Finite size scaling and multifractality at the Anderson transition for the three Wigner-Dyson symmetry classes in three dimensions

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The disorder induced metal–insulator transition is investigated in a three dimensional simple cubic lattice and compared for the presence and absence of time reversal and spin–rotational symmetry, i.e. in the three conventional symmetry classes characterized by parameter $\beta = 1, 2,$ and $4$. Large scale numerical simulation has been performed on systems with linear sizes up to $L = 100$ at the band center, $E = 0$. The multifractal dimensions, exponents $D_q$ and $\alpha_q$, have been determined in the range of $-1 \leq q \leq 2$. The finite-size scaling of the generalized multifractal exponents provides the critical exponents for the different symmetry classes in accordance with values known from the literature using high precision transfer matrix techniques. The multifractal exponents and their $\beta$ dependence provide further characterization of the Anderson transition as a function of $\beta$.

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I. INTRODUCTION

Metal-insulator transition, and disordered systems are in the forefront of condensed matter research since the middle of the last century and yet this topic has quite some open questions and is still actively investigated. In the last few years experimental evidences have been obtained about this topic in remarkable journals in particular reporting Anderson localization of ultrasound in disordered elastic networks light in disordered photonic lattices in the transverse direction or in an ultraslow atomic system in a disordered laser trap. Richardella et al. examined the MIT in a dilute magnetic semiconductor Ga$_{1-x}$Mn$_x$As, that is a strongly interacting and disordered system. They found a clear phase transition together with multifractal local density of states (LDOS) at the Fermi energy, showing, that multifractality is a robust and important property of disordered systems. Multifractal properties consistent with the theory of Anderson localization are also found in the ultrasound system. On the theoretical side we know, that disorder plays a crucial role in integer quantum Hall effect, and lately it was shown, that a large overlap of multifractal wave functions of disordered systems can increase the superconducting critical temperature or the multifractal fluctuations of the LDOS close to criticality induces a new phase due to the presence of local Kondo effects induced by local pseudo gaps at the Fermi energy. Moreover, Anderson localization was also reported in the spectrum of the Dirac operator of QCD at high temperature through spectral statistics and multifractal analysis shows also promising results also. All in all, Anderson localization and multifractality are widely applicable and important topics.

The latter models show that there is an increased interest in understanding the nature of the Anderson transition in the presence of various global symmetries. A comprehensive review of the current understanding is given in Ref. The symmetry classes were introduced first to describe random matrix ensembles, but the naming conventions are the same in the field of disordered systems. The classification considers two global symmetries: time-reversal and spin-rotational symmetry. As it turns out, beside these symmetries there are three further symmetry classes according to the presence of chiral symmetry, and there are four Bogoliubov-de Gennes classes also, corresponding to particle-hole symmetry prominent in hybrid (superconductor-normal) systems. The effect of symmetry classes on the Anderson transition has already been investigated earlier using spectral statistics, there is much less work based on the multifractal analysis of the eigenstates.

Our goal in this article is to fill in this gap and apply multifractal finite size scaling (MFSS), developed originally by Rodriguez, Vasquez, Rmer and Slevin to the Anderson models in the three conventional Wigner-Dyson (WD) classes. The organization of the article is the following. In Sect. we define the model and describe its numerical representation. In Sect. we briefly describe the finite size scaling analysis of the generalized multifractal exponents of the critical eigenstates, in Sect. we give the results obtained for the three universality classes and finally in Sect. we summarize our results.

II. MODELS AND NUMERICAL REPRESENTATION

A. The model

In this article we investigate Anderson models belonging to the three WD classes, without chiral and particle-hole symmetry. We will investigate the case of diagonal disorder and nearest neighbor hopping therefore the Hamiltonian reads as

$$
\mathcal{H} = \sum_{i\sigma} \varepsilon_i c^\dagger_{i\sigma} c_{i\sigma} - \sum_{ij\sigma\sigma'} t_{ij\sigma\sigma'} c^\dagger_{i\sigma} c_{j\sigma'} + h.c., \quad (1)
$$
where \( i, j \) and \( \sigma, \sigma' \) stand for site- and spin index, \( \varepsilon_{ij} \)-s are random on-site energies, which are uniformly distributed over the interval \( [-W, W] \), \( W \) acts as disorder strength. Using a uniform distribution is just a convention, other distributions of disorder, e.g. Gaussian, binary, etc. can be used as well.

In the orthogonal class time-reversal and spin-rotational symmetry are preserved. In this case the Hamiltonian is invariant under orthogonal transformations – hence the name –, therefore it is a real symmetric matrix. Since spin does not play any role, we will consider a spinless Anderson-model. In the numerical simulations the Hamiltonian is represented by an \( N \times N \) real symmetric matrix, where \( N = L^3 \), and \( L \) is the linear system size. The diagonal elements, are are uniformly distributed random numbers, off-diagonal elements are zero, except if \( i \) and \( j \) are nearest neighbors:

\[
H_{ij}^O = \begin{cases} 
\varepsilon_i \in U \left[-\frac{W}{2}, \frac{W}{2}\right], & \text{if } i = j \\
-1, & \text{if } i \text{ and } j \text{ are neighboring sites} \\
0, & \text{otherwise}
\end{cases}
\]  \( (2) \)

Setting the hopping elements to 1 is equivalent to choosing the energy unit. To avoid surface effects, we used periodic boundary conditions. However, this case was investigated very carefully by Rodriguez et al.\(^{14}\) we will consider this symmetry class to verify our numerical method, and to have complete description of all the WD classes.

In the unitary class time-reversal symmetry is broken, which can be realized physically by applying magnetic field. It can be shown, that either spin rotational symmetry is broken or not, the model will belong to the unitary class.\(^{12}\) The Hamiltonian is invariant under unitary transformations therefore it is a quaternion hermitian matrix. We will discuss the case when spin-rotational symmetry is present, because this way we can use spinless fermions again, that keeps matrix size \( N \times N \). However, one has to store about twice as much data compared the orthogonal case, because here every off-diagonal matrix element is a complex number. Obviously finding an eigenvalue and an eigenvector takes more time, too.

For the numerical simulations we followed Slevin and Ohtsuki. Let us consider a magnetic field pointing to the \( x \) direction with flux \( \Phi \), measured in units of the flux quantum, \( \frac{\Phi}{\Phi_0} \). Its effect can be represented by a unity phase factor, the Peierls substitution for the hopping elements of the Hamiltonian matrix. The upper triangular of the Hamiltonian reads as

\[
H_{ij}^U = \begin{cases} 
\varepsilon_i \in U \left[-\frac{W}{2}, \frac{W}{2}\right], & \text{if } i = j \\
-1, & \text{if } i \text{ and } j \text{ are neighboring sites} \\
-\epsilon^{2\pi i \Phi z}, & \text{if } i \text{ and } j \text{ are neighboring sites in the z direction} \\
0, & \text{otherwise}
\end{cases}
\]  \( (3) \)

Complex hermiticity sets the off-diagonal elements in the lower triangular part, \( j < i \). Periodic boundary conditions and flux quantization force a restriction for the magnetic flux namely, that \( \Phi \cdot L \) must be an integer. In the thermodynamic limit arbitrary small magnetic field drives the system from the orthogonal to the unitary class. However, in a finite system the relation of the system size, \( L \), and the magnetic length, \( L_H = \frac{1}{\sqrt{2\pi \Phi}} \), matters. In case of weak magnetic field, \( L \ll L_H \), the system belongs to the orthogonal class, in case of strong magnetic field, \( L \gg L_H \), it belongs to the unitary class. Since we used system sizes of multiples of 10 lattice spacings, see Tab. I, we chose \( \Phi = \frac{1}{5} \). This leads to \( L_H \approx 0.789 \), therefore this choice clearly fulfills the above two conditions.

In the symplectic class time-reversal symmetry is present, and spin-rotational symmetry is broken, that describes a system with spin-orbit interaction. In this case the Hamiltonian is invariant under symplectic transformations therefore it is a quaternion hermitian matrix. For the numerical simulations we followed Asada, Slevin and Ohtsuki.\(^{16}\) Since in this case we have to deal with the spin index also, the Hamiltonian is an \( 2N \times 2N \) complex hermitian matrix. Diagonal elements corresponding to the \( i \)th site and hopping elements between site \( i \) and \( j \) are \( 2 \times 2 \) matrices because of the spin indexes, having a form

\[
\epsilon_i = \begin{pmatrix} 
\varepsilon_i & 0 \\
0 & \varepsilon_i
\end{pmatrix} 
\]

\[
t_{ij} = \begin{pmatrix} 
e^{i\alpha_{ij}} \cos \beta_{ij} & e^{i\gamma_{ij}} \sin \beta_{ij} \\
-e^{-i\gamma_{ij}} \sin \beta_{ij} & e^{-i\alpha_{ij}} \cos \beta_{ij}
\end{pmatrix}
\]  \( (4) \)

where \( \varepsilon_i \) is an uniformly distributed random on-site energy from the interval \( [-W, W] \), \( \alpha_{ij}, \beta_{ij} \) and \( \gamma_{ij} \) were chosen to form an SU(2)-invariant parametrization, leading to the so-called SU(2) model: \( \alpha_{ij} \) and \( \gamma_{ij} \) are uniform random variables from the interval \([0, 2\pi]\), and \( \beta \) has a probability density function \( p(\beta) d\beta = \sin(2\beta) d\beta \) in the range \([0, \frac{\pi}{2}]\). The upper triangular of the Hamiltonian has the following form:

\[
H_{ij}^S = \begin{cases} 
\epsilon_i, & \text{if } i = j \\
t_{ij}, & \text{if } i \text{ and } j \text{ are neighboring sites} \\
0, & \text{otherwise}
\end{cases}
\]  \( (5) \)

The off-diagonal elements are defined following the property of complex hermiticity. To store the Hamiltonian requires about eight times more memory compared to the orthogonal case, because here every off-diagonal element contains four complex number. Finding an eigenvalue is way much slower than for the unitary case, mainly because of the linear size of the matrix is twice as large.

\[ \text{B. Numerical method} \]

MFSS deals with the eigenvectors of the Hamiltonian, that is a large sparse matrix. Recent high precision calculation use Jacobi-Davidson iteration with incomplete LU preconditioning, therefore we decided to use...
TABLE I: System sizes and number of samples for the simulation for the 3D Anderson model belonging to the conventional WD classes.

| system size ($L$) | number of samples |
|-------------------|-------------------|
| 20                | 15000             |
| 30                | 15000             |
| 40                | 15000             |
| 50                | 15000             |
| 60                | 10000             |
| 70                | 7500              |
| 80                | 5000              |
| 90                | 4000              |
| 100               | 3500              |

The choice of the investigated range of $W$ is influenced by 3 effects. If $q$ is large, the $q$th power in Eq. (7) enhances the numerical and statistical errors, leading to a

$$R_q = \sum_{k=1}^{\lambda-d} \mu_k^q = \lambda^{\tilde{\tau}_q} \quad S_q = \frac{d R_q}{dq} = \sum_{k=1}^{\lambda-d} \mu_k^q \ln \mu_k,$$

where $\lambda = \frac{L}{d}$ and $\tilde{\tau}_q$ is the finite system mass exponent. $\tau_q$, corresponding to the thermodynamic limit, and its derivative reads as:

$$\tau_q = \lim_{\lambda \to 0} \frac{\ln R_q}{\ln \lambda} \quad \alpha_q = \frac{d \tau_q}{dq} = \lim_{\lambda \to 0} \frac{S_q}{R_q \ln \lambda}.$$  

$\tau_q$ can be rewritten in the following form:

$$\tau_q = D_q(q-1) = d(q-1) + \Delta_q,$$

where $D_q$ is the generalized fractal dimension, and $\Delta_q$ is the anomalous scaling exponent. Employing a Legendre-transform on $\tau_q$, and obtain the singularity spectrum, $f(\alpha)$:

$$f(\alpha_q) = qa \alpha_q - \tau_q.$$  

$\tau_q$, $\alpha_q$, $D_q$ and $\Delta_q$ are often referred to as multifractal exponents.

According to recent results a symmetry relation exists for $\alpha_q$ and $\Delta_q$ given in the form:

$$\Delta_q = \Delta_{1-q} \quad \alpha_q + \alpha_{1-q} = 2d$$

For numerical approaches one has to define the finite-size version of these MFEs at a particular value of disorder:

$$\tilde{\alpha}^{ens}_q(W,L,\ell) = \frac{\langle S_q \rangle}{\langle R_q \rangle \ln \lambda},$$

$$\tilde{D}^{ens}_q(W,L,\ell) = \frac{1}{q-1} \frac{\ln \langle R_q \rangle}{\ln \lambda},$$

where $\langle \rangle$ stands for ensemble averaging over the different disorder realizations. Typical averaged versions can be also defined as

$$\tilde{\alpha}^{typ}_q(W,L,\ell) = \langle S_q \rangle \frac{1}{\ln \lambda},$$

$$\tilde{D}^{typ}_q(W,L,\ell) = \frac{1}{q-1} \frac{\ln \langle R_q \rangle}{\ln \lambda}.$$
Equations (16a)–(16b) can be summarized in one equation:

\[ \tilde{D}_q(W, L, \ell) = D_q + \frac{q}{\ln A_q} T_q \left( \frac{L}{\xi}, \frac{\ell}{\xi} \right) \]  

(16b)

These two effects together lead to a regime where the physically interesting quantities and confidence intervals of the fit parameters. This fit procedure will provide us the physically interesting quantities and confidence intervals. In the next subsections we are going to present different methods for the finite size scaling.

### A. Finite size scaling at fixed λ

At fixed λ, \( G_q \) in Eq. (18) can be considered as the constant term of \( G_q \), therefore

\[ \tilde{G}_q(W, L, \ell) = G_q + \frac{1}{\ln \lambda} G_q \left( \frac{L}{\xi}, \frac{\ell}{\xi} \right) \]  

(17)

where the constant λ has been dropped. \( G_q \) can be expanded with one relevant, \( g(w) \), and one irrelevant operator, \( \eta(w) \), the following way using \( w = W - W_c \):

\[ G_q \left( \rho L^q, \eta L^{-y} \right) = G_q^r \left( \rho L^q \right) + \eta L^{-y} G_q^{ir} \left( \rho L^q \right) \]  

(20)

### B. Finite size scaling for varying λ

In order to take into account different values of λ the scaling law given in Eq. (17) has to be considered. The expansion of \( G \) in (17) is

\[ G_q \left( \rho L^q, \rho \ell^q, \eta' L^{-y'}, \eta' \ell' \right) = G_q^r \left( \rho L^q, \rho \ell^q \right) + \eta' L^{-y'} G_q^{ir} \left( \rho L^q, \rho \ell^q \right) \]

According to Rodriguez et al. [14] the most important irrelevant term is the one containing the finite box size, \( \ell \), therefore we took into account that one only. This leads to

\[ \tilde{G}_q(W, L, \ell) = G_q + \frac{1}{\ln \lambda} \left( G_q^r \left( \rho L^q, \rho \ell^q \right) + \eta \ell' \eta' L^{-y'} G_q^{ir} \left( \rho L^q, \rho \ell^q \right) \right) \]  

(24)
The Taylor-expansions of the above functions are

\[
G_q^r \left( gL^\frac{r}{2}, g\ell^\frac{r}{2} \right) = \sum_{i=0}^{n_r} \sum_{j=0}^{n_r} a_{ij} g^i L^{\frac{r}{2}} \ell^{-\frac{i}{j}}
\]  

(25)

\[
G_q^{ir} \left( gL^\frac{r}{2}, g\ell^\frac{r}{2} \right) = \sum_{i=0}^{n_r} \sum_{j=0}^{n_r} b_{ij} g^i L^{\frac{r}{2}} \ell^{-\frac{i}{j}}
\]  

(26)

\[
\varrho(w) = w + \sum_{i=2}^{n_r} c_i w^i
\]

\[
\eta(w) = 1 + \sum_{i=1}^{n_r} d_i w^i
\]  

(27)

The advantage of this method is, that it provides the MFE, since it is one of the parameters to fit, \( G_q \). There are many more data to fit compared to the fixed \( \lambda \) case. Fixed \( \lambda \) means, that at a given system size one can use GMFEs obtained at a certain value of \( \ell \) – the one that leads to the desired \( \lambda \) – , while in this case one can fit to GMFEs obtained at different values of \( \ell \). However, these GMFEs are correlated, because they are the results of the coarse graining of the same wave functions with different sizes of boxes. During the fitting procedure one has to take into account these correlations, see Sect. 3. Since the relevant and irrelevant scaling functions have two variables, \( gL^\frac{r}{2} \) and \( g\ell^\frac{r}{2} \), one has to fit a two-variable function with number of parameters \( 3n_r(n_r + 1)/2 + 3n_{ir}(n_{ir} + 1)/2 + n_r + n_{ir} - 1 \). We can see, that the number of parameters grows as \( \sim n_{r/ir}^2 \), instead of \( \sim n_{r/ir} \), as for fixed \( \lambda \). This makes the fitting procedure incorporating the correlations definitely much more difficult.

C. General principles for the FSS fit procedures

In this section we discuss the details of the methods and criteria we used during the MFSS. In order to fit the scaling law Eq. (19) and (24) we used the MINUIT library. To find the best fit to the data obtained numerically the order of expansion of \( G_q^{ir} \), \( g \) and \( \eta \) must be decided by choosing the values of \( n_r, n_{ir}, n_q \) and \( n_{ir} \). Since the relevant operator is more important than the irrelevant one we always used \( n_{rel} \geq n_{ir} \) and \( n_q \geq n_{ir} \). To choose the order of the expansion we used basically three criteria. The first criterion we took into account was how close the ratio \( \chi^2/(N_{df} - 1) \) approached one \( (N_{df} \) stands for number of degrees of freedom). Let us denote the numerically obtained datapoints by \( y_i \), the fit function value by \( f_i \) at the \( i \)th parameter value, and \( C \) the correlation matrix of the numerically obtained data points, that can be computed numerically with a similar expression to the variance. With these notations \( \chi^2 \) reads as

\[
\chi^2 = \sum_{i,j} \frac{(y_i - f_i) (C^{-1})_{ij} (y_j - f_j)}{\sigma^2_i}
\]  

(28)

for more details see Ref. 13. If the data points are not correlated, \( \chi^2 \) is a diagonal matrix, and the expression leads to the usual form:

\[
\chi^2 = \sum_i \frac{(y_i - f_i)^2}{\sigma^2_i}
\]  

(29)

The number of degrees of freedom, \( N_{df} \) is the number of data points minus the number of fit parameters. A ratio \( \chi^2/(N_{df} - 1) \approx 1 \) means, that the deviations from the best fit are in the order of the standard deviation (correlation matrix). The second criterion was, that the fit has to be stable against changing the expansion orders, i.e. adding a few new expansion terms. From the fits that fulfilled the first two criteria we chose the simplest model, with the lowest expansion orders. Sometimes we also took into account the error bars, and we chose the model with the lowest error bar for the most important quantities \( (W, \nu, \text{etc...}) \), if similar models fulfilled the first two criteria.

The error bars of the best fit parameters were obtained by a Monte-Carlo simulation. The data points are results of averaging, so due to central limit theorem they have a Gaussian distribution. Therefore we generated Gaussian random numbers with parameters corresponding the mean of the raw data points and standard deviation (correlation matrix) of the mean, and then found the best fit. Repeating this procedure \( N_{MC} = 100 \) times provided us the distribution of the fit parameters. We chose 95% confidence level to obtain the error bars.

IV. RESULTS OF THE MFSS FOR THE ANDERSON MODELS IN THE WD SYMMETRY CLASSES

With the numerical method described in Sect. 3 we computed an eigenvector for every disorder realization of the Hamiltonian. From the eigenvectors every GMFE is computable, for the orthogonal and unitary class the \( |\Psi_i|^2 \) expression in Eq. 6 is trivial, and it means summation for the spin-index for the symplectic class, because spatial behavior is in our interest. At fixed \( q \) and \( \Delta_q \) are linear transforms of \( D_q \), therefore we used only the \( \alpha_q \) and \( D_q \) GMFEs for the MFSS. We investigated the range \( -1 \leq q \leq 2 \), because GMFEs behave the best in this regime for the reasons described in Sect. 3.

A. Results of the MFSS at fixed \( \lambda = 0.1 \)

The typical behavior of the GMFEs is presented in Fig. 1. In all cases there is a clear sign of phase transition: With increasing system size the GMFEs tend to opposite direction on both sides of their crossing point. Note, that there is no well-defined crossing point due to the irrelevant term in Eq. 20. Applying the MFSS method described in Sect. 3.1 with the principles of Sect. 3.1C to the raw data leads to a very well fitting function, see the red lines on Fig. 1. After the subtraction of the irrelevant part from the raw data, plotting it
as a function of $\theta L^2$ results a scaling-function also, see the insets of Fig. 1.

The MFSS provided us the critical point, $W_c$, the critical exponent, $\nu$, and the irrelevant exponent, $y$ at every investigated values of $q$, the results are visible in Fig. 2. The parameters of the critical point correspond to the system itself, therefore it should not depend on the quantity we used to find it. In other words it should be independent of $q$, the averaging method and the GMFE we used. From Fig. 2 it is clear, that this requirement is fulfilled very nicely. There is a small deviation for the irrelevant exponent, $y$, obtained from $\alpha^{\text{typ}}$ at $q = -1$ and $q = -0.75$ in the unitary and symplectic class, but since $y$ describes the sub-leading part, it is very hard to determine, and we cannot exclude some sort of underestimating the error bar of this exponent. Another interesting feature of the results is, that the error bars are getting larger as $q$ goes above 1. As written in Sect. III C large $q$ enhances the errors through the $q$th power in Eq. (7), leading to bigger error bars. Similar effect can be seen around $q \approx -1$, where the relatively less precise small wave-function values dominate the sums in Eq. (7), that can also contribute to the deviation of $y$ obtained from $\alpha^{\text{typ}}$ in this regime. These two effects together lead to our investigated interval $-1 \leq q \leq 2$, where GMFEs behave the best. The results are strongly correlated, since they were obtained from the same wave functions, therefore they cannot be averaged. We chose a typical $q$-point for every symmetry class to describe the values of the critical parameters, see Tab. 1.

In the orthogonal class the critical parameters are in excellent agreement with the most recent high precision results of Rodriguez et. al [13], $W_c^{\text{Ro}} = 16.517$ (16.498..16.533), $\nu^{\text{Ro}} = 1.612$ (1.593..1.631) and $y^{\text{Ro}} = 1.67$ (1.53..1.80), obtained from $\alpha_0$ with the same method (fixed $\lambda$). This agreement verifies our numerics and fit method, and makes it reliable for the other two universality classes.

In the unitary class the critical parameters match with the results of Slevin and Ohtsuki [12], $W_c^{\text{U}} = 18.375$ (18.358..18.392) and $\nu^{\text{U}} = 1.43$ (1.37..1.49), obtained by transfer matrix method (they did not published the value of the irrelevant exponent). They used magnetic flux $\Phi = \frac{1}{4}$, while we used $\Phi = \frac{1}{2}$, and according to Drse et al., $W_c$ depends on the applied magnetic flux. However, on Fig. 2 of Ref. [22] is seen, that the critical points at $\Phi = \frac{1}{4}$ and $\Phi = \frac{1}{2}$ are very close to each other, hence the agreement between our critical point and the result of Slevin and Ohtsuki.

In the symplectic class the critical parameters agree more or less with the results of Asada et. al [10], $W_c^{\text{S}} = 20.001$ (19.984..20.018), $\nu^{\text{S}} = 1.375$ (1.359..1.391) and $y^{\text{S}} = 2.5$ (1.7..3.3), obtained by transfer matrix method. However, the difference seems not very large, our critical point is considerably different, even though we used exactly the same model. Due to bigger computational resources we could investigate much bigger system sizes than they did, therefore it is possible, that they underestimated the role of the irrelevant scaling, resulting in a somewhat higher critical point.

The critical points are higher in the unitary and in the symplectic class, then in the orthogonal class showing, that broken time-reversal or spin-rotational symmetry requires more disorder to localize wave-functions. The relationship between the $W_c^{\alpha}$ and $W_c^{\text{S}}$ probably depends on the applied magnetic flux, and the strength of the spin-orbit coupling. However, because of their close value of the critical exponents, $\nu^{\alpha}$ and $\nu^{\text{S}}$ are the same within our confidence interval, the following relation appears: $\nu^{\alpha} > \nu^{\text{U}} > \nu^{\text{S}}$. The situation for the irrelevant exponent is similar namely, that they are the same within error bar, but $y^{\alpha}$ seems to be slightly higher than $y^{\text{U}}$, that is a bit higher than $y^{\text{S}}$.

B. Results of the MFSS at varying $\lambda$

As it was mentioned in Sect. III C GMFEs obtained by typical averaging are equal to ensemble averaged GMFEs only in a range of $q$, $q_0 < q < q_\ell$. Since we intended to compute the MFEs also, we restricted our analysis to ensemble averaged GMFEs, and left the label $\text{ens}$ from the notations.

We fitted the formula Eq. (24) to the raw data. To do that, we had to choose a range of the box size $\ell$, that is used for the MFSS. We always used the widest range of $\ell$, that resulted convergence, $\chi^2/(N_{df} - 1) \approx 1$. We found, that for our dataset for different values of $q$ for $\alpha_0$ or $D_q$ different ranges of $\ell$ were the best. We used minimal box sizes $\ell_{\text{min}} = 2$ or $\ell_{\text{min}} = 3$ and maximal box sizes corresponding to $\lambda_{\text{max}} = 0.1$ or $\lambda_{\text{max}} = 0.66$. At $q = 0.4$ and $q = 0.6$ fit method had sometimes convergence troubles and resulted large error bars, because these points are close to the special case of $q = 0.5$ where by definition $\alpha_{0.5} = \lambda$. Artifacts from this regime were also reported in Ref. [13], therefore we decided not to take into account these points for $\alpha$. Results of the MFSS fit are visible in Fig. 3. The results are independent of $q$ and the used GMFE, as for the fixed $\lambda$ method. In Sect. IV A we already saw, that according to the arguments of Sect. III C error bars are getting bigger, if $q$ grows beyond 1. This phenomena is seen here much more amplified, while in Ref. [13] similar effect is visible on a moderate level. The difference between our results is probably due to the fact, that they used system sizes up to $L = 120$, that was not possible for us, mainly because of the long runtime and large memory usage for the symplectic model. They also use $\ell_{\text{min}} = 1$ and $\ell_{\text{min}} = 2$, while $\ell_{\text{min}} = 1$ was never suitable for our dataset. We have less data and less number of samples compared to them, and noise get bigger as $\ell$ decreases, because of the smoothing effect of boxing described in Sect. III C.

As written in Sect. IV A the results for different values of $q$ are strongly correlated, therefore we chose one of them with the lowest error bars, that represents well the results for that universality class.
FIG. 1: Dots are the raw data for different GMFEs in the the conventional WD symmetry classes. Red line is the best fit obtained by MFSS. Insets are scaling functions on a log-log scale, after the irrelevant term was subtracted. Error bars are shown only on the large figures, in order not to overcomplicate the insets.

FIG. 2: Critical parameters of the Anderson models in WD classes obtained by MFS at fixed \( \lambda = 0.1 \). First row corresponds to the orthogonal class, second row corresponds to the unitary class, third row corresponds to the symplectic class.
FIG. 3: Critical parameters of the Anderson models in WD classes obtained by two-variable MFFS with varying $\lambda$. First row corresponds to the orthogonal class, second row corresponds to the unitary class, third row corresponds to the symplectic class.

TABLE II: Result of the MFSS at fixed $\lambda = 0.1$ for the selected values of $q$. 

|   | exp $\alpha_{\text{exp}}$ | $W_c^\lambda$ | $\nu^\lambda$ | $\eta^\lambda$ | $N_\chi$ | $\chi^2$ | $\eta_1, \eta_2, \eta_3, \eta_4$ |
|---|---------------------------|---------------|---------------|---------------|----------|----------|-------------------------------|
| ort | $\alpha_{\text{ort}}$ | 16.524 (16.511, 16.538) | 1.598 (1.576, 1.616) | 1.763 (1.679, 1.842) | 172 | 170 | 3 2 1 0 |
| uni | $\alpha_{\text{uni}}$ | 18.373 (18.358, 18.386) | 1.424 (1.407, 1.436) | 1.633 (1.516, 1.751) | 198 | 179 | 4 2 1 0 |
| sym | $\alpha_{\text{sym}}$ | 19.838 (19.812, 19.869) | 1.369 (1.305, 1.430) | 1.508 (1.309, 1.743) | 171 | 151 | 4 2 1 0 |
The critical parameters listed in Tab. IV are in a very nice agreement with our previous results for the fixed method of $\lambda = 0.1$, see Sect. IV A, and also with the results of Ref. 56. Comparing the critical parameters for the orthogonal case with the results of Rodriguez et. al.57 obtained by the same method, $W^{0}_{c, Rod} = 16.530$ (16.524..16.536), $v^{0}_{Rod} = 1.590$ (1.579..1.602), we see a nice agreement again. Moreover these results are more accurate with this method compared to the fixed $\lambda$ method, leading to (for $g^O$ and $g^U$ only almost) significantly different critical exponents and irrelevant exponents for the different WD classes, $\nu^O > \nu^U > \nu^S$ and $g^O \geq g^U > g^S$.

C. Analysis of the multifractal exponents

The resulting MFEs are listed in Tab. V and depicted in Fig. 4. However, curves are very close to each other, at most of the $q$ values there is a significant difference between the data points of different symmetry classes, that is clear from Tab. V or Fig. 6. For the orthogonal class one can find matching results with the listed MFE’s in Ref.56.

We tested the symmetry relation Eq. (11) for $\alpha_q$ and $\Delta_q$, the results are listed in Tab. V and depicted on Fig. 3. The symmetry relation is fulfilled in the range $-0.25 \leq q \leq 1.25$, and small deviations are visible outside this interval – for the orthogonal class only at $\alpha_{-1}$ and $\alpha_{2}$. In this regime error bars are growing very large, coming from mainly the large errors of $\alpha_{q \geq 1.5}$ and $D_{q \geq 1.5}$. Similar effects were already seen for the critical parameters in Fig. 3. It is really hard to estimate the correct error bars in this large $q$ case, and the deviation from the symmetry are small, therefore we believe, that differences appear only because of slightly underestimated error bars of $\alpha_{q \geq 1.5}$ and $D_{q \geq 1.5}$. All in all we found numerical results basically matching with Eq. (11).

Assuming, that $\Delta_q$ is an analytic function of $q$, using the symmetry relation Eq. (11), one can expand $\Delta_q$ in Taylor series around $q = \frac{1}{2}$:

$$\Delta_q = \sum_{k=0}^{\infty} c_k \left( q - \frac{1}{2} \right)^{2k} = \sum_{k=0}^{\infty} c_k \left( q(q-1) + \frac{1}{4} \right)^k = \sum_{k=0}^{\infty} c_k \sum_{i=0}^{k} \binom{k}{i} (q(q-1))^i \left( \frac{1}{4} \right)^{k-i} = \sum_{k=1}^{\infty} d_k (q(1-q))^k,$$

(30)

where the condition $\Delta_0 = \Delta_1 = 0$ forced by the definition of $\Delta_q$ (see Eq. 11) was used in the last step, leading to $k = 1$ as lower bound for the summation. Similar expression can be derived for $\alpha_q$ using the connection $\alpha_q = d + \frac{d}{q} \Delta_q$ derived from Eqs. (30)–(31):

$$\alpha_q = d + (1 - 2q) \sum_{k=1}^{\infty} a_k (q(1-q))^{k-1},$$

(31)

where $a_k = kd_k$. One can obtain the $d_k$ and $a_k$ coefficients by fitting the expressions Eq. (30)–(31). We used only the range $q \leq 1.25$, because beyond this regime – as written above – error bars are growing extremely large, and there are small deviations from the symmetry relation Eq. (11) also. We plotted $\Delta(q)$ and $\alpha(q)-d$ in Fig. 6 to make visible the presence of higher order terms of the expansion.

We fitted expressions Eq. (30)–(31) up to third order in all cases, the resulting expansion coefficients are listed in Tab. V. From the data listed one can see, that the expansion coefficients fulfill the relation $a_k = kd_k$. However $\alpha_q$ and $\Delta_q$ were obtained from the same wavefunctions, they are results of completely independent fit-procedures. Therefore the fact, that they satisfy the equation $a_k = kd_k$, confirm our result for their value.
Table III: Critical parameters of the Anderson models in the WD symmetry classes obtained by two-variable MFSS with varying \( \lambda \). First column is the symmetry class, second is the GMFE used for the MFSS, third is the critical point, fourth is the critical exponent, and fifth is the irrelevant exponent.

| class | exp     | \( W_c \)       | \( \nu \)     | \( y \)     |
|-------|---------|----------------|-------------|-------------|
| ort   | \( \alpha_0 \) | 16.524 (16.513..16.534) | 1.595 (1.582..1.609) | 1.749 (1.697..1.786) |
| uni   | \( D_{0.1} \) | 18.371 (18.363..18.380) | 1.437 (1.426..1.448) | 1.651 (1.601..1.707) |
| sym   | \( \alpha_0 \) | 19.836 (19.831..19.841) | 1.383 (1.359..1.412) | 1.577 (1.559..1.595) |

Table IV: Expansion coefficients of Eqs. (30)-(31) obtained by a fit depicted in Fig. 6.

| class | \( \alpha(q)^d \) | \( \alpha(q)^{1-q} \) |
|-------|----------------|----------------|
| ort   | 1.044 (1.041..1.047) | 1.097 (1.095..1.098) |
| uni   | 0.095 (0.085..0.105) | 0.096 (0.091..0.100) |
| sym   | 0.018 (0.012..0.025) | 0.017 (0.014..0.020) |
| \( a_1 \) | 1.046 (1.043..1.049) | 1.099 (1.096..1.102) |
| \( a_2 \) | 0.179 (0.164..0.193) | 0.185 (0.174..0.197) |
| \( a_3 \) | 0.042 (0.032..0.053) | 0.043 (0.035..0.050) |

Even though \( \varepsilon \ll 1 \) should hold, one can try to extrapolate to three-dimensions, \( \varepsilon = 1 \). This leads to \( d^O_1 \approx 0.699 \), \( d^O_2 \approx 0.301 \), \( d^U_1 \approx 0.707 \) and \( d^U_2 \approx -0.451 \). As one can see, these values are rather far from our numerical results, but this is not surprising for an \( \varepsilon \)-expansion at \( \varepsilon = 1 \). These results capture well the tendency at least, that \( d^O_1 \) is slightly smaller, than \( d^U_1 \). On the other hand it leads to \( d^O_2 \) and \( d^U_2 \) having opposite sign, that is far from our numerical results. It is interesting to mention, that the first-loop term, that is proportional to \( \varepsilon \) and leads to parabolic \( \Delta_q \), results \( d^O_1 = 1 \) and \( d^U_1 = \alpha_0 - d = 1 \), that are very close to our numerically measured values.

In this sense parabolic approximation is better for the orthogonal class, as compared to the fourth-loop order approximation. If higher order terms were obtained, or \( \Delta_q \) were expanded using another approach, our coefficients could provide relatively accurate values as a compared with analytical results.

V. SUMMARY

In this paper we examined the three-dimensional Anderson models belonging to the conventional WD symmetry classes with the help of multifractal finite size scaling using two methods: a simpler method for fixed \( \lambda \) leading to a single-variable scaling function, and a more complicated method for varying \( \lambda \) resulting in a two-variable scaling function. Both methods confirmed the presence of multifractality in all three symmetry classes, and we obtained critical parameters listed in Tabs. II and III in agreement with each other and with previous results known from the literature. The more complicated varying \( \lambda \) method provided more precise values for the critical parameters, listed in Tab. III and significantly different critical exponents for the different WD symmetry classes.

Applying the method of varying \( \lambda \) we also calculated the multifractal exponents, that basically fulfill the ex-
| q | class | $\alpha_k$ | $D_k$ | $f(\alpha_k)$ | $\alpha_k + \alpha_k$ | $\Delta \alpha_k$ |
|---|---|---|---|---|---|---|
| -1 | ctt | 0.555 (5.429.626) | 1.962 (4.304.935) | 2.297 (2.345.250) | 6.275 (2.360.666) | -0.103 (0.042.549) |
| | uni | 0.567 (5.629.570) | 3.970 (4.666.396) | 2.269 (2.303.224) | 6.331 (2.615.444) | -0.130 (0.195.062) |
| -0.75 | sym | 0.575 (5.690.579) | 4.001 (3.994.401) | 2.251 (2.298.222) | 6.379 (1.097.554) | -0.134 (0.237.063) |
| | ctt | 0.590 (5.878.557) | 1.713 (4.088.742) | 2.582 (2.599.264) | 6.133 (4.598.603) | -0.035 (0.054.312) |
| | uni | 0.533 (3.175.349) | 1.743 (3.749.754) | 2.565 (2.573.557) | 6.176 (6.131.629) | -0.062 (0.098.025) |
| | sym | 0.540 (3.506.543) | 1.773 (3.770.377) | 2.549 (2.558.253) | 6.221 (6.113.634) | -0.060 (0.114.023) |
| -1 | ctt | 0.755 (4.856.486) | 1.492 (3.488.396) | 2.800 (2.803.276) | 6.061 (3.959.619) | -0.008 (0.045.025) |
| | uni | 0.754 (4.955.526) | 1.517 (3.524.526) | 2.784 (2.787.281) | 6.103 (3.603.606) | -0.019 (0.041.001) |
| 0.75 | sym | 0.498 (4.577.348) | 1.254 (2.532.255) | 2.945 (2.946.944) | 6.016 (5.951.694) | -0.000 (0.012.010) |
| | ctt | 0.500 (4.567.406) | 1.276 (2.566.268) | 2.943 (2.945.941) | 0.037 (5.958.401) | -0.006 (0.031.002) |
| | uni | 0.496 (4.603.404) | 1.274 (2.474.275) | 2.941 (2.941.941) | 0.033 (5.967.672) | -0.004 (0.011.003) |

TABLE V: MFE $\alpha_k$, $D_k$ and $f(\alpha_k)$, and values for the corresponding symmetry relation Eq. (11) obtained for the WD symmetry classes.

Expected symmetry relation Eq. (11), small deviations were detected for large $q$—values probably due slightly underestimated error bars. However, the MFEs of different symmetry classes seem to be very close to each other, in most cases our work shows significant differences between them. We expanded the MFEs in terms of the variable $q(-1)$, and determined the expansion coefficients up to third order numerically. The expansion coefficients of Eq. (30) fulfill the expected relation $\alpha_k = k \alpha_k$ giving a further confirmation for the validity of our results for the MFEs listed in Tab. V. We also compared the numerical results to available analytical estimates, and found sometimes similar, but sometimes opposite qualitative behavior for expansion coefficients for the orthogonal and the unitary classes. Nevertheless, we believe that the numerical precision of our results should be used as tests for future renormalization or other type of expansion approximations. Therefore our results await analytical comparison.
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