UNIVERSAL STATISTICS OF ENERGY LEVELS AT THE METAL-INSULATOR TRANSITION

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The nearest-neighbor level spacing distribution is numerically investigated by direct diagonalizing a disordered Anderson Hamiltonians for quantum systems. The level statistics scaling is examined near the metal-insulator transition and the correlation exponent is found. We suggest a new universal level spacing distribution at the critical point of the transition, which is related to the multifractality of the electron wavefunctions.

Introduction

The level statistics in the energy spectrum of a disordered system became a subject of modern condensed matter theory. Particular interest comes also from theories of critical phenomena. The distribution of energy values of quantum-chaotic systems is assumed to obey certain probability laws, which are invariant with respect to unitary transformations. When the fluctuations of randomness of the atomic and/or impurity potential are increased, a quantum system undergoes a second order phase transition, which is origin of the Anderson metal-insulator transition. In condensed matter physics this transition is referred to as a localization-delocalization transition. A metallic phase is known to be described by the random matrix theory, developed by Wigner and Dyson [1]. In the insulating regime, the electron levels of the strongly localized states fluctuate like random stochastic variables [2]. The study of the crossover between the chaotic (Wigner) and ergodic (Poisson) statistics which is induced by the phase transition was started in [3] and became the subject of several subsequent investigations [4-6].

The nearest neighbor spacing distribution $P(s)$ is accepted as a characteristic entity for description of the level statistics. In the metallic regime $P(s)$ is very close to Wigner surmise

$$P_w(s) = \pi s/2 \exp(-\pi s^2/4), \quad (1)$$

where s is measured in units of the mean spacing Δ. In the localized regime the level spacings are distributed according to the Poisson law

$$P_p(s) = 1/\Delta \exp(-s/\Delta), \quad (2)$$

because the levels are entirely uncorrelated. Both distribution laws are universal and do not depend on the properties of the system (Fig.1.). The investigation of the non-trivial crossover of $P(s)$ between these two universal limits, namely between the Wigner and the Poissonian limits, which accompanies the disorder-induced metal-insulator transition, was performed in [2-4].

It is well known that $P(s)$ exhibits critical behavior and is scale invariant at the critical point. In fact this distribution gives a unique method to study the critical behavior of the localization length. The invention of a *third universal* level statistics precisely at the transition [2,3] excited large interest in finding an explicit analytical expression of the critical spacing distribution $P_{cr}(s)$. The form of the critical distribution is different for various symmetries. For example, for the orthogonal symmetry $P_{cr}(s)$ is proportional to s for small spacings s. For larger spacings s it is shown that $P_{cr}(s)$ behaves similar to the Poisson asymptotic limit $P(s) \rightarrow P_p(s)$ for $s >> \Delta$, because the Thouless energy at the transition point is order of the mean level spacing Δ. This simple exponential asymptotic form of the critical level spacing distributions is valid not only for the orthogonal symmetry (with spinless electrons an without magnetic field), but also for other

universality classes: the unitary (in the presence of the magnetic field) and the symplectic (in the presence of the spin-orbit coupling) classes.

Method and results

By exact diagonalizing the Anderson Hamiltonians with the advanced procedures developed especially for clusters of huge sizes up to 10^7 lattice sites, we investigate the finite-size scaling properties of the probability distribution of neighboring spacings and find the critical parameters, characteristic of the second phase transition. Our main result is that the critical P(s) is scale invariant for various symmetries and approaches the integrability limit for asymptotically large spacings. In addition, the critical index of the correlation length is extracted on the basis of finite-size scaling analysis with the system size L and disorder degree W of the random impurity potential. The Anderson model is defined by the Hamiltonian

$$H_A = \Sigma_n \varepsilon_n a^+_n a_n + \Sigma_{n \neq m} (a^+_n a_m + c.c.), \quad (3)$$

where $a^+_n(a_n)$ is the creation (annihilation) operator of an electron at a site n, with m denoting the nearest neighbors of n. The site energies ε_n are measured in units of the overlap integral between adjacent sites. They are independent random variables that are distributed around zero according to the box distribution of width W. A simple cubic lattice with periodic boundary conditions was used. It is known from the transfer-random-matrix method, that in the center of the energy band the critical disorder degree $W = W_{cr} \approx 16{,}5$ [4]. The electron spectrum was properly unfolded by fitting the integrated density of states to polynomial splines. It should be noted that the numerical diagonalization of giant sparse matrices of rank 10^6- 10^7 is highly nontrivial task. As expected the $P(s)$ is indeed scale-invariant at the W_{cr} that means it does not depend on the system size. The best fit using the χ^2 -criterion over large range of spacings provides the exponent, which is very close to the theoretical value. This value has been calculated by the transfer matrix method $\nu = 1.5$ in the vicinity of the metal-insulator transition at the orthogonal symmetry [6].

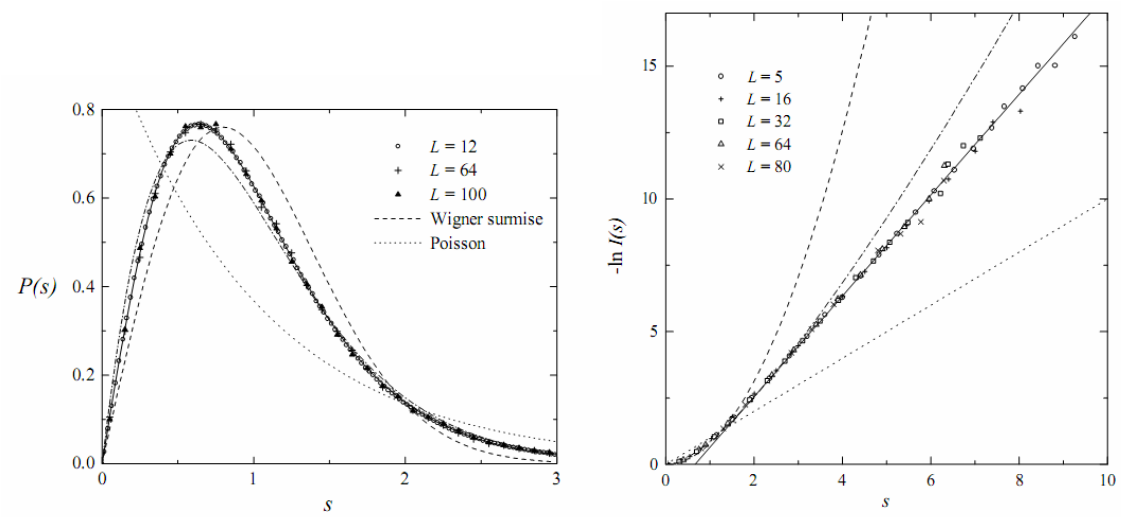

Fig. 1. (*left*) Level spacing distribution $P(s)$ for various system sizes at the critical point of the metal-insulator transition ($W=W_{cr}$). Wigner and Poisson distributions correspond to Eq.(1) and Eq.(2), respectively. Dash-dotted line is the result of the perturbative theory with β=1.24. Full line is the derivative of $I_{cr}(s)$ from the interpolation formula Eq.(6).
(*right*) Cumulative probability of neighboring spacings $I(s)$ for various system sizes L. Solid line is Eq.(5) with β=1.00 Dash-dotted line is power law with β=1.24. Dashed and dotted lines are $I_W(s)$ and $I_P(s)$, respectively from Eq. (4).

It is important that exponential tail of *P(s)* contributes to the relative accuracy only with the small weight. Therefore its influence can be neglected. Is it imperative furthermore to investigate the asymptotical behavior of the level spacing distribution at large *s*, particularly without including data from the region $0 \le s \le 2$. In what follows, we consider the cumulative level spacing distribution probability density function $I(s) = \int P(s)ds$. It gives the probability to find neighboring energy levels with the separation $E > s\Delta$. The integration does not change the asymptotic form of the probability function, which is exponential for any symmetry. Since s>0, I(s) = 1, and by the normalization to the total number of the spacings in a given energy interval $\int I(s)ds = 1$. The Wigner surmise and the Poisson distribution yield

$$I_w(s) = \exp(-\pi s^2/4), \quad \text{and} \quad I_p(s) = \exp(-s), \tag{4}$$

respectively. The numerical study of the cumulative probability *I(s)* is analogous to that of the density of states while unfolding the electron spectrum. By arraging the spacings in a descending sequence one can very accurately construct the desired histograms of *I(s).* Using the common statistical hypothesis at large *s*

$$\ln I_{cr}(s) = - A_{cr} s^{\beta} \quad , \tag{5}$$

we calculated A_{cr} and β for various system sizes. Our results show that independent of size the index gives $\beta = 1.00 \pm 0.05$ (see Fig.1 right). This means that the asymptotic behavior is better described by the *linear law* for large spacings, so that $I_{cr}(s) \propto \exp(-A_{cr} s)$ with the universal value $A_{cr} \approx 1.9 \pm 0.1$. This is very similar to the insulating regime, although the decay rate A_{cr} is almost twice larger that unity (Poissonian integrability). This is due to quantum mechanical level repulsion.

Our linear asymptotic result is in a direct contrast to the fractional power law with $\beta \approx 1.2$-1.4 obtained previously by other research groups. This controversy provides new constructive point of view on the universal form of the level statistics that changes conventional approaches to the description of the critical phenomena in the condensed matter physics. We propose that the index A_{cr} directly related to the multifractal nature of the electron wavefunctions (Fig.2).

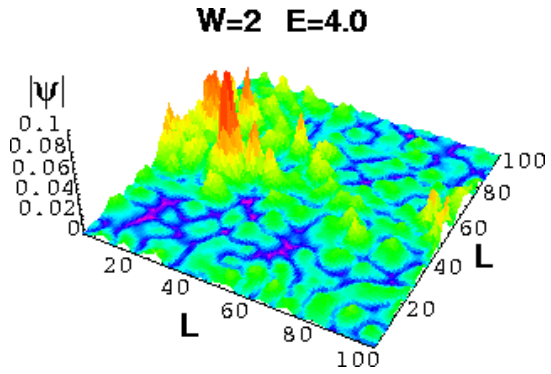

Fig.2. The typical amplitude distribution of the multifractal electron wave function of the electron at the critical region of the metal-insulator transition, obtained numerically for the 2D Anderson model with the lattice size of *L*=100 for fixed *W* and *E* (*W* is the disorder parameter, *E* is the electron energy). The fundamental symmetry corresponds to the orthogonal case. (See also Ref. [5])

In addition, the equivalence of averaging over the spectrum and over the realizations of the random potential within a statistical ensemble was proven. Indeed, due to diminishing the spacing with the system size $\Delta \propto L^3$, the averaging for smaller cubes is performed over many samples, while for our largest systems L=100 an 200 a single realization without ensemble averaging is even sufficient to get similar distributions with comparable precision.

For numerically describing a crossover between small and large s, we propose an explicit form of the new interpolation probability function

$$I_{cr}(s) = \exp\{\mu - (\mu^2 + A^2_{cr}\, s^2)^{1/2}\}, \qquad (6)$$

with a coefficient $\mu =$ 2,21. Although we do not provide here a rigorous analytical proof, it gives an excellent fit all over the range of the computed spacings [2]. The corresponding $P_{cr}(s)$ fulfills the both normalization conditions. It is interesting that this exponent is related to the index of multifractality of the critical eigenstates. Therefore we suggest that the statistical properties of the electron energy spectra define the multifractal nature of the wavefunctions at the criticality. Similar to the chaotic counterpart in classical mechanics the critical index of the localization length in quantum systems depends strongly on the dimensionality [5] and basic symmetry [6].

Conclusions

A presence of a random impurity potential leads to the effect of the localization of electron states, which is an origin of the disorder induced metal- insulator transition. Quantum interference of electron waves is responsible for a dramatic change in transport properties. Extensive numerical simulations support conclusions of previous analytical approaches. Correlations in spectra of disordered systems play an important role in describing the Anderson transition. The energy level statistics exhibits critical behavior and experiences a crossover from the random matrix theory towards the uncorrelated Poissonian statistics. An existence of a *novel critical statistic* allows one a self-contained description within a finite-size single parameter scaling hypothesis and extracting the critical exponents. Fundamental symmetries (orthogonal, unitary and symplectic) and the spatial dimensionality significantly influence the critical statistics, corresponding to different physical situations. By using various numerical techniques (like the advanced Lanczos diagonalization [6], transfer matrix methods, Monte-Carlo algorithms) one can successfully study quantum features of transport characteristics and the spectral fluctuations of the disordered systems close to the metal-insulator transition in the presence of a magnetic field and a spin-orbit interaction.

References

1. Mehta M.L., Random Matrices, Academic Press, Boston, 1991, 523p.

2. Zharekeshev I. Kh. and Kramer B., Asymptotics of Universal Probability of Neighboring Spacings at the Anderson Transition, Phys. Rev. Lett. 1997, 79, 717-721.

3. Shklovskii B.I., Shapiro B., B. R. Sears B.R., Lambrianides P., and H. B. Shore H.B., Statistics of spectra of disordered systems near the metal-insulator transition, Phys. Rev. B, 1993, 47, 17, p. 11487-11491.

4. Zharekeshev I. Kh. and Kramer B., Universal Fluctuations in Spectra of Disordered Systems at the Anderson Transition, Japanese. J. Appl. Phys.,1995, 34, 4361-4366.

5. Efetov K.B., Supersymmetry in disorder and chaos. Cambridge University Press, 1999, Pp. xiii + 441.

6. Zharekeshev I.Kh., Kramer B., Numerical-scaling study of the statistics of energy levels at the Anderson transition, in book: Statistical and Dynamical Aspects of Mesoscopic Physics, Editors D. Reguera, G. Platero, L.L. Bonilla, and J.M. Rubi, Lecture Notes in Physics 547, (Springer-Verlag, Berlin 2000) p. 237-251.

ЭНЕРГИЯ ДЕҢГЕЙЛЕРІНІҢ МЕТАЛДЫҚ ИЗОЛЯТОРҒА АУЫСҚАН КЕЗДЕГІ УНИВЕРСАЛДЫҚ СТАТИСТИКАСЫ

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Кванттық жүйеде фазалық ауысу сындық нүктесінде энергияның көршілес деңгейлерінің арасындағы қашықтықтардың үлестірілу мүмкіндігі алғашқы рет зерттелген.

УНИВЕРСАЛЬНАЯ СТАТИСТИКА УРОВНЕЙ ЭНЕРГИИ НА ПЕРЕХОДЕ МЕТАЛЛ-ИЗОЛЯТОР

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Изучается вероятность распределения расстояний между соседними уровнями энергии в критической точке фазового перехода в квантовой системе.