Universality of the metal-insulator transition in three-dimensional disordered systems

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The universality of the metal-insulator transition in three-dimensional disordered system is confirmed by numerical analysis of the scaling properties of the electronic wave functions. We prove that the critical exponent \( \nu \) and the multifractal dimensions \( d_q \) are independent on the microscopic definition of the disorder and universal along the critical line which separates the metallic and the insulating regime.

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One of the main problem of the disorder induced metal-insulator transition (MIT) is the proof of its universality. In the pioneering work [1], it was conjectured that if the sample size exceeds all the length parameters of the model, then the conductance, \( g \), is the only parameter which governs MIT. This scaling hypothesis has been confirmed by various numerical analysis, with the help of the finite-size scaling [2, 3]. Generally accepted scenario of the Anderson localization is that disorder broadens the conductance band. Electron states in the tail of the band become localized, separated from delocalized (metallic) states by the mobility edges, \( E_c \). System exhibits the MIT if the Fermi energy, \( E_F \), crosses the mobility edge. With increased disorder, \( E_c \) moves towards the band center. There is a critical value of the disorder, \( W_c \), for which \( E_c \) reaches band center, \( E_c = 0 \). For disorder \( W > W_c \), all electronic states inside the band become localized. Phase diagram in the energy-disorder plane was calculated in [4] and is schematically shown in the upper panel of Fig. 1.

At the band center, \( E = 0 \), the universality of the MIT was confirmed by detailed numerical analysis of the disorder and system size dependence of Lyapunov exponents in quasi-one dimensional systems [5, 6], mean conductance [7], conductance distribution [8], and level statistics [8, 9]. These studies determined the value of the critical exponent \( \nu \), which determines the divergence of the correlation length, \( \xi \sim \left| W - W_c \right|^{-\nu} \), as \( \nu = 1.57 \pm 0.02 \) [8, 9]. The analysis of MIT along the critical line (non-zero energy \( E \)) is more difficult because the critical region is narrower and finite size effects are stronger [10]. Critical exponent, \( \nu_c \), was obtained only in models with random hopping [11], and very recently in [12].

In this paper, we present numerical proof of the universality of MIT. By scaling analysis of the electronic wave functions in the vicinity of two critical points, shown in the upper panel of Fig. 1, we prove that the critical exponent \( \nu \) and fractal dimensions \( d_q \) of the wave function (defined below) are universal along the critical line.

Electron eigenenergies and wave functions are calculated for three-dimensional Anderson Hamiltonian,

\[
\mathcal{H} = W \sum_r \varepsilon_r c_r^\dagger c_r + \sum_{\langle rr' \rangle} c_r^\dagger c_{r'},
\]

where \( r \) counts the sites of the three-dimensional (3D) lattice of the size \( L^3 \), \( \varepsilon_r \) is the random energy distributed either with the Box distribution, \( P_B(\varepsilon) = (2/W)\Theta(W/2 - |\varepsilon|) \) or with the Gaussian distribution, \( P_G(\varepsilon) = \sqrt{2\pi W^2} \exp\left(-\varepsilon^2/2W^2\right) \). Parameter \( W \) measures the strength of the disorder. For \( E = 0 \), the critical disorder \( W_c \approx 16.5 (6.15) \) for the Box (Gauss) distribution of random energies, respectively.

The quantities of interest are inverse participation ratios (IPR), \( I_q(E_n) \). By definition, [13]

\[
I_q(E_n) = \sum_r |\Phi_n(r)|^{2q}.
\]

FIG. 1: (Color online) Top panel shows schematic phase diagram for 3D Anderson model. Solid line separates metallic (shaded area) and localized states. Open circles shows the position of critical points studied in this paper. Note that the mobility edge, \( E_c \), lies outside the unperturbed energy band. Two bottom panels present numerical data for \( I_2 \), given by Eq. (2) for cubes of the size \( L = 8 \) (middle) and \( L = 16 \) (bottom) and with Gaussian disorder \( W = 2 = 0.325 W_c \). In the metallic region, \( I_2 \) decreases when \( L \) increases, while \( I_2 \) becomes \( L \)-independent in the tail of the band, where electronic states are localized.
Here, $E_n$ and $\Phi_n(r)$ is the $n$th eigenenergy and eigenfunction of the Hamiltonian $H$, respectively.

The size dependence of IPR indicates the character of the eigenstate. If the $n$th eigenstate is conductive, the wave function is distributed throughout the sample and $|\Phi_n(r)| \propto L^{-d/2}$. Inserting in Eq. (2) we obtain that $I_q(E_n) \propto L^{d(1-\eta)}$. For localized state, $\Phi_n(r)$ is nonzero only in a small region, where $|\Phi_n(r)| \sim 1$. Hence, $I_q(E_n) \sim 1$, too. These size dependences are shown in two bottom panels of Fig. 1.

Different size dependence of $I_q(E)$ enables us to use IPR as a scaling variable for the calculation of the critical parameters in the same way as Lyapunov exponents \(2\), the conductance $\nu$ \(3\), or level statistics $\nu$ \(4\). However, in contrast to the Lyapunov exponent or mean conductance, IPR is not a size independent constant at the critical point, but decreases as

$$I_q(E = E_c) \sim L^{-d_q},$$

where $d_q$ are fractal dimensions. This makes the scaling analysis slightly more difficult. On the other hand, fractal dimensions, $d_q$, represent a new set of parameters, which can be used for the verification of the universality of the MIT. We expect that $d_q$ are universal constants for all critical points along the critical line.

The energy spectrum of the Hamiltonian depends on the system size, $L$, and on the microscopic details of the disorder in a given sample. Therefore, we have to calculate an average values, defined as follows. For each system size, we consider a statistical ensemble of $N_s$ samples which differ only in the realization of random energies, $\epsilon_r$. For each sample, we calculate all eigenenergies, $E_n$, lying in a narrow energy interval, $E - \delta, E + \delta$, and calculate corresponding $I_q(E_n)$. For the $i$th sample, the number of eigenstates, $n_i$, depends on the microscopic realization of the disorder. Also, since the values of $I_q$ might fluctuate in many orders in magnitude in the critical region \(13\) (these fluctuations are shown in Fig. 6), it is more convenient to study logarithm of $I_q$. Thus, our scaling variable is then defined as

$$Y_q(E) = \frac{1}{N_{\text{stat}}} \sum_i \sum_{|E_i - E| < \delta} \ln I_q(E_n), \quad (4)$$

where $N_{\text{stat}} = \sum_i n_i$. In our calculations, $N_{\text{stat}} \sim 10^5$ ($5 \times 10^5$ for $L \geq 50$) and $\delta = 0.025$. With these parameters, we calculate $Y_q(E)$ with relative accuracy better than 0.2%. Numerical data were collected by LAPACK subroutines for $L \leq 16$. For larger system size ($L \leq 54$) we use our own program based on the Lanczos algorithm.

We expect that $Y_q$ is a good scaling variable, so that it behaves in the vicinity of the critical point as

$$Y_q(E, L) = Y_q^c - d_q \ln L + A(E - E_c) L^{1/\nu}, \quad (5)$$

for the fixed disorder $W_c$, and

$$Y_q(W, L) = Y_q^c - d_q \ln L + A(W - W_c) L^{1/\nu}, \quad (6)$$

for the fixed energy $E = 0$.

For a given $q$, we fit obtained numerical data for $Y_q$ to Eqs. (5) or (6). Obtained results are in Figs. 2, 3 and 4. Typical data for $q = 2$ and $q = 5$ are given in Table I.

Figure 2 shows the $L$-dependence of $Y_5$ for Gaussian disorder $W_2 = 2$ and for energies close to the critical energy, $E_c \approx 6.58$. We see that at the critical point,

![Figure 2](image.png)

FIG. 2: (Color online) $Y_5(E, L)$ as a function of system size $L$ for various energies $E = 6.50, 6.55, \ldots, 6.60$ (from bottom to top). Thin solid lines are fits, Eq. (5). Thick solid line is $(\ln I_5) = Y_5^c - 4 d_5 \ln L$ (Eq. (1) for the critical energy $E_c \approx 6.58$. The same fit for other three critical points are also shown (described by legend). Data confirm universal $L$-dependence of $Y_5$ for three critical points. The different behavior for the critical point $BE_c$ is due to strong finite-size effect, discussed in the text.

| $q$ | $E_c$ | $W_c$ | $\nu$ | $d_q$ | $L_{\text{min}}$ | $L_{\text{max}}$ |
|-----|------|------|------|------|----------------|----------------|
| 2   | 6.50 | 2    | 0.64 | 0.38 | 3.10           | 4.54           |
| 5   | 6.50 | 2    | 0.64 | 0.38 | 3.10           | 4.54           |
| 2   | 6.50 | 5    | 0.64 | 0.38 | 3.10           | 4.54           |
| 5   | 6.50 | 5    | 0.64 | 0.38 | 3.10           | 4.54           |

TABLE I: Critical exponent, $\nu$, and fractal dimensions, $d_q$, calculated by scaling analysis of the inverse participation ratio, $I_q$, for four critical points. Calculated position of critical points, $E_c$, $W_c$, is given in the 3rd column. $GW_c$ - Gaussian disorder, band center, $GE_c$ - Gaussian disorder, band tail, $BW_c$ - Box disorder, band center, $BE_c$ - Box disorder, band tail. Data for system of the size $L_{\text{min}} \leq L \leq L_{\text{max}}$ were used in the scaling analysis.
\( E = E_c, \quad Y_q(E_c) \) decreases logarithmically,

\[
Y_q(E_c, L) = Y_q^c - d_q \ln L,
\]

in agreement with Eq. (4). Outside the critical point, the \( L \) dependence of \( Y_q \) changes due to the presence of the term \( \sim (E - E_c) L^{1/\nu} \). Similar analysis, performed for other critical points confirms the universality of the relationship (7). This indicates that parameters \( Y_q^c, d_q \) and \( A \) are universal.

There are two sources of inaccuracy of the scaling analysis: (i) if the critical region is not sufficiently narrow, then the linear term \( \sim E - E_c \) could not be sufficient to describe a correct \( E \)-dependence of numerical data and higher order terms of the expansion (5) must be considered. To test the accuracy of the linear approximation, we add also cubic term, \( \sim (E - E_c)^3 \) in Eq. (6). We found that such correction does not influence obtained critical parameters and might be neglected. (ii) for small system size, \( L \), the variable \( Y_q \) suffers from finite-size effects (FSE) [2]. The role of FSE can be estimated by the scaling analysis for data of restricted system size, \( L \geq L_{\text{min}} \).

For three critical points, \( GE, GW, \) and \( BW \); the position of critical points is given in Table I, we found that data for \( L > L_{\text{min}} \sim 16 \) are already free of FSE. However, we were not able to obtain reliable critical parameters for the critical point \( BE_c \). As shown in Table I and Fig. 2, our numerical data for this critical point are still far from limiting values. For this critical point we can only demonstrate the convergence of critical parameters to expected universal values when \( L_{\text{min}} \) increases (inset of Fig. 3). Larger samples are necessary to prove this convergence numerically.

Figure 3 summarizes our data for fractal dimensions, \( d_q \). Data confirm that the spatial distribution of the wave function is universal, independent on the position of the critical point along the critical line. Presented data for \( d_q \) are in agreement with previously reported values [10].

Figure 4 presents obtained data for the critical exponent, \( \nu \). We see that \( \nu \) converges to the generally accepted value, \( \nu \sim 1.57 \) [2, 4], when either \( L_{\text{min}} \) or \( q \) increases. In order to show the effect of the system size, we plot for each value of \( q \) a few data obtained with increasing minimal system size used in the scaling procedure. Inset of Fig. 4 presents our data for the critical point \( BE_c \). Because of strong finite-size effects, much larger systems are necessary for the estimation of reliable values the critical exponent.

To understand the origin of the FSE, we calculated the density of states, \( \rho(E) \), in the critical region of all four critical points. As shown in left Fig. 4 \( \rho(E = 0) \) changes only in a few \% when disorder varies around the critical value, \( W_c \). Contrary to the band center, the density \( \rho(E) \) around the mobility edge \( GE_c \) decreases significantly (almost by factor of two) in the critical region (right Fig. 5). In the case of critical point \( BE_c \), this decrease is even more significant. Intuitively, one expects that the one-parameter scaling works better when electronic states inside the critical region have the same, or at least comparable, density. Since the interval of energies, \( \Delta E = 0.3 \), used in the case of \( GE \) is already sufficient to correct correct critical parameters, we expect that the the energy interval for \( BE \) must be \( \Delta E \approx 0.2 \). However, narrower interval of energies requires larger system.
The universality of the spatial distribution of the critical wave function is confirmed also by Fig. 6 which shows the probability distribution of \( \ln I_q \) for three critical points, \( GE_c, GW_c \) and \( BW_c \). The width of the distribution, \( \sigma_q = \sqrt{\text{var} \ln I_q} \approx 3.4 \), is close to the limiting value reported in Ref. [17]. However, the distribution \( P(\ln I_q) \) is not system size invariant. The mean value of \( \ln I_q \) decreases when system size increases, while the distribution always possesses a long tail for \( \ln I_q \sim 1 \).

In conclusion, we investigated numerically the wave function of electron in the critical regime of the metal-insulator transition. By the scaling analysis of the logarithm of the inverse participation ratio, \( I_q \), we calculated the critical exponent, \( \nu \), and fractal dimensions, \( d_q \). We found that these parameters depend neither on the microscopic details of the disorder nor on the position of the critical point. This result confirms that the metal-insulator transition is universal along the critical line which separates metallic and insulating regimes.

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