Critical level statistics at the Anderson transition in four-dimensional disordered systems

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1 Introduction

The statistical description of electronic spectra at the Anderson transition is one of the subjects of central interest. This quantum phase transition implies that there exists a non-vanishing value of the disorder of the random potential, at which the system undergoes the crossover between a conducting and an insulating phases with delocalised and localised electron states, respectively. The spatial dimensionality $d$ of the system plays an important role in determining the critical properties of both the conductivity and the level statistics. According to the one-parameter scaling theory of localisation, all single-electron states in the one and two dimensions are localised even for arbitrarily weak randomness, provided that the time-reversal and the spin-rotational symmetries are preserved. Therefore, the lowest integer dimension for which the disorder-induced metal-insulator transition (MIT) occurs for non-interacting particles is $d = 3$. Numerous computer simulations performed on transport electron properties have confirmed the scaling hypothesis (see, for example, [2, 3] and references therein). Furthermore, the MIT has been also found at the next higher integer dimensionality $d = 4$, by applying the transfer-matrix method (TMM) [4, 5]. The energy level statistics in two dimensions (2D) do not exhibit critical behaviour [6, 7], while in 3D they do [6, 8, 9, 10] in agreement with the earlier results obtained by the TMM [3]. A new universal scale-independent level spacing distribution $P(s)$ has been predicted exactly at the MIT in 3D [1]. This distribution differs characteristically from the results of the ‘classical’ random matrix theory (RMT) by Wigner and Dyson [11, 12], which is valid for weakly disordered conductors [13, 14]. An analytical approach...
has been developed recently \[15, 16\], which supposes that the shape of the \( P(s) \) at the mobility edge is given by a combination of the dimensionality \( d \) and the critical exponent \( \nu \) of the correlation length. At present this relation is intensively investigated for models of different basic symmetry, namely for the orthogonal \[17, 18, 19\], the unitary \[20, 21\] and the symplectic \[22, 23, 24\] critical ensembles. Here the critical disorders and the exponents are known, and the dependence of \( P(s) \) on \( \nu \) and \( d \) could be determined quantitatively. In order to obtain further insight, it is of great interest to study also critical parameters and the level statistics at higher dimensions.

In this paper we report results of detailed numerical calculations on the level statistics using the Anderson model for the 4D hypercubic lattice. We show that the nearest-neighbour level spacing distribution \( P(s) \) exhibits critical behaviour. Its shape is size-invariant at the transition, and its form considerably differs from that in 3D. Using the level statistics method in terms of the complete distribution of having \( n \) levels in a given energy interval we detect the metal-insulator transition, which corresponds to the disorder \( W_c = 34.5 \pm 0.5 \). We perform the finite size scaling analysis in order to find the one-parameter scaling function and to determine the correlation length exponent \( \nu \), which is smaller than that in 3D. Combining the results obtained for the statistic \( J_0 \) (defined below) and the variance of the level number we argue that the critical spectral fluctuations are stronger in 4D than in 3D, being closer to the Poissonian statistics.

2 Model and computational procedure

The model for the 4D disordered system is defined by the Anderson Hamiltonian

\[
H = \sum_n \epsilon_n c_n^\dagger c_n + V \sum_{n \neq m} (c_n^\dagger c_m + c_n c_m^\dagger),
\]

(1)

where \( c_n^\dagger \) (\( c_n \)) is the creation (annihilation) operator of an electron at a lattice site \( n \), and \( m \) denotes the sites adjacent to the site \( n \) (their number equals 8 for the simple hypercubic lattice). The site energies \( \epsilon_n \) are randomly distributed according to a box distribution with a width \( W \), which plays the role of the disorder parameter. The second term describes the hopping between the nearest-neighbour sites in the lattice. Our considerations are restricted to the particles without spin and with no magnetic field. It was earlier found by the TMM \[4\] that the MIT at the band centre \( E = 0 \) is close to the disorder \( W = 33.2 \). For 3D the critical disorder is smaller, \( W \approx 16.5 \) \[2\].

After numerical diagonalisation of the Hamiltonian \( \{1\} \) with periodic boundary conditions using the Lanczos algorithm we obtained the exact discrete spectrum of the electrons for simple 4D hypercubic lattices of various sizes ranging from \( L^4 = 4^4 \) to \( 10^4 \) and for different disorders \( W \). Linear and energy scales are measured in units of the lattice constant and the overlap integral between adjacent sites (\( V = 1 \)), respectively. The levels were taken from energy intervals centred at \( E = 0 \) so that they belong to the critical energy region, defined by the condition \( L < \xi = (|E - E_c|/E_c)^{-\nu} \), where \( \xi \) is the correlation length and \( E_c \) is the mobility edge. The number of realizations for a given size \( L \) was such that the total number of eigenvalues amounted as much as \( 10^5 \). We have checked that the density of states \( \rho = (\Delta L^4)^{-1} \) around the band centre slightly varies with the energy (\( \Delta \) is the mean level spacing). Therefore, the careful unfolding procedure has been applied for the spectra of all pairs of \( \{W, L\} \).
3 The critical level spacing distribution $P_c(s)$

A traditional way to study the statistical properties of disordered spectra is to consider the level spacing distribution $P(s)$ which is defined as the probability density of nearest neighbouring levels. It is known that in the metallic region $P(s)$ is very close to the Wigner surmise \[13\] for the Gaussian orthogonal ensemble (GOE) of random matrices \[11\], namely

$$P_{\text{GOE}}(s) = \frac{\pi}{2} s \exp \left( -\frac{\pi}{4} s^2 \right),$$  \hspace{1cm} (2)$$

where $s$ is measured in units of the mean level spacing $\Delta$. In the localised region the energy levels are completely uncorrelated, and hence the spacings are distributed according to the Poisson law

$$P_P(s) = \exp(-s).$$  \hspace{1cm} (3)$$

In a similar way as for the 3D Anderson model \[6\] \[8\] \[10\], the third, universal distribution $P_c(s)$ is supposed to be revealed exactly at the critical point, which is different from both of the above laws. For systems of finite size the level statistics is expected to change continuously from $P_{\text{GOE}}(s)$ through $P_c(s)$ to $P_P(s)$, when increasing the strength of fluctuations of the random impurity potential. When increasing the size of the system the distribution tends towards either $P_{\text{GOE}}(s)$ \[4\] or $P_P(s)$ \[4\], depending on whether the disorder is below or above its critical value, respectively.

Fig. 1 shows the function $P(s)$ calculated at the disorder $W$ very close to the critical point. The fact that the data within numerical errorbars lie on a common curve independent on $L$, defines the critical level spacing distribution $P_c(s)$ (see also section 5). In comparison with $d = 3$ the critical $P_c(s)$ for $d = 4$ is closer to $P_P(s)$. It is worth
Fig. 2: Large-$s$ part of the critical level spacing distribution $P_c(s)$ of the Fig. 1 for various system sizes $L$. Dashed-dotted straight line, $\ln P_c(s) = -1.4s$, is the best fit to the data. Dashed and dotted curves are $P_{GOE}(s)$ and $P_V(s)$, respectively.

noticing that our numerical data deviate considerably from the interpolation formula $P_c(s) = B s \exp(-A s^{1+1/d\nu})$ derived analytically in \cite{14}, where the coefficients $A$ and $B$ are defined by the normalisation conditions.

For small spacings we found the linear increase $P_c(s) = B s$, as consistent with the orthogonal symmetry. However, the linear slope $B \approx 2 B_{GOE}$ is larger than in $d = 3$ \cite{6} and, consequently, in the RMT. This indicates that the level repulsion becomes weaker with increasing $d$. The behaviour of $P_c(s)$ at larger spacings is well described by the sub-Poissonian form $P_c(s) \propto \exp(-A s)$ with $A = 1.4 \pm 0.1$. One can see in Fig. 2 that $P_c(s)$ changes by several orders of magnitude in the interval $2 < s < 10$. As expected, this asymptotic decay is slower compared to $d = 3$, where the exponential rate is $A \approx 1.9 \frac{19}{19}$, but faster than the Poissonian decay.

4 The probability distribution $Q_n(s)$

In order to perform the finite size scaling analysis and to study how the level statistics behave around the critical point, we have calculated the dependence of the statistics of neighbouring spacing on the disorder $W$ for different $L$. To include the entire range of spacings, we use here the probability distribution of having $n$ eigenvalues in a given energy interval of the width $s$:

$$Q_n(s) \equiv \int_s^\infty I_n(s') ds' = \int_s^\infty ds' \int_{s'}^\infty p_n(s''), ds'',$$

where $I_n(s)$ being the cumulative distribution of $n$ successive levels. The function $Q_n(s)$ is known for the metallic limit from the RMT \cite{12}. In the insulating limit the Poisson process $Q_n(s) = s^n \exp(-s)/n!$ governs the completely uncorrelated spectrum.

In what follows we investigate the probability to have no level, $n = 0$, within the bin $s$, which implies the level statistics for the case of nearest neighbour spacings. In
order to show \((L, W)\)-dependence we plot in Fig. 3 the absolute deviation from the Poisson process \(\Delta Q_0(s) = -[Q_0(s) - \exp(-s)]\). The data for the metallic phase, i.e. for \(W < W_c\), turn out to be closer to the GOE. The larger the system size, the closer the level statistics to this limit. When \(W > W_c\) the data approach zero, however with the opposite size effect. Closer to the critical disorder all of the data within statistical uncertainties start to fall onto a common intermediate curve independent of \(L\). This is the manifestation of critical behaviour. Similar scaling properties are also observed for \(Q_{n>0}(s)\).

4.1 The spectral statistic \(J_n\)

To parameterise the distribution \(Q_n(s)\) we deal with a global statistical quantity defined as follows

\[
J_n = \int_0^\infty Q_n(s)ds, \tag{5}
\]

which takes the whole range of the spacings into account. For \(n = 0\) one can easily show that it is related to the spacing variance \(\langle \delta^2 s \rangle\) as

\[
J_0 = \frac{1}{2}\langle s^2 \rangle = \frac{1}{2}(\langle \delta^2 s \rangle + 1). \tag{6}
\]

For investigating the critical properties of the spectra at the Anderson transition the statistic \(J_0\) was for the first time introduced in [17]. It proved to be more efficient than those which have previously been used in studying the 2D and 3D cases [4, 8, 10]. This is due to that since the probability density \(P(s) = p_0(s)\) and the cumulative distribution \(I_0(s)\) are normalised to unity, one had to choose some spacing \(s^*\) in order to weigh the functions after or before this point [6, 8, 11] for a given pair of the
parameters \{W, L\}. This leads however to loosing part of the information obtained from the diagonalisation and, as a result, decreases the accuracy. In contrast, the set of parameters \(J_n\) does not require \(s^*\). Therefore, \(J_n\) is more successful, in our opinion, for demonstrating the scaling properties of the level statistics with less number of realizations and, as consequence, to locate the MIT more precisely. For the GOE \(J_0 = 0.643\), \(J_1 = 0.922\), ..., \(J_{n=\infty} = 1\). In the localised regime, one has simply \(J_n = 1\) for any \(n\). For \(d = 3\) the set of the critical numbers \(J_n^c\) has been obtained in [17], for example, \(J_0^c \approx 0.714\) and \(\langle s^2 \rangle \approx 1.42\). In the presence of strong spin-orbit interactions, where the MIT occurs even for \(d = 2\), another set \(J_n^c\) describes the critical symplectic ensemble [22].

### 4.2 The finite size scaling and the critical exponent

We have calculated the dependence of \(J_0\) on \(W\) near the transition for various system sizes. All computed data lie within the interval between \(J_0^{\text{GOE}}\) and \(J_0^P\), gradually growing from the former to the latter limit, when increasing the disorder \(W\). The increase of \(J_0\) develops faster with \(L\). For an infinite system this change would transform to a discontinuous crossover between these two limits exactly at the transition \(W_c\). One observes from Fig. 4 that \(J_0(W)\) exhibits critical behaviour. The common crossing point \(J_0^c \approx 0.79\) (\(\langle s^2 \rangle \approx 1.57\)), where the size effect on the statistics changes sign, corresponds to the transition. Intersection of the curves of different \(L\) enables us to determine the fixed point more precisely, \(W = W_c = 34.5 \pm 0.5\). The obtained value is in reasonable agreement with that computed previously by the TMM [4, 5]. However it markedly deviates from the linear relation \(W_c(d) = (d - 2)W_c(d = 3)\).
Fig. 5: One-parameter scaling dependence of the statistic $J_0$ on $L/\xi$ for different system sizes $L$ and disorders $W$. Full straight line is the RMT result $J_0 = 0.643$ [12]. Dotted line is (8) with $J^0_0 = 0.79$ and the coefficient $C = 0.043$.

At the fixed point the correlation length diverges with the exponent $\nu$:

$$\xi(W) \propto |W - W_c|^{-\nu}. \quad (7)$$

By using the lowest terms of the expansion for the function $J_0(W, L)$ near $W_c$

$$J_0(W, L) \approx J^0_0 + C(W - W_c)L^{1/\nu} = J^0_0 + C \left( \frac{L}{\xi} \right)^{1/\nu}, \quad (8)$$

one extracts the critical exponent of the correlation length. Inset of Fig. 5 shows that the data within the numerical errors are well described by the linear approximation

$$\ln \frac{dJ_0(W, L)}{dW} \propto \nu^{-1} \ln L. \quad (9)$$

The estimated value $\nu = 1.1 \pm 0.2$ is consistent with previous findings [5]. It appeared to be smaller than that for $d = 3$ ($\nu \approx 1.45$ [10]). On the other hand, it is still larger than the standard mean-field result $\nu_{MF} = 1/2$, valid for the upper bound $d_u$ of the Anderson transition [25]. Based on our results one can argue that $d = 4$ is definitely lower than $d_u$, which is believed to be equal infinity [26].

By introducing the scaling variable $\xi$, which is identified as the correlation length, it is possible to replot all of the data in Fig. 5 into a single-parameter function, as shown in Fig. 5. The resulting curve $J_0(L/\xi)$ consists of two branches characteristic of different regimes of the disorder-induced MIT. The decaying branch corresponds to the metallic phase ($W < W_c$) and the growing one belongs to the insulating phase ($W > W_c$). Outside of the critical region, i.e. $L/\xi > 1$, the numerical data deviate from the linear approximation (8). The one-parameter finite size scaling procedure allows one to find the dependence of the correlation length $\xi$ on the disorder. Close to $W_c$ the numerical results of $\xi(W)$ shown in Fig. 5 give a satisfactory agreement with (7), while far apart from the fixed point one observes a considerable discrepancy. Thus, the critical behaviour of the spectral statistics in 4D is typical for the Anderson transition and analogous to that for the 3D case [5, 8, 10].
5 Variance of the energy level number

While the spacing distribution $P(s)$ and, consequently, $J_0$ probe the short-range correlations in the electron spectra, the variance of the number of levels $\langle \delta^2 N(E) \rangle$ in a given energy interval $E$, which describes the global spectral rigidity, can provide the information about fluctuations on scales much larger than $\Delta$. It is defined as a width of the distribution of $N$ levels in the interval $E$: $\langle \delta^2 N(E) \rangle = \sum_{N=0}^{\infty} (N - \langle N \rangle) Q_N(E)$. In the extreme insulating limit $W \gg W_c$ the number variance obeys the ordinary Poisson law $\langle \delta^2 N(E) \rangle = \langle N(E) \rangle$. For any finite $W$ the eigenfunctions can spatially overlap, so that the fluctuations $\langle \delta^2 N \rangle$ are reduced below the Poisson limit due to level repulsion. When the system is a good conductor, i.e $W \ll W_c$, the electron states are spread over the entire volume. Therefore the number variance for $\langle N \rangle \gg 1$ can be approximated by the Dyson formula

$$\langle \delta^2 N \rangle = \frac{2}{\pi^2} \ln \langle N \rangle + \gamma, \quad \gamma \approx 0.44,$$

valid for the Gaussian orthogonal ensemble of random matrices [12, 13]. Thus, the relative variance $(\delta^2 N)/\langle N \rangle$ for large $\langle N \rangle$, which is also known as a spectral compressibility $\kappa$, changes from zero to unity as $W$ increases. Of particular interest is the question how does the relative variance behave at $W = W_c$. For instance, in 3D systems it was numerically shown that its critical value equals a constant $\kappa_c \approx 0.27$ [17]. It may also be worth considering in more detail the number variance for weakly disordered 4D systems in order to compare with the results of the diffusive theory [14].

Fig. 6 shows the numerical results of the relative number variance around the transition. The size dependence below and above the critical point is very similar to that of $\Delta Q_0(s)$ in Fig. [3]. With increasing $L$ the data approach the Dyson result [14] if $W < W_c$, while $\kappa \to 1$ if $W > W_c$, respectively. At $W = W_c = 34.5$ the ratio $\langle \delta^2 N \rangle/\langle N \rangle$ is almost insensitive to $L$. This justifies again the existence of the intermediate scale-invariant statistics at the long-range energy correlations. The ratio $\langle \delta^2 N \rangle/\langle N \rangle$ at the MIT decreases very slowly with increasing the mean level number $\langle N \rangle$. 

![Fig. 6: Disorder dependence of the correlation length $\xi(W)$ for 4D disordered system. Dotted line is (7).](image)
Recently the analytical theory has been proposed [27] suggesting that the compressibility at the mobility edge is totally characterised by properties of the critical eigenstates and is directly determined in terms of the multifractal exponent \(\mu = d - D_2\) and \(\kappa_c\) as

\[
\kappa_c = \lim_{\langle N \rangle \to \infty} \frac{d\langle \delta^2 N \rangle}{d\langle N \rangle} = \frac{\mu}{2d} < \frac{1}{2}. \tag{11}
\]

The results of \(\mu\) and \(\kappa_c\) obtained numerically so far for lower dimensions \(d \leq 3\) satisfy reasonably this relation. Our 4D-data for sufficiently large values \(\langle N \rangle > 20\) yet obey at least the condition for the above upper limit, going down to \(\kappa_c \approx 0.45 - 0.5\). This value appears to be larger than that of 3D, indicating that the critical spectral rigidity diminishes. However the accuracy of \(\langle \delta^2 N \rangle\) is still not high enough to reach a precise saturation value at \(\langle N \rangle \gg 1\) and, as a result, to provide a reliable estimate of \(\mu\) from (11). In addition, an independent computational analysis of the multifractality of eigenfunctions in 4D would be needed.

6 Conclusions

We have numerically calculated the critical distribution of neighbouring spacings \(P(s)\) at the metal-insulator transition for the 4D Anderson model. The disorder-induced crossover between the Wigner and the Poisson statistics for finite systems is shown to obey a one-parameter scaling law as for lower dimensions. The finite size scaling analysis of the level statistics allows one to locate the critical disorder \(W_c\) and to detect the correlation length exponent \(\nu\). Comparing the obtained results with lower dimensions we are led to the conclusion that the spectral correlations at criticality depends on the spatial dimensionality, becoming weaker with increasing \(d\). The further systematic study of the dimensionality dependence would be desirable in order to answer the question how the critical level statistics favours the Poissonian limit, when approaching the upper bound of the Anderson transition [28]. Another interesting problem for simulations in 4D could be spectral fluctuations in a weakly disordered
metal to check the non-perturbative theory \[28\].

7 Acknowledgements

We thank L. Schweitzer, A.D. Mirlin and M. Schreiber for useful discussions. I.Kh.Zh. thanks DFG for the financial support during his stay at the University of Hamburg. The support from the TMR-Network (contract FMRX CT96-0042) and the Sonderforschungsbereich 508 “Quantenmaterialien” of the University of Hamburg is gratefully acknowledged.

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