

# FINITE SIZE SCALING ANALYSIS OF DISORDERED ELECTRON SYSTEMS

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## 1. Introduction

The quantum mechanics defines two possible eigenstates of the quantum particle: in the *extended* state the particle can propagate freely across the system, while in the *bound* state the particle is trapped in the vicinity of the potential minima. In 1958 P. W. Anderson [1] proved that in disordered systems also the third quantum state exists in which the particle is *localized*. The physical origin of the localization consists in the wave character of the propagation as a consequence of the interference of various components of the wave function, scattered on random impurities. Although the particle in the localized state is spatially localized, the center of the localization is not given by any potential minima.

The most simple quantum model which enables us to investigate localization is the disordered tight binding model, which describes the propagation of electron on the disordered  $d$ -dimensional lattice:

$$E\phi(\vec{r}) = W\epsilon(\vec{r})\phi(\vec{r}) + V\sum_{\vec{r}'}\phi(\vec{r}') \quad (1)$$

In the model, electron hops from one lattice position  $\vec{r}$  to the neighboring position  $\vec{r}'$ . The random potential  $\epsilon(\vec{r})$  ( $|\epsilon(\vec{r})| \leq 1/2$ ) mimics the disorder.  $W$  measures the disorder strength. For zero disorder,  $W = 0$ , the model describes the propagation of electron on the  $d$ -dimensional regular lattice with energies  $E$  from the conducting band  $-2d \leq E/V \leq +2d$ . For non-zero values of  $W$ , the electron still can hop from one lattice site the neighboring one. Since these sites possess different potentials  $\epsilon(\vec{r})$ , the electron propagation at long distances is more difficult than on the regular lattice. Anderson proved that for each value of  $W$  there exists the energy  $E_c$  (mobility edge) such that electron propagation is possible only for energies  $|E| < E_c$  and all electronic states with energies  $|E| > E_c$  are localized [2]. Further increase of the disorder causes decrease of  $E_c$ . For the critical value  $W = W_c$  the mobility edge  $E_c$  reaches the band center ( $E_c = 0$ ) and all electron states are localized. Phase diagram in the  $E - W$  plane is shown the Fig. 1.

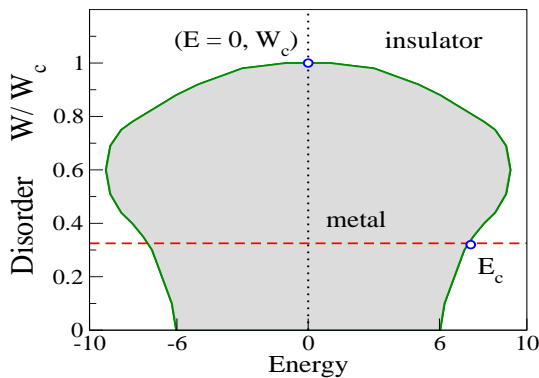


Fig. 1: Phase diagram of the disordered electron system in the energy-disorder plane. The system is either metallic (electron can move through the sample) or insulator (electron is localized). Solid line between the regions of the metallic and the insulating regime is a critical line of the metal-insulator transition. Shown are also two critical points discussed in Sect. 4.

Owing to the randomness of the model (1), any physical quantity of interest  $X$  is a statistical variable which fluctuates as a function of the realization of the disorder. We have to consider large statistical ensemble of disordered samples which differ only by the realization of random energies  $\epsilon$ , and to calculate the probability distribution  $P(X)$ . The distribution  $P(X)$  is in general not self-averaging, but converges to the size-independent functions [3]. As an example, we show in Fig. 2 the probability distribution of the electron conductance (defined below by Eq. 4) for the three dimensional disordered model (Eq. 1) at the critical point  $E = 0$ ,  $W = W_c$  shown in Fig. 1.

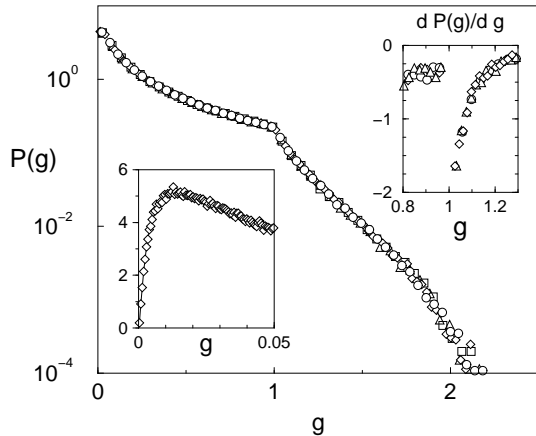


Fig. 2: The probability distribution  $P(g)$  of the electron conductance at the critical point calculated numerically for three dimensional cubes  $L \times L \times L$  with  $L = 10, 12, 14$  and  $18$ . Note the logarithmic scale on the vertical axis. Insets show that  $P(g) \rightarrow 0$  when  $g \rightarrow 0$  and that  $P(g)$  is not analytic for  $g = 1$  [3]. Both the distribution  $P(g)$  and the mean conductance  $\langle g \rangle$  depend on the boundary conditions even in the limit of infinite system size  $L$ .

Analytical description of the transport in disordered systems is possible only in the limit of weak disorder. For strong disorder, the relevant data can be calculated numerically for finite size of the system. The extrapolation to the infinite system size is possible with the use of the *finite size scaling method* [4].

In this paper, we describe in Sect. 2 the finite size scaling method and demonstrate its application to the analysis of two different physical quantities: the conductance of the two dimensional system with spin-dependent hopping term  $V$  (Sect. 3) and the electron wave function in the three dimensional model (Sect. 4). We show that known numerical data enable us to described quantitatively the critical regime of the metal-insulator transition.

## 2. Scaling analysis and universality

Any physical variable  $X$  is a function of system parameters and the size  $L$ . Scaling analysis assumes that in the vicinity of the critical point  $X$  becomes the function of only one parameter, namely the ratio of the system size  $L$  and the correlation length  $\xi$ ,

$$X = X(L/\xi). \quad (2)$$

The correlation length  $\xi$  diverges to infinity at the critical point,

$$\xi(\tau) \sim |\tau|^{-\nu}. \quad (3)$$

Parameter  $\tau$  measures the closeness to the critical point:  $\tau = E - E_c$  or  $W - W_c$ , and  $\nu$  is the critical exponent. The scaling theory predicts that the metal-insulator transition is universal: the value of the critical exponent  $\nu$  depends only on the dimension  $d$  and the physical symmetry of the model.<sup>1</sup> Our main task is the estimation the critical exponents of various models and verification of the universality of the metal-insulator transition.

<sup>1</sup>For instance, additional magnetic field breaks the time reversal symmetry, therefore systems with and without magnetic field possess different values of  $\nu$ .

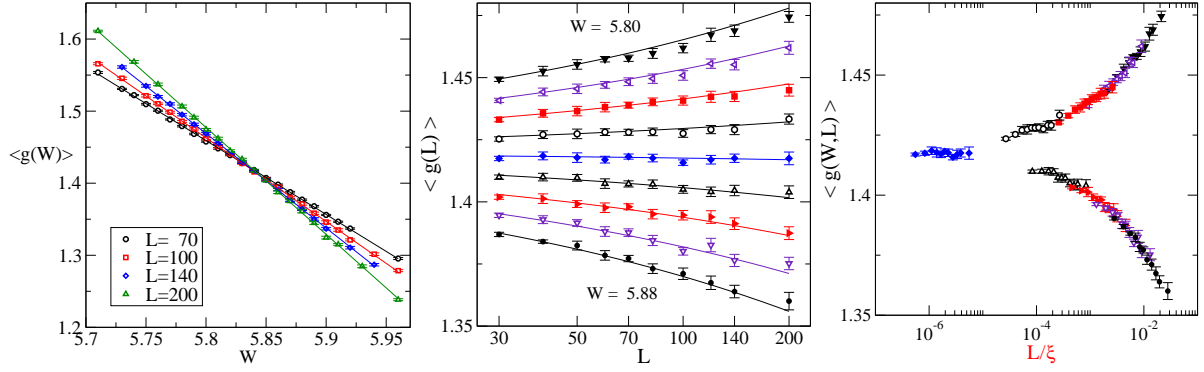


Fig. 3: *Two dimensional model with spin variable hopping. The energy of the electron is  $E = 0$  (band center). Left: The mean conductance as a function of the disorder for four values of the size of the system. Note that the conductance does not depend on the size  $L$  when  $W = W_c \approx 5.84$ . Middle: The mean conductance as a function of the size of the system  $L$  for a few fixed values of  $W$ . In the metallic (insulating) regime, mean conductance increases (decreases), respectively, when the size of the system  $L$  increases. At the critical point,  $\langle g \rangle$  is constant, in agreement with the scaling assumption. Right Figure demonstrates that the mean conductance is a function of ratio  $L/\xi$ , in agreement with the scaling relation (2).*

### 3. Mean conductance of two dimensional disordered models

The most important variable which characterizes the electron transport in disordered systems is the conductance  $G$ . Using the Economou-Soukoulis formula [5]

$$G = \frac{e^2}{h} g, \quad g = \frac{e^2}{h} \text{Tr } t^\dagger t, \quad (4)$$

the conductance can be expressed in terms of transmission amplitudes  $t$  which determine the probability that the electron propagates through the sample. The last can be calculated by the transfer matrix method [6]. In two dimensional systems, the mean conductance equals to the conductivity.

We calculate numerically the dimensionless conductance  $g$  for the two dimensional model with spin dependent hopping term  $V$  [7]<sup>2</sup>. The left and the middle Fig. 3 confirm that the mean conductance  $\langle g \rangle = g_c$  does not depend on the size of the system at the critical point  $W \approx 5.85$ . When expanding Eq. (2) in powers of  $L/\xi \ll 1$ , we obtain with the use of Eq. (2)

$$\langle g(W, L) \rangle = g_c + A \frac{L}{\xi(W)} + \dots = g_c + A(W - W_c)L^{-1/\nu} + \dots \quad (5)$$

Left Fig. 3 shows that indeed the mean conductance  $\langle g \rangle$  is a linear function of  $W$  in the vicinity of the critical point. Since  $W - W_c$  changes its sign when  $W$  crosses  $W_c$ , we expect that  $\langle g \rangle$  as a function of  $L$  increases (decreases) when the system is insulator (metal). This is shown in middle Fig. 3. Right Figure 3 shows that the mean conductance depends only on one parameter  $L/\xi$ , in agreement with the scaling theory. Detailed analysis of the data enables us to calculate the critical exponent [6]

$$\nu = 2.80 \pm 0.04 \quad (6)$$

<sup>2</sup>In this model, two orientations of electron spin must be considered. The random potential  $\epsilon$  does not depend on spin but electron can change the orientation of spin when hops from one site to the neighboring one. Therefore, the hopping term  $V$  in Eq (1) is a  $2 \times 2$  matrix.

Two dimensional disordered models with constant spin independent hopping term  $V$  do not possess the metallic phase [7]. The critical disorder is zero,  $W_c = 0$ . Consequently, for any non-zero value of the disorder the mean conductance should decrease with increasing size of the system. Numerical data shown in Fig. 4 seem to contradict this prediction. An increase of the mean conductance with increasing  $L$ , observed for weak disorder, resembles the metallic phase. However, this increase is *the finite size effect*. The scaling behavior described by Eq. (2) is namely observable only when the size of the system  $L$  increases over any characteristic length of the system. In the present model, the electron mean free path  $\ell \sim W^{-2}$  is extremely large when the disorder  $W$  is small. The decrease of the mean conductance, predicted by the scaling theory, is observable only for large size of the system  $L \gg \ell$ . For instance, Fig. 4 shows that for the disorder  $W = 2$  the mean conductance  $\langle g \rangle$  decreases only when the size of the system  $L \geq 200$ . For  $W = 1$ , the expected decrease of  $\langle g \rangle$  starts at  $L \approx 800$ .

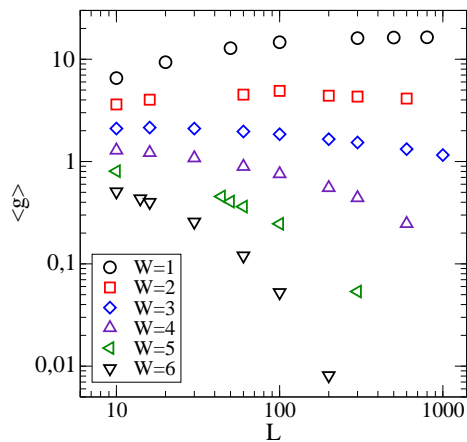


Fig. 4: The system size dependence of the mean conductance of the two dimensional model defined by Eq. (1). Note the logarithmic scale on the vertical axis. For weak disorder the conductance increases with  $L$ . With the use of data for  $L \leq 300$  only, one can conclude that there is a metallic regime for  $W < 4$ . However, this is a typical finite size effect since the decrease of the conductance is observed for further increase of the system size  $L$  [6].

#### 4. Inverse participation ratio

Inverse participation ratio (IPR) enables us to investigate the spatial distribution of the electron inside the disordered sample. IPR is defined as

$$I_q(E_n) = \sum_{\vec{r}} |\Phi_n(\vec{r})|^{2q}, \quad (7)$$

where  $\Phi_n(\vec{r})$  is the  $n$ -th electron eigenfunction with the eigenenergy  $E_n$ . The size dependence of IPR enables us to distinguish between the metallic and localized regime. In the localized regime, we expect that only a few lattice sites are occupied with  $|\Phi_n| \sim 1$ . Therefore  $I_q \sim 1$  does not depend on the size of the system. In the metallic regime, electron occupies all sites of the lattice,  $|\Psi_n(\vec{r})|^2 \sim L^{-d}$ , and  $I_q(E_n) \sim L^{-d(q-1)}$ . Of particular interest is the critical point, where the wave function is multifractal [9], and

$$I_q \sim L^{-d_q(q-1)}. \quad (8)$$

Parameters  $d_q$  are *multifractal dimensions*. Since the electron eigenenergies and eigenstates can be calculated numerically for relatively large models, the analysis of the IPR enables us to find the critical point and calculate the critical exponent. In real calculation, we have to take into account the statistical character of disordered quantum systems. Therefore, we consider  $N_{\text{stat}}$  samples, which differ only in the realization of the disorder. For each sample, we find all

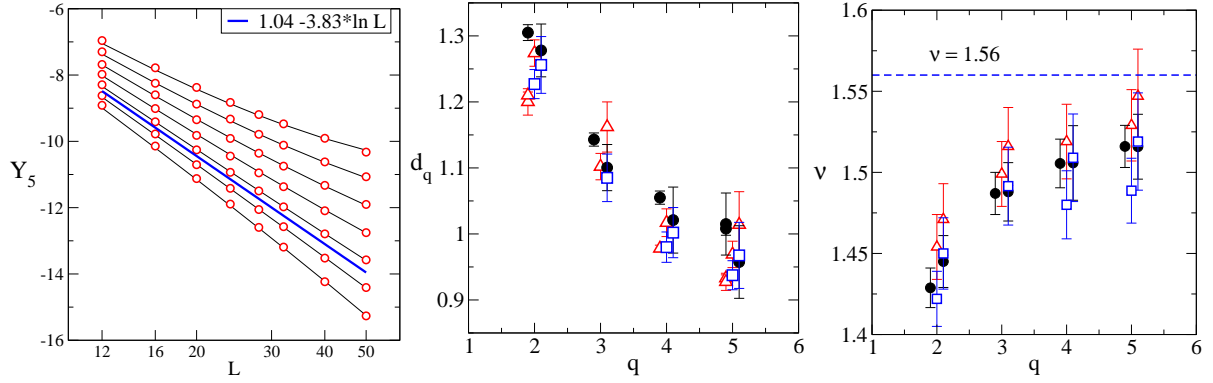


Fig. 5: Numerical data for the inverse participation ratios  $Y_q$  defined by Eq. (9) used for the numerical analysis of the metal-insulator transition at two critical points shown in Fig. 1 [10]. Left: Inverse participation ratio  $Y_5$  as a function of the size of the system for energies  $E = 6.50, 6.55, \dots, 6.80$  (from top to bottom). Thick solid line is  $Y_5$  for the critical point  $E_c = 6.58$  (Eq. 11). The middle and the right Figures shows multifractal dimensions  $d_q$  and critical exponent  $\nu$ , respectively, estimated from the scaling analysis of  $Y_q$  ( $q = 2 - 5$ ). Note that the estimation of the critical exponent  $\nu$  is more accurate for higher values  $q$  since  $|\Psi(\vec{r})|^{2q}$  is “more localized” for higher  $q$ . The most accurate estimation of the critical exponent  $\nu \approx 1.56$ , found by scaling analysis of other variables [11,12] is shown in the right Figure by the dashed line.

eigenstates with energies  $E_n$  inside the narrow energy interval  $E - \delta E, E + \delta E$  and calculate the quantity  $Y_q(E)$

$$Y_q(E, L) = \frac{1}{N_{\text{stat}}} \sum_{\text{samples}} \sum_{|E-E_n|<\delta} \ln I_q(E_n). \quad (9)$$

Fig. 1 shows that close to the critical point  $E_c$  the variable  $Y_q(E, L)$  fulfills the scaling relation

$$Y_q(E, L) = Y_q^c - d_q \ln L + A(E - E_c)L^{-1/\nu} \quad (10)$$

[10] with logarithmic size dependence at the critical point,

$$Y_q(E_c, L) = Y_q^c - d_q \ln L. \quad (11)$$

This enables us to find the critical energy  $E_c$ . The slope of the  $\ln L$  dependence determines the fractal dimension  $d_q$ . The scaling analysis of  $Y_q(E)$  in the vicinity of the critical point, enables us to estimate the critical exponent  $\nu$ . Obtained results are summarized in Fig. 5.

## 5. Conclusion

We demonstrated the application of the finite size scaling method to the analysis of the transition of the disordered system from the metallic to the insulating regime. The method enables us to calculate the critical point and the critical exponent which determines the divergence of the correlation length in the vicinity of the critical point.

The universality of the metal-insulator transition was verified by numerical analysis of various physical parameters and the critical exponent was calculated with high accuracy for different disordered models (for review, see [2,6] and references therein). In spite of this success,

obtained numerical results are still not generally accepted [13]. One reason is that experimental verification of calculated data is difficult since the electron-electron interaction, always presented in real materials, is not included into the theory. This difficulty can be overcome by experiments on disordered photonic structures. Since the localization results from the scattering of waves propagating through disordered media, it should be, and it really has been, observed also in photonic structures [14,15].

Numerically obtained value of the critical exponent for the three dimensional disordered model (1) has been recently supported by the semi-analytical work [16] and verified by experimental optical measurements [17,18] equivalent to the three dimensional disordered model (1).

Another unsolved problem of the localization is the disagreement between numerical results and predictions of the analytical theories. At present, no analytical theory confirms numerically obtained values of critical exponents. The reason for this disagreement lies in the statistical character of the process of localization. The theory must consider all possible scattering processes on randomly distributed impurities. All physical variables are statistical quantities with broad probability distributions. It is in general not known how to calculate analytically their mean values. We believe that detailed numerical analysis of various disordered systems bring inspiration for the formulation of analytical theory.

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