SCALING OF LEVEL STATISTICS
AT THE METAL–INSULATOR TRANSITION

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Abstract. Using the Anderson model for disordered systems the fluctuations in electron spectra near the metal–insulator transition were numerically calculated for lattices of sizes up to $28 \times 28 \times 28$ sites. The results show a finite–size scaling of both the level spacing distribution and the variance of number of states in a given energy interval, that allows to locate the critical point and to determine the critical exponent of the localization length.

The statistical description of energy spectra of disordered quantum systems is based on the random–matrix theory [1–3]. One of the main properties of the spectra of random–matrices is the repulsion between their eigenvalues. For a disordered metal, such a correlation of energy levels is caused by a pronounced overlap of delocalized one–electron states. By increasing the disorder of a random potential the system is known to undergo a metal–insulator transition (MIT). On the insulating side of the MIT, the energy levels of the localized states are not correlated due to vanishing of the level repulsion. A central question in the problem of level statistics is how a character of spectral fluctuations varies when the system changes from the delocalized to the localized regime.

On the metallic side of the MIT the distribution function $P(s)$ of neighboring spacings between levels can be described by the Wigner formula [4]

$$P_W(s) = \frac{\pi}{2} s \exp\left(-\frac{\pi}{4}s^2\right),$$

(1)

where $s$ is measured in units of the mean inter–level spacing $\Delta$. In the

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H.A.Cerdeira et al. (eds.), Quantum Dynamics of Submicron Structures, 93-98
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localized regime the spacings are distributed according to a Poisson law

\[ P_P(s) = \exp(-s). \] (2)

The crossover of \( P(s) \) between the Wigner (1) and the Poisson statistics (2) which accompanies the MIT was extensively investigated both numerically [5–8] and analytically [9, 10]. It was pointed out by Shklovskii et al [7] that the level spacing distribution exhibits critical behavior near the MIT. Therefore we focus on the finite–size scaling properties of the distribution \( P(s) \). In addition, we analyze the variance of the number of energy levels \( \langle \delta N(E)^2 \rangle \) as a function of the average level number \( \langle N(E) \rangle \) in a specified energy interval \( E \), and study its universal peculiarities at the critical point.

One of the simplest models describing a disorder–induced MIT is the Anderson model

\[ H = \sum_n \epsilon_n a_n^+ a_n + \sum_{n \neq m} (a_n^+ a_m + a_n a_m^+). \] (3)

Here \( a_n^+ \) and \( a_n \) are the creation and annihilation operators of an electron at a site \( n \) in a lattice; \( m \) denote the nearest neighbors of \( n \). The on-site energy \( \epsilon_n \) is measured in units of the overlap integral between adjacent sites and is uniformly distributed variable in the interval from \(-W/2\) to \(W/2\). The parameter \( W \) specifies the degree of the disorder of the system. The critical disorder of the MIT which occurs in the middle of the band corresponds to \( W_c \approx 16.5 \) [11]. For a finite system when \( W \ll W_c \), the level statistic is close to (1) and when \( W \gg W_c \) it obeys (2) [5].

In order to find the electron spectrum in the critical region we diagonalized numerically the real symmetric Hamiltonian (3) for simple cubic lattices of the size \( L \times L \times L \) with periodic boundary conditions. The Lanczos algorithm for eigenvalue problem was used in a version that was especially designed for very sparse and big matrices with hierarchic structure. We applied the algorithm for cubes with \( L = 6, 8, 12, 16, 20, 24, 28 \) at various degree of the disorder close to \( W_c \). We consider an energy interval which is centered at \( \epsilon = 0 \) and has such a width that it contains a half of all eigenvalues. As we are interested in sample–to–sample fluctuations in the spectra the calculations were carried out for ensembles of different random configurations. After unfolding the spectrum the histograms of several spectral distributions were constructed by use of \( 10^5 \) spacings calculated for each pair of \( \{L, W\} \).

Fig. 1 displays the distribution function \( P(s) \) calculated near the MIT for two cubes of sizes \( L = 6 \) and \( L = 28 \). By increasing the disorder \( W \) the spacing distribution for both \( L \) varies continuously from \( P_W(s) \) to \( P_P(s) \) over all range of spacings. Results of calculations for other, intermediate sizes confirm this continuous crossover. But the behavior of this crossover substantially depends on the size of the cube. One can see that \( P(s) \) changes
Figure 1. The level–spacing distribution $P(s)$ for various disorders near the transition. Continuous curves correspond the Wigner (1) and the Poisson (2) distributions for the metallic and insulating phases, respectively.

faster between (1) and (2) for $L = 28$ than for $L = 6$. The size–dependence of $P(s)$ is observed on both sides of the MIT. However at the transition point when $W_c = 16.5$ the spacing distribution has almost the same form for all $L$ from 6 to 28. The independence of the level spacing distribution on the size of system at $W_c$ is in good agreement with predictions of the new universal level statistics at $L \to \infty$ which exists exactly at the transition[7].

In order to study the scaling properties of the spacing distribution in more detail we introduce the quantity $\alpha = \int_{s_0}^{s} (P(s) - P_W(s)) ds / \int_{s_0}^{s} (P_P(s) - P_W(s)) ds$, which describes a normalized deviation of $P(s)$ from the Wigner distribution (1). We chose $s = 0.473$, the crossing point of $P_W(s)$ and $P_P(s)$, in order to study $P(s)$ in the range of small spacings. In this case $\alpha$ corresponds to a “strength” of the repulsion of two consecutive levels when the separation between them is less than average spacing $\Delta$. In the thermodynamic limit $\alpha = 0$ for $W < W_c$, and $\alpha = 1$ for $W > W_c$. For finite $L$ it is reasonable to assume a scaling law

$$\alpha(W, L) = f(L/\xi(W)),$$

where $\xi(W)$ is the correlation length of the transition.

Fig. 2 shows the $L$-dependence of the parameter $\alpha$ near the critical point. In the insulating regime $\alpha$ grows with $L$ approaching its limit $\alpha = 1$, whereas in the metallic phase $\alpha$ decreases to zero. The change of the sign of the size effect takes place at the critical point. Therefore we can determine very accurately the critical value of the disorder $W_c = 16.35 \pm 0.15$. Similar results for smaller systems were earlier obtained in Ref. [7, 8] for $s_0 = 2$ which corresponds to using $P(s)$ only in the range of asymptotically large spacings. In order to obtain the scaling curve (4), on which all data points collapse, we shifted $\ln L$ by $\ln \xi(W)$ separately for each $W$. The overlap between adjacent values of $W$ allows to fit most of the points onto two branches for $W < W_c$ and $W > W_c$ corresponding to localized and
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The quantity $\alpha$ as a function of the size $L$ at different degrees of disorder near the metal–insulator transition.

Figure 2. The quantity $\alpha$ as a function of $L/\xi$ at different degrees of disorder near the metal–insulator transition. We calculated also the critical exponents of the localization length $\nu$. Using the singularity of $\xi$ near the transition point $\xi(W) \propto |W - W_c|^{-\nu}$ one can expand the relation (4) to a power series. Taking into account only the linear term, $\alpha(W, L) = \alpha_c + \text{const} L^{1/\nu} (W - W_c)$, and applying the $\chi^2$–criterion to fit the data plotted in Fig. 2 we found that $\nu = 1.45 \pm 0.1$.

Another important quantity which is used to describe the level statistics is the magnitude of fluctuations of the number of energy levels $\delta N(E)$ in a given energy interval $E$. The variance $\langle (\delta N(E))^2 \rangle$ characterizes the “stiffness” of the spectrum. From the statistical viewpoint it is reasonable to investigate the dependence of the variance $\langle (\delta N(E))^2 \rangle$ on the average number of levels $\langle N(E) \rangle$ in the vicinity of the MIT. Here $\langle ... \rangle$ denotes the averaging over the random configurations with the same disorder $W$. In the metallic regime the variance is known to be defined by the Dyson formula, $\langle \delta^2 N \rangle_M = 2/\pi^2 (\ln(\langle N \rangle) + C)$, where $C \approx 2.18$, provided that $\langle N \rangle \gg 1$ [1]. In the strongly localized regime the levels are not correlated, hence $\langle \delta^2 N \rangle_I = \langle N \rangle$, that is much larger than $\langle \delta^2 N \rangle_M$. Decreasing disorder suppresses the fluctuations $\delta N$, so that the variance changes from $\langle (\delta N)^2 \rangle_I$ to $\langle (\delta N)^2 \rangle_M$ [5].

Exactly at the transition the variance behaves linearly with the average level number, $\langle \delta^2 N \rangle_c = \kappa \langle N \rangle$ [5, 10], as in the insulating regime. However the numerical factor $\kappa$ is less than unity.

We calculated the dependence of the ratio $\langle (\delta N(E))^2 \rangle / \langle N(E) \rangle$ on the average number of levels within a given interval $E$ for different lattice sizes $L$ at the disorder $W$ varying from 12 to 20, as shown in Fig. 4. It is obvious that near the MIT this ratio exhibits the critical behavior. In approaching the transition, $W = W_c$, it becomes size–invariant (Fig. 4c). Such a behavior is closely related to the universality of the critical level spacing distribution,
as mentioned above. In addition, one can observe that at the MIT the relative fluctuations of the level number \(\langle \delta N^2 \rangle / \langle N \rangle\) decreases with the energy, when \(\langle N \rangle \equiv E/\Delta \sim 1\), and then varies very weakly over two orders of magnitude of \(\langle N \rangle\), tending to a constant value \(\kappa \approx 0.32\). For \(E > 200\Delta\) the numerical errors becomes larger due to the finite number of realizations. Our results are consistent with the suggestion about the proportionality between the variance and the average level number \([5]\), but deviate from the power law proposed recently in \([13]\).

Determining the ratio \(\langle \delta N^2 \rangle / \langle N \rangle\) as the function \(F(E, L, W)\), one can analyze the scaling properties similarly to those of \(P(s)\). For example, the disorder dependence for the given energy width \(E = 20\Delta\) is shown in Fig. 5. Near the critical point, \(|W - W_c| < 1\), the function can be linearized \(F(E, L, W) = \kappa + A L^{1/\nu} (W - W_c)\). The factor \(A\) depends on the energy \(E\), in contrast to that for \(\alpha\), whose critical behavior is not sensitive to the choice of \(s\). In order to obtain the one–parameter scaling law one should take in account the typical volume per one electron state lying in the interval \(E\), \(L_0^3 = L^3 \langle \Delta/E \rangle\), instead of the total volume \(L^3\), i.e. \(F - \kappa \propto (L_0/\xi)^{1/\nu}\). Fig. 6 shows \(\langle \delta N^2 \rangle / \langle N \rangle\) vs. \(L_0/\xi(W)\), where \(\xi(W)\) is taken from the analysis of \(\alpha\). All data belong to the common two–branch curve regardless to \(L, W\), and chosen \(\langle N \rangle\). Indeed, the fluctuations \(\delta N\) in the interval \(E\) are mainly defined by the states confined within the correlation volume \(\xi\), which are separated by the energy \(\Delta_\xi = \Delta (L/\xi)^3\). The number of those states is \(N_\xi = E/\Delta_\xi\). Therefore \(F = \kappa + N^{-1/3\nu}_\xi \text{sign}(W - W_c)\).

In conclusion, we have used the level spacing distribution \(P(s)\) as a scaling variable in order to detect the critical behavior at the disorder–induced
Figure 5. Disorder dependence of the ratio $\langle \delta N^2 \rangle / \langle N \rangle$ at the given number of levels $\langle N \rangle \equiv E/\Delta = 20$ for various sizes $L$.

Figure 6. $\langle \delta N^2 \rangle / \langle N \rangle - \kappa$ as a function of $L_o/\xi(W)$ for different $L$ and various $\langle N \rangle$ from 10 to 100.

metal–insulator transition. The results for the critical exponent $\nu$ and the critical disorder $W_c$, which were obtained by numerically diagonalizing the Anderson Hamiltonian for up to $28^3$ lattice sizes, are consistent with those obtained earlier by using completely different approaches [12]. Our calculations showed that the universality of the level statistics at the transition is revealed not only in the form of $P(s)$ but also in the dependence of the variance of the number of electron states in an energy interval of a given width on their mean number $\langle N \rangle$. We also analyzed the scaling behavior of the function $\langle \delta^2 N \rangle = F(\langle N \rangle)$. At the MIT this function is found to be $L$–invariant with a leading linear term, $\langle \delta^2 N \rangle_c = \kappa \langle N \rangle$, where $\kappa \approx 0.3$.

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