Scaling law and critical exponent for α_0 at the 3D Anderson transition

Louella J. Vasquez[1,*], **Keith Slevin**[2,**], **Alberto Rodriguez**[1], and **Rudolf A. Römer**[1]

[1] Department of Physics and Centre for Scientific Computing, University of Warwick, Coventry, CV4 7AL, United Kingdom

[2] Department of Physics, Graduate School of Science, Osaka University, 1-1 Machikaneyama, Toyonaka, Osaka 560-0043, Japan

We use high-precision, large system-size wave function data to analyse the scaling properties of the multifractal spectra around the disorder-induced three-dimensional Anderson transition in order to extract the critical exponents of the transition. Using a previously suggested scaling law, we find that the critical exponent ν is significantly larger than suggested by previous results. We speculate that this discrepancy is due to the use of an oversimplified scaling relation.

1 Introduction

The metal to insulator transition (MIT) in the three-dimensional (3D) Anderson model of localization is one of the most interesting quantum critical phenomena [1,2]. The transition is characterized by the divergence of the correlation length ξ near the critical point. Here we consider non-interacting electrons subjected to a random potential (e.g. uniform distribution of disorder $[-W/2, W/2]$), the correlation length near the mobility edge E_c diverges as $\xi(E_c, W) \propto |W - W_c|^{-\nu}$ with W_c as the critical value of the disorder. The critical exponent ν characterizes the critical divergence and is the same for all models in a given universality class, here the 3D orthogonal class. To accurately estimate ν, several quantities have been used in previous work such as the reduced localization length obtained from transfer-matrix calculations, which gives $\nu = 1.57 \pm 0.02$ [3], and energy level statistics studies, which gives $\nu = 1.44 \pm 0.2$ [4].

An alternative approach is a direct study of the multifractal spectrum of the wavefunction at the MIT [5–8]. In principle, the system size dependence of different characteristics of the multifractal spectrum $f(\alpha)$ can be used for such a scaling study. In this work, we will determine ν using the parameter α_0 as the scaling variable. α_0 is the location of the maxima of both the multifractal spectrum and the probability density function (PDF) of the variable $\alpha = -\ln|\psi_i|^2/\ln L$ [8]. Hence ν will be estimated from the raw statistics of wave function intensities $|\psi_i|^2$. In the regime of extended states where the disorder is weak, α_0 approaches the dimension of the support $d = 3$ upon increasing system size L such that in the zero disorder limit only one value $\alpha(W = 0) = 3$ exists. Whereas in the localized region, α_0 increases with L. At the critical point of the MIT, α_0 is scale invariant, i.e. a constant independent of L. These characteristics are consistent with a second order phase transition and it has been suggested [9, 10] that near the critical

*   Corresponding author   E-mail: L.J.A.Vasquez@warwick.ac.uk
**   E-mail: slevin@margaux.phys.sci.osaka-u.ac.jp

point α_0 follows the scaling relation

$$\alpha_0(W) - \alpha_0(W_c) \propto |W - W_c|L^{\frac{1}{\nu}}. \tag{1}$$

However, no high-precision numerical test of this relation has ever been performed and one of the aims of the present study is to test its validity based in part on the high-quality wave function data presented in Refs. [6–8].

In order to estimate ν from finite-size data, we employ the usual finite-size scaling method [3], starting from the assumption that all values of $\alpha_0(W, L)$ can be described by a common scaling curve $\mathcal{F}(\chi_r L^{1/\nu}, \chi_i L^y)$. There are two corrections to the universal scaling as in (1): (i) nonlinearities in W of the scaling variables and, (ii) a correction due to an irrelevant scaling variable χ_i that takes into account the systematic shifting with L of the crossing point in the plot of $\alpha_0(W, L)$ vs W and that should disappear for large enough system sizes. After Taylor expansions of both arguments in $\mathcal{F}$, the scaling curve becomes $\alpha_0(W, L) = \sum_{l=0}^{n_I} \sum_{j=0}^{n_R} \chi_i^l L^{ly} a_{lj} \chi_r^j L^{j/\nu}$, with $a_{10} = a_{01} = 1$, $\chi_r(\omega) = \sum_{n=1}^{m_r} b_n \omega^n$, $\chi_i(\omega) = \sum_{n=0}^{m_i} c_n \omega^n$, $w = 1 - W/W_c$, b_n and c_n are coefficients. We will obtain the values of α_0 from the scaling of the generalized inverse participation ratios and also directly from the PDF as described in the following sections.

2   Determination of α_0 from the generalized inverse participation ratio

Given a lattice with volume L^d, the generalized inverse participation ratios (gIPR) are defined as $P_q = L^d \langle |\psi_i|^{2q} \rangle$. Here the average $\langle \cdots \rangle$ is over all sites and disorder realizations. The scaling law for P_q is expressed as $P_q(\lambda) \propto \lambda^{\tau_q}$ where λ is an effective length scale. The Legendre transformation of the mass exponents τ_q is the multifractal spectrum $f(\alpha) = q\alpha_q - \tau_q$ with $\alpha_q = \mathrm{d}\tau_q/\mathrm{d}q$. The α_0 corresponds exactly to the moment $q = 0$, that is $\alpha_0 = \mathrm{d}\tau_q/\mathrm{d}q|_{q=0}$. Let us briefly discuss our numerical procedure to obtain α_0 based on the scaling law of the gIPR [6, 7]. We consider a cubic lattice with linear length L and divide it equally into boxes of size l such that the effective length scale becomes $\lambda = l/L$. Using the box probability $\mu_k = \sum_{i=1}^{l^3} |\psi_i|^2$, the gIPR is now $P_q = \lambda^{-d} \langle \mu_k^q \rangle$. Finally, from the definition of τ_q in the scaling law we have $\alpha_0 = \langle \ln \mu_k \rangle / \ln \lambda$. To determine α_0 for a fixed L, the box size is varied with values in the range of $l \in [5, L/2]$ and α_0 is computed to be the slope of the linear plot of $\langle \ln \mu_k \rangle$ versus $\ln \lambda$. Fig. 1 shows the values of α_0 versus W and the fit obtained from the finite size scaling method. Here we have considered system sizes in the range $L \in [20, 30, \cdots, 100]$ with 10^4 eigenstates for each L and W.
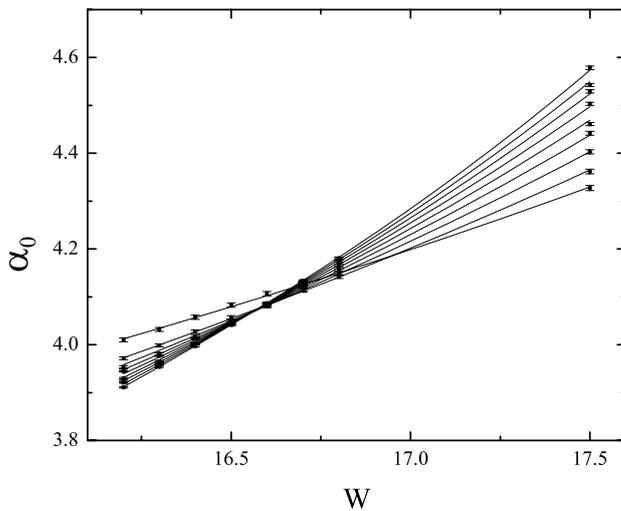

Fig. 1   Position α_0 of the maximum of $f(\alpha)$ shown as a function of disorder W for $W \in [16.2, 16.3, \cdots, 16.8, 17.5]$. Errors as shown denote one standard deviation. The fit (lines) used has the following parameters: $n_I = 1$, $n_R = 3$, $m_i = 1$, $m_r = 1$ and $y \sim -5$. Starting in the weak disorder regime, the different lines correspond to different L from $L = 20$ (top) to $L = 100$ (bottom). The estimated critical parameters are $W_c = 16.56 \pm 0.01$ and $\nu = 2.56 \pm 0.06$. The goodness of fit is 0.1.

3   Determination of α_0 from the probability density function

The distribution of $|\psi_i|^2$ is well-defined by the spread of the α values being that $|\psi_i|^2 = L^{-\alpha}$. The PDF $\mathcal{P}_L(\alpha)$ for $\alpha = -\ln|\psi_i|^2/\ln L$ satisfies $\mathcal{P}_L(\alpha) = \mathcal{P}_L(\alpha_0)L^{f(\alpha)-d}$. Since $f(\alpha) \leq d$, the maximum of the PDF is exactly located at $\alpha = \alpha_0$. This relation between $\mathcal{P}_L(\alpha)$ and $f(\alpha)$ gives a direct correspondence between the two. Here, the PDF was numerically determined by the histogram of α values [8]. To avoid the effects of bin size caused by the histogram method, the maximum of the PDF is instead more precisely estimated from the inflection point of the cumulative distribution function (CDF). Since in the first approximation the $\mathcal{P}_L(\alpha)$ near the maximum can be regarded to be a Gaussian distribution [8, 11], we fit the CDF with $[1 + \mathrm{Erf}(\alpha - \alpha_0/\sqrt{2}b)]/2$ by taking 10% of the total points around its inflection point (α_0). The scaling plot as obtained by the current method is shown in Fig. 2.
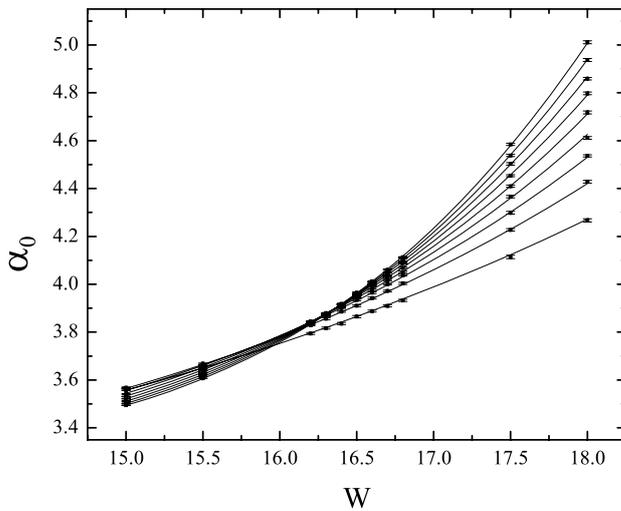

Fig. 2 Values of α_0 versus W for $W \in [15.0, 15.5, 16.2, 16.3, \cdots, 16.8, 17.5, 18.0]$, errors and lines as before in Fig. 1. The fit has the parameters: $n_I = 1$, $n_R = 5$, $m_i = 0$, $m_r = 3$ and $y \sim -1.5$. The corresponding critical parameters are $W_c = 16.47 \pm 0.04$ and $\nu = 2.36 \pm 0.07$. Goodness of fit is 0.1.

4   Conclusions

The multifractal spectrum $f(\alpha)$ is scale invariant at criticality [6,7]. This means that in principle *all* values of α_q can be used as a scaling parameter to determine the critical exponent of the transition. Here, we have concentrated on α_0, which is the most easily obtained of all the α_q, as it is simply given by the position of the maxima of $f(\alpha)$ and the PDF. In addition, we have also performed a similar finite-size scaling analysis for α_1 (where $f'(\alpha)\big|_{\alpha=\alpha_1} = 1$) and α_2 (obtained from the usual inverse participation ratio $L^d \langle|\psi_i|^4\rangle$). Results will be presented elsewhere. We find, quite surprisingly, that the extracted estimates for ν are consistently larger than commonly accepted [3, 4]. Their values are in the range of $2.1 \sim 2.5$. Since the size of the samples studied as well as the number of disorder realization is quite large, we are confident that these results are not due to insufficient numerical accuracy. Hence we speculate that it is the functional form of (1) which is incorrect. We assume a proper derivation of the scaling form of $f(\alpha)$ and the α_q will again allow the standard values to be reconfirmed.

References

[1] R. A. Römer and M. Schreiber, The Anderson Transition and its Ramifications – Localisation, Quantum Interference, and Interactions, Lecture Notes in Physics, Vol. 630, Chap. Numerical investigations of scaling at the Anderson transition (Springer, Berlin, 2003), pp. 3–19.

[2] F. Evers and A. D. Mirlin, Rev. Mod. Phys. **80** (October), 1355–1417 (2008).

[3] K. Slevin and T. Ohtsuki, Phys. Rev. Lett. **82**, 382–385 (1999), ArXiv: cond-mat/9812065.

[4] F. Milde, R. A. Römer, and M. Schreiber, Phys. Rev. B **61**, 6028–6035 (2000), ArXiv: cond-mat/9909210.

[5] A. Rodriguez, L. J. Vasquez, and R. A. Römer, Eur. Phys. J. B **67**, 77–82 (2009).

[6] L. J. Vasquez, A. Rodriguez, and R. A. Römer, Phys. Rev. B **78**, 195106 (2008), cond-mat:0807.2217v1.

[7] A. Rodriguez, L. J. Vasquez, and R. A. Römer, Phys. Rev. B **78**, 195107 (2008), cond-mat:0807.2209v1.

[8] A. Rodriguez, L. J. Vasquez, and R. A. Römer, Phys. Rev. Lett. **102**, 106406 (2009), cond-mat:0812.1654.

[9] M. Janssen, Int. J. Mod. Phys. B **8**, 943 (1994).

[10] B. Huckestein and L. Schweitzer, Physica A **191**, 406–409 (1992).

[11] F. Wegner, Nucl. Phys. B **316**, 663–678 (1989).