Finite-Size Scaling of the Level Compressibility at the Anderson Transition

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Abstract. We compute the number level variance \( \Sigma_2 \) and the level compressibility \( \chi \) from high precision data for the Anderson model of localization and show that they can be used in order to estimate the critical properties at the metal-insulator transition by means of finite-size scaling. With \( N, W, \) and \( L \) denoting, respectively, linear system size, disorder strength, and the average number of levels in units of the mean level spacing, we find that both \( \chi(N, W) \) and the integrated \( \Sigma_2 \) obey finite-size scaling. The high precision data was obtained for an anisotropic three-dimensional Anderson model with disorder given by a box distribution of width \( W/2 \). We compute the critical exponent as \( \nu \approx 1.45 \pm 0.12 \) and the critical disorder as \( W_c \approx 8.59 \pm 0.05 \) in agreement with previous transfer-matrix studies in the anisotropic model. Furthermore, we find \( \chi \approx 0.28 \pm 0.06 \) at the metal-insulator transition in very close agreement with previous results.

PACS. 71.30.+h Metal-Insulator transition – 71.23.An Theories and Models; Localized states – 72.15.Rn Localization effects (Anderson or Weak localization)

1 Introduction

The Anderson metal-insulator transition (MIT) in disordered systems has been vigorously studied for a long time [1, 2] and still continues to attract much attention [3]. For non-interacting electrons in disordered systems the scaling hypothesis of localization has been successfully validated by theoretical [4, 5] and numerical [6–10] approaches. The latter approaches use well-known techniques of finite-size scaling (FSS) [11]. FSS at the Anderson MIT has a noteworthy history, reaching a first peak with the seminal results for, e.g., the AM with anisotropic hopping [20–22], the off-diagonal AM [23, 24], and the AM in a magnetic field [25, 26], confirmed this value of \( \nu \) within the error bars [27]. Also, \( \nu \) is identical for the MIT as a function of disorder or energy [28]. We emphasize that a properly performed Slevin/Ohtsuki scaling procedure needs to assume various fit functions and that the final estimates are to be suitably extracted from many such functional forms and starting parameters [21, 22]; bootstrap [17–19] or Monte Carlo methods [21, 23] then need to be employed for a precise estimate of error bars.

Regarding experiments, we note that similarly precise data (0.1%) are much harder to obtain for our experimental colleagues. Nevertheless, recent advances in this direction based on careful finite-temperature analysis of the conductivity data show a clear trend towards increasing \( \nu > 1 \) [28, 29]. The roles of sample inhomogeneities, mag-
netic effects and other possible experimental influences are also discussed. The statistical properties of spectra of disordered single-electron systems are closely related to the localization properties of the corresponding wave functions. In the 3D AM we have the insulating, the critical, and the metallic phases, respectively. For the insulating regime, the localized states even if they are close in energy have an exponentially small overlap and their levels are uncorrelated. Accordingly, in the thermodynamic limit the normalized distribution of the spacing s between neighboring energy levels follows the Poisson law

\[ P_P(s) = \exp(-s). \]  

In the metallic regime, the large overlap of delocalized states induces correlations in the spectrum leading to level repulsion. In this case, if the system is invariant under rotational and under time-reversal symmetry, the normalized spacing distribution closely follows the Wigner surmise of the Gaussian orthogonal ensemble (GOE) of random matrices.

\[ P_{WD}(s) = \frac{\pi}{2} s \exp \left( -\frac{\pi}{4} s^2 \right). \]  

The third symmetry class at the MIT is usually called the critical statistics due to its fractal nature of the critical states (see and references therein). The proposed linear increase of \( \Sigma_2 \) at the MIT as a function of \( n \) at the transition has been a matter of discussion. In general, there is consensus that \( \Sigma_2 \) has a quasi-Poisson behavior as in Equation (2) at the MIT.

In this paper we show how \( \Sigma_2 \) and \( \chi \) can be used together with FSS to obtain reliable estimates of the critical exponent \( \nu \). We employ various FSS schemes to check the accuracy of our results. Our study goes beyond previous investigations of the level number variance due to a considerably enhanced accuracy in the scaling data. Based on raw spectral data of an anisotropic version of the AM, we find that \( \nu \) is consistently larger than 1 in contradiction to a recently raised objection to the FSS method of Ref. [17], cp. Appendix. The values of \( \nu \) that we obtain are in good agreement with the above mentioned recent estimates for the isotropic case [1, 19, 22, 23, 7]. The mean value of \( \chi_c \) at the MIT is \( \approx 0.28 \pm 0.06 \).

2 The Model Hamiltonian

We consider the 3D Anderson model of localization described by a Hamiltonian in the lattice site basis as

\[ H = \sum_i \varepsilon_i |i\rangle \langle i| + \sum_{ij} t_{ij} |i\rangle \langle j|. \]  

The states \( |i\rangle \) are orthonormal and correspond to particles located at the \( N^3 \) sites \( i = (x, y, z) \) of a regular cubic lattice with periodic boundary conditions. The site energies \( \varepsilon_i \) are taken to be random numbers uniformly distributed in the interval \( [-W/2, W/2] \); \( W \) defines the disorder strength. The hopping integrals \( t_{ij} \) are restricted to nearest neighbors and depend only on the three spatial directions. In this paper we consider weakly coupled planes defined by \( t_x = t_y = 1, t_z = 0.1 \). We emphasize that we have chosen the strong anisotropy simply because we have the most accurate data (the relative error ranges from 0.2 to 0.4%) available for this value from a previous study [21, 53]. This high accuracy (for spectral data) has been achieved by averaging over 10 samples for system size 50\(^3\) and then increasing the number of samples up to 699 for system size 13\(^3\) such that always at least 10\(^5\) eigenenergies have been computed for each \( N \) and \( W \). Since it was shown in Refs. [21, 53] numerically that the universality class of the model is not changed by the anisotropy, we therefore need not generate similarly precise data for the isotropic model in order to show scaling of \( \Sigma_2 \) and \( \chi \).

The Hamiltonian [7] was diagonalized numerically using a Lanczos method. In order to perform any statistical calculations the eigenspectrum is "unfolded" so that the average spacing between adjacent eigenvalues is one. Spectra unfolding amounts to a kind of renormalization of the eigenvalues in order to extract the universal spectral
properties. One way to perform spectral unfolding is to subtract the regular part from the integrated density of states and consider only the fluctuations [12]. This can be achieved by different means; however, there is no rigorous prescription and the “best” criterion is the insensitivity of the final result to the method employed. This criterion is fulfilled in the present study.

3 Finite-Size Scaling

According to the one-parameter-scaling hypothesis [61], a quantity $X$ at different disorders $W$ and energies $E$ scales onto a single scaling curve, i.e.,

$$X(N; W, E) = f(\xi(W, E)/N),$$

(8)

where the scaling function $f$ is a generalized homogeneous function [61] and $\xi$ denotes the correlation length. The MIT in the 3D AM is a second-order phase transition and as such it is characterized by a divergent correlation length with power-law behavior $\xi_\infty = |W - W_c|^{-\nu}$. The task of FSS now is to determine the infinite-size quantities $f$ and $\xi(W, E)$ from finite-size data and to obtain the critical exponent $\nu$ and the critical disorder $W_c$ or the critical energy $E_c$.

The essential idea of the FSS procedure of Ref. [17] is to construct a family of fit functions which include corrections to scaling due to an irrelevant scaling variable and due to non-linearities of the disorder dependence of the scaling variables. The former is only necessary when the accuracy of the data allows us to observe systematic shifts of the intersection points for different $W$ (or $E$) and $N$. In all current FSS studies of spectral properties such an accuracy has not been reported, only studies using the transfer-matrix method allow for an identification of irrelevant variables.

Following Refs. [17, 21, 22], we thus assume a scaling form without irrelevant variables to be

$$X = \tilde{f}(g_r N^{1/\nu}),$$

(9)

where $g_r$ is the relevant scaling variable. Taylor expanding $\tilde{f}$ up to order $n_r$, we get

$$\tilde{f} = \sum_{i=0}^{n_r} b_i g_r^i N^{i/\nu}.$$  

(10)

Non-linearities are taken into account by expanding $g_r$ in terms of $u = 1 - W/W_c$ (or $u = 1 - E/E_c$) up to order $m_r$

$$g_r(u) = u + \sum_{k=2}^{m_r} b_k u^k.$$  

(11)

The fit function is adjusted to the data by choosing the orders $n_r$ and $m_r$ up to which the expansions are carried out.

4 Results

4.1 The spectral rigidity

In Figure 1 we show the computed $\Sigma_2$ data for, e.g., three disorders, $E \in [-4.1, 4.1]$ (50% of the spectrum), and various system sizes. In a previous study [21], we have shown that similar level-statistics results can be obtained when only 20% of the spectrum close to the band center are taken into account [12]. The dependence of $W_c$ on energy has been considered previously in, e.g. Ref. [4]. A large band of states around $E = 0$ shows the same multifractal characteristics as a narrow band [23]. Thus it is justified to take a large part of the spectrum into account when computing spectral statistics. It is evident from the figure that there is a systematic size dependence as a function of disorder. For large disorder $W = 12$ and upon increasing the system size the data approach the insulating (Poisson) behavior. Similarly, for small disorder $W = 6$ the curves tend towards the metallic (GOE) behavior. And close to the MIT at $W_c \approx 8.625$, the data for all system sizes collapse onto a single curve. A similar trend as in Figure 1 has been observed for $\Sigma_2$ in the four-dimensional isotropic AM [25].

4.2 FSS with integrated $\Sigma_2$ data

In order to perform FSS, we could now use the data of Figure 1 and plot them at each value of $\langle n \rangle$ as a function of disorder. However, such an approach is of limited usefulness since it is apriori unclear how to weigh data from different $\langle n \rangle$ values. Furthermore, the fluctuations in the data lead to rather large error bars in the obtained
estimates of $\nu$ and $W_c$. Instead, we define the integrated quantity

$$\eta(N,W) = \frac{1}{L_0} \int_0^{L_0} \Sigma_2(L) dL$$

with $L = \langle n \rangle$. This is similar to the FSS analysis of $\Delta_3$-statistics [29]. The integral is also considered up to $L_0 = 30$ only because the relative error in $\Sigma_2$ becomes rather large for larger $L_0$ values and hence the calculation is less reliable. It is evident from Figure 2 that $\eta(N,W)$ shows the desired system-size dependence for various values of $W$ exhibiting insulating, critical and metallic behavior for $W$ larger, close to, and smaller than $W_c \approx 8.625$. In order to obtain $\xi$ from finite system-size data we now use the FSS procedure of Section 3. For the non-linear fit, we used the Levenberg-Marquardt method [17]. In Figure 3, we show that the data from different system sizes collapse on two branches corresponding to localized and extended behavior. This clearly shows that $\eta$ exhibits one-parameter FSS. We then compute the critical exponent $\nu$ and the critical disorder $W_c$ for various parameters. The results are tabulated in Table 1. The average values are $\nu \approx 1.43 \pm 0.13$ and $W_c \approx 8.62 \pm 0.04$, respectively. Here and in the following, the error intervals are standard errors, i.e., denoting one standard deviation.

4.3 FSS with $\chi$

We now turn our attention to computing $\chi$. First we note that $\Sigma_2(L)/L$ ($L = \langle n \rangle$) as plotted in Figure 2 is already a crude approximation of $\chi$. Since there is a systematic size dependence, this already indicates that $\chi$ should obey FSS. In order to proceed more accurately, we now fit the $\Sigma_2(L)/L$ data with an ansatz function containing irrelevant scaling exponents $y_k$, i.e.

$$\frac{\Sigma_2(N,W,L)}{L} \approx \chi + \sum_{k=1}^{m} a_k (N,W)L^{-y_k}$$

up to order $m$. Thus in the limit $L \to \infty$, the constant term will be equal to the desired value of the level compressibility $\chi$. The data used in the fits range from $L = 0$ up to $L \approx 140$. Data for larger $L$ values ($\approx 250$) was ignored due to reduced statistical accuracy. In Figure 3, we show some typical fits for large system sizes.

We next perform FSS of $\chi$ as explained above. However, a non-linear fit procedure of (increasingly fluctuating) large $L$-data with exponents as fitting parameters is
Fig. 4. The one-parameter scaling dependence of $\chi$, obtained from Equation (13) for, e.g., $y_1 = 1$ and $y_2 = 2$, on $\xi$ for disorders $W \in [7, 11]$, system sizes 24, 30, 40, and 50, with $n_c = 3$, $m_r = 1$. The dashed line indicates the value $\chi_c = 0.27(1)$ at the MIT obtained from this fit.

Fig. 5. The one-parameter scaling dependence of $\chi^+\,$, obtained from Equation (13) for $y_1 = 1$ and $y_2 = 2$ fitted up to $L = 30$, on $\xi$ for disorders $W \in [7, 11]$, system sizes 24, 30, 40, and 50, with $n_c = 3$, $m_r = 1$.

4.4 FSS with $\chi$ from truncated data.

In order to suppress the problems with large-$L$ fluctuations, we have truncated the $\Sigma_2/L$ data at $L = 30$ and performed the FSS procedure as before with Equation (13) using fixed $y_1 = 1$ and $y_2 = 2$. As shown in Figure 5, the $\chi$ data for different system sizes and different $W$ values collapse again onto a single scaling curve with two branches. Due to the truncation, the estimated values $\chi^+$ can only serve as upper limits to the true value $\chi_c$ at the MIT. But the resulting values for $\nu$ and $W_c$ are of much better accuracy and are shown in Table 2. For the average critical exponent we obtain $\nu \approx 1.44 \pm 0.13$ and for the average critical disorder $W_c \approx 8.66 \pm 0.04$.

4.5 FSS with a polynomial fit

In order to proceed more accurately with the determination of $\nu$ and $W_c$, we now fit $\Sigma_2(L)$ data for small $L$ with a polynomial in $L$, i.e.,

$$\frac{\Sigma_2(N, W, L)}{L} \approx \chi_p + \sum_{k=1}^m b_k(N, W)L^k$$

(14)

up to order $m$. We then identify a rough estimate of the level compressibility with the linear expansion coefficient $\chi_p$. This implies a systematic shift of $\chi$ and the value of $\chi_p$ at the MIT will also be shifted towards a larger value when compared to $\chi_c$. However, $\nu$ and $W_c$ can be determined with increased precision: the quality of the fit, cp. Figure 5, is very good and certainly better than in the two previous cases. As a check to the numerical reliability of this method, we vary the value of $L$ included in the fit function (14) by fitting the $\Sigma_2/L$ data for various ranges
Fig. 6. \( \chi_p(N, W) \) obtained by fitting the \( \Sigma_2 \) data with \( m = 3 \) in Equation (4). System-size dependence is clearly seen. The solid lines are fit functions from FSS of Equation (9) with \( n_r = 3 \) and \( m_r = 1 \).

Fig. 7. The one-parameter scaling dependence of \( \chi_p \) on \( \xi \) for different system sizes \( N \) and disorders \( W \in [6, 12] \).}

of \( L = 10, 15, 20, 25 \) and \( 30 \). We find that there is only a negligible change in the obtained values of \( \nu \) and \( W_c \).

After FSS, \( \chi_p \) data for all system sizes and all \( W \) collapse onto two curves as shown in Figure 6. Results for \( \nu \) and \( W_c \) for various FSS functions and different \( m \) are shown in Table 1. For the average critical exponent we obtain \( \nu \approx 1.47 \pm 0.10 \) and for the average critical disorder \( W_c \approx 8.56 \pm 0.05 \).

The values of \( \nu \) calculated from the \( \eta \) and the three \( \chi \)-based approaches are compatible with each other and are also comparable to values from other methods \( [18, 72] \). for instance the transfer-matrix method which gives \( \nu \approx 1.62 \pm 0.07 \) \( [24] \). We can therefore claim that both \( \chi \) and \( \eta \) are good FSS parameters to characterize the MIT. Nevertheless, a simple fitting procedure in the large \( L \) limit, although in principle correct, will encounter many numerical problems.

5 Conclusion

States at the 3D MIT are multifractal entities \( [18, 59] \). This implies that, while not being extended, their spatial structure nevertheless results in a long-ranged, power-law overlap of electronic densities in energy \( [18, 72] \), i.e.,

\[
\langle |\Psi_i|^2|\Psi_k|^2 \rangle \propto |E_i - E_k|^{-(1-D_2/d)}
\]

where \( D_2 \) is the correlation dimension \( [59] \) and the connection \( \chi_c = (d-D_2)/2d \) has been conjectured \( [70] \). In order to describe generic features of such multifractal states, various critical random matrix models have been suggested and studied \( [63, 71, 72] \), albeit mostly for the unitary class of models. Using the above relation of \( D_2 \) (see Refs. \([59, 63]\) for numerical estimates at the MIT in anisotropic 3D AMs) with \( \chi_c \), we find that the computed value \( \chi_c \approx 0.29 \pm 0.06 \) is compatible with \( D_2 \approx 1.3 \pm 0.1 \), which can be calculated easily from the \( f(\alpha) \) spectra published in Refs. \( [24, 59, 71, 72] \). On the other hand, it has been shown that in the limit of “strong multifractality”, the above connection between \( \chi_c \) and \( D_2 \) no longer holds \( [70] \). Previous estimates of \( D(2) \) in the isotropic 3D AM range from 1.4–1.7 \( [55, 71, 72, 80] \). Certainly, our multifractal \( [59, 63] \) is not an infinitely sparse multifractal wave \( (D(2) = 0) \) as sometimes expected for the critical ensembles \( [16] \).

In summary, our results show that \( \chi \) (and \( \eta \)) can indeed be used to compute, with the help of FSS, estimates of \( \chi_c \), \( W_c \) and \( \nu \) which are in good agreement with transfer-matrix and other spectral analysis. We are confident that the remaining small difference in values can be further shrunk when larger system sizes become available for the spectral statistics.

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A Another FSS procedure

In a recent communication to the cond-mat archives \( [56] \), the FSS method used in the present paper has been criticized and the results obtained by various groups \( [17–26] \) for the critical exponent \( \nu \) of the localization length at the MIT in the 3D AM have been questioned. These claims are based on the observation that there still is some disagreement between analytical, numerical and experimental results for the critical exponent \( [1] \). Ref. \([70] \) proposes
yet another procedure to deal with corrections to scaling. Furthermore, it is hinted that the numerical data support $\nu \approx 1$, whereas the present manuscript and recent numerical papers find $\nu \approx 1.5 \pm 0.2$ [17, 19].

We have tested the method proposed by Ref. [50] first with transfer-matrix data [20, 22, 23] with $\varepsilon \approx 0.1$%; we find $\nu = 1.75 \pm 0.17$ for the anisotropic and $1.55 \pm 0.04$ for the random-hopping AM. The FSS of section 3 gives $\nu = 1.61 \pm 0.07$ [20] and $\nu = 1.54 \pm 0.03$ [22, 21], respectively, for the same set of data. Note that the first value (1.75) is so high because systematic shifts of $W_c$ due to an irrelevant scaling variable are not taken into account in [20]. Using for a second test the energy-level-statistics data of the present manuscript with $\varepsilon \approx 1\%$, we find $\nu = 1.51 \pm 0.25$. Last, for artificially generated data with precisely known $W_c = 16.5$ and varying $\nu \in [0.5, 2.0]$ the results of the method of Ref. [50] are comparable to the results of the Kramer/MacKinnon FSS [10] and slightly less reliable than the present FSS as shown in Figure 8. We conclude that the method proposed in Ref. [50] also yields $\nu \approx 1.58$ and not $\nu \approx 1$ for the MIT of the AM.

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Table 2. Parameters for FSS of $\chi$ as in (13) with $y_1 = 1$, $y_2 = 2$ and the resulting estimates for $\chi_c$, $\nu$ and $W_c$. The numbers in the 3rd and 4th column denote orders $n_r$ and $m_r$ used in the expansions (10) and (11), respectively, for which the best fits have been obtained. The 5th column is for fits based on $\Sigma_2$ data up to $L = 140$, the 6 – 8th columns are for fits up to $L = 30$ only. The goodness-of-fit $Q$ [64] is less than 0.1 in all cases.

| $W$      | $N$      | $n_r$ | $m_r$ | $L_{max} = 140$ | $L_{max} = 30$ |
|----------|----------|-------|-------|-----------------|-----------------|
| 7-11.0   | 13-50    | 3     | 1     | 0.27(9)         | 0.31(5)         |
| 7-11.0   | 13-50    | 1     | 3     | 0.16(3)         | 0.31(3)         |
| 8-9.25   | 13-50    | 3     | 1     | 0.26(12)        | 0.30(5)         |
| 8-9.25   | 13-50    | 1     | 3     | --              | 0.31(5)         |
| 8-9.25   | 13-50    | 3     | 2     | 0.31(1)         | 0.33(1)         |
| 8-9.25   | 13-50    | 2     | 3     | 0.37(2)         | 0.37(6)         |
| 8-9.25   | 24-50    | 3     | 3     | 0.27(1)         | 0.32(1)         |
| 7-11.0   | 24-50    | 3     | 1     | 0.27(1)         | 0.32(1)         |
| 7-11.0   | 24-50    | 1     | 3     | 0.26(2)         | 0.32(1)         |
| 8-9.25   | 24-50    | 3     | 1     | 0.19(13)        | 0.32(1)         |
| 8-9.25   | 24-50    | 1     | 3     | 0.36(18)        | 0.32(2)         |
| 7-11.0   | 13-50    | 3     | 3     | 0.31(1)         | 0.33(1)         |

average: | 0.28(6) | 0.32(3) | 8.66(4) | 1.44(13) |
Table 3. Values of the critical disorder strength $W_c$ and the critical exponent $\nu$ values computed from Equation (14) with various $m$ values. The numbers in the 4th and 5th column denote orders $n_r$ and $m_r$ used in the expansions (10) and (11), respectively for which the best fits have been obtained. The goodness-of-fit $Q$ is larger than 0.99 in all cases.

| $m$ | $W$  | $N$  | $n_r$ | $m_r$ | $W_c$   | $\nu$   |
|-----|------|------|-------|-------|---------|---------|
| 2   | 7...11.0 | 13...50 | 3     | 1     | 8.65(2) | 1.36(3) |
| 2   | 7...11.0 | 13...50 | 1     | 3     | 8.63(2) | 1.52(4) |
| 2   | 8...9.25  | 24...50 | 3     | 1     | 8.57(3) | 1.43(6) |
| 2   | 8...9.25  | 24...50 | 1     | 3     | 8.53(3) | 1.65(7) |
|     | average: |       |       |       | 8.60(3) | 1.49(5) |
| 3   | 7...11.0 | 13...50 | 3     | 1     | 8.67(2) | 1.29(3) |
| 3   | 7...11.0 | 13...50 | 1     | 3     | 8.61(1) | 1.42(3) |
| 3   | 8...9.25  | 24...50 | 3     | 1     | 8.55(4) | 1.45(8) |
| 3   | 8...9.25  | 24...50 | 1     | 3     | 8.53(4) | 1.51(8) |
|     | average: |       |       |       | 8.59(3) | 1.42(6) |
| 4   | 7...11.0 | 13...50 | 3     | 1     | 8.54(4) | 1.32(9) |
| 4   | 7...11.0 | 13...50 | 1     | 3     | 8.51(4) | 1.40(9) |
| 4   | 8...9.25  | 24...50 | 3     | 1     | 8.45(10)| 1.56(26)|
| 4   | 8...9.25  | 24...50 | 1     | 3     | 8.42(11)| 1.68(28)|
|     | average: |       |       |       | 8.48(7) | 1.49(18)|
|     | total average: |   |       |       | 8.56(5) | 1.47(10)|
