). None of the FSE are explicitly included in (2). Nevertheless, it still enables us to test the sensitivity of the critical parameters to the size of the analysed systems. To do so, we considered different sets of input data $z_j(L, W)$ with the restriction $L_{\min} \leqslant L \leqslant L_{\max}$ ($L_{\min} \leqslant 12$). Then, the $L_{\min}$- and $L_{\max}$- dependences of W_c and α were analysed. While the influence of the choice of $L_{\max}$ is, as supposed, negligible, both W_c and z_{jc} increase with $L_{\min}$. We found $L_{\min}$ - 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 $L_{\min} = 12$. The estimation of the critical exponent α does not depend on the choice of interval of L. The obtained data are in good agreement with the estimation (4) for all LEs under consideration.

The weak $L_{\min}$ sensitivity of the critical exponent agrees with the assumption that FSE influence primarily the W-independent part of z_j [12]. Figure 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 'higher order'.

Slevin and Ohtsuki [13] fitted $z_1(W, L)$ (resp. its inverse z_1^{-1}) to the more general function

$$z_1^{\text{fit}}(L, W) = z_{jc} + \sum_{n=0}^{N_x} \sum_{m=0}^{N_y} A_{nm} x^n y^m \tag{7}$$

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 β represents the second critical (irrelevant) scaling exponent. We fit our data to function (7) with $b_1 = b_2 = 0$ and $n + m \leqslant 1$:

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

More sophisticated fits do not provide us with any reasonable improvement of the accuracy of the 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 $L_{\min}$ large enough the role of the irrelevant scaling exponent is negligible. The finite-size effects become small and difficult to measure. The value of the irrelevant critical exponent β obtained from the fitting function (8) decreases to ~ -20 for large $L_{\min}$.

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

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

$$16.50 \leqslant W_c \leqslant 16.53 \qquad \text{and} \qquad 1.50 \leqslant \nu \leqslant 1.54. \tag{9}$$

These values are in a very good agreement with [12].

Our results (9) differ from those obtained by the many-parametric fitting procedure in [13] (table 1.). None of the analysed statistical ensemble provides us with such a high value of ν. This discrepancy is probably caused by different input data. Contrary to previous treatments [12, 13], we collected data for large system size in order to simplify the fitting function. The main disadvantage of this strategy is 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 $L_{\min}$ indicates that the fitting function (8) is still insufficient to reflect the corrections to scaling completely. The only way to obtain 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 ν 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 a unambiguous function of the first one. Evidently, the same holds also for any function of the zs. This indicates the validity of the one-parameter scaling theory.

We show for the first time, that the numerical data for the higher LEs could be used for calculation of the critical parameters of the metal–insulator transition. The numerical accuracy

of higher LEs is much better than that of z_1. The price we pay for it is a stronger influence of the finite-size effects which means 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 have discussed methods of eliminating the finite-size effects and have estimated the critical disorder and the critical exponent ν by relation (9).

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