CRITICAL STATISTICAL ENSEMBLES IN ELECTRON NANOSYSTEMS AT THE LOCALIZATION TRANSITION

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The statistical properties of spectra in the electron nanostuctures are studied with and without magnetic field. It is shown that the spectral correlations exhibit universal scale-independent behaviour characteristic of critical statistical ensembles

Introduction

The crossover from integrability to chaos is one of the important issues in physics of complex systems. Non-ergodicity and nonlinear behavior of open systems out of equilibrium is often caused by the influence of the external conditions, for example, by the adiabatic connection to the environment or by imposing strong external fields. The description of dynamical aspects of time-dependent evolution of statistical parameters can be based on the formalism of canonical ensembles (when the number of particles N in an open nanosystem is fixed) and grand-canonical ensembles (when N is large and not fixed). As a counterpart for the transition between full integrability and complete chaos in quantum electronic systems (e.g. quantum dots coupled to a bath reservoir) can serve a delocalization-localization transition.

On the other hand, the latter is characterized by a sharp crossover of the electronic conductivity from the metallic regime to the insulating one. A striking signature of this metal-insulator transition is a presence of the criticality, meaning that a set of thermodynamical quantities exhibit critical behavior. It turns out, that the distributions of strongly fluctuating parameters at the critical point of the transition obey generic common laws and can be analyzed by the finite-size scaling scenarios. Moreover, a new set of the statistical ensembles, named *critical* ones, have been introduced especially for characterizing the critical point.

The problem of localization of quantum particles in a disordered nanosystem has attracted great attention during last decades, triggered by the discovery of new quantum phenomena in condensed matter physics. After the first formulation of the modern theory of solids in the 1930's it was thought for a long time that the effect of disorder on the state of electrons in solid structures can be described in terms of the perturbations of low orders. Indeed, the standard quantum-mechanical implementation of Boltzmann transport approach appeared to work perfectly everywhere, expect for certain unexplainable observations like, for example, the negative magnetoresistance of doped semiconductors in a weak magnetic field. It was only in 1958 that Philipp Anderson suggested the currently well-known concept of quantum localization of electrons by the potential disorder [1]. He proposed that in a tight-binding model of electrons on a lattice with chaotically varying site energies V the electrons of a given energy E would become localized if the spread of the on-site energies V meaning the disorder degree is sufficiently large.

In the other words, the behavior of the electronic states would change drastically from extended to localized behavior. In the former case the disorder manifests itself mainly through a decay of phase coherence in the averaged one-particle propagator, while in the latter case the probability amplitude decreases exponentially as one goes away from the centre of localization. It is not surprising, since even in a classical system the disorder may cause the localization of particles. However the quantum nature of electrons make them harder to overcome narrow passages and channels, despite the fact that

quantum particles can tunnel under barriers, i.e. through classically forbidden regions. Hence, quantum particles in nanoclusters tend to be localized more easily than their classical counterparts.

Quantum transport in open nanosystems

The first qualitative consequence of the quantum nature of particles for transport in disordered open nanosystems is reflected in the fact that the mean free path l cannot become shorter that the wavelength of the electrons λ_F. For electrons in the centre of the band λ_F is of the order of the lattice spacing a, but for energies near the band edge λ_F may be larger than lattice constant a. In a classical system the shortest possible mean free path is always given by the average distance between the scattering centers, irrespectively of the particle energy. If the disorder increases beyond the point where $l \approx \lambda_F$ or else, if the energy of the electrons decreases for a fixed disorder, the nature of the electronic states is expected to change from extended to localized. As a consequence, the electrical conductivity of the nanosystem or mobility of carriers is expected to vanish to zero.

This scenario, where a change in the electron energy induces a metal-insulator transition, was explored early by Mott [2]. He introduced the term 'mobility edge' for the critical energy separating extended and localized states. These two types of states are not likely to coexist at a given energy, since any small change in the potential would cause admixtures of extended states with a localized state, and would thus delocalize it. On the basis of qualitative considerations and experimental data Mott concluded that the Anderson transition in a three-dimensional system should be discontinuous, the conductivity jumps from a finite value, called minimum metallic conductivity downwards to zero. The advent of the computer, which made the exact diagonalization of finite-size systems possible, and the advances in electrical transport measurements near the metal-insulator transition at low temperatures have changed this picture.

It is well established now that there is, in fact, no minimum metallic conductivity and that the transition is continuous, much like a continuous phase transition in usual thermodynamics. A continuous phase transition is necessarily associated with a characteristic length ξ, localization length, which tends to infinity as the transition is approached. At the transition a natural unit of length does not exist anymore and the system is therefore considered as being *scale-invariant*. The ensuing scaling behavior was discovered by Thouless [3] who noticed that the conductance of a finite-size block scales with the size in a universal way.

In this paper we also consider the electronic spectra rather than the conductivity. Its statistics also undergo the phase transition similar to the conductance. Mostly concentrated on the critical point of the metal-insulator transition, the various classes of the ensembles are numerically investigated depending on the presence of the external magnetic field. It has earlier shown that the probability function of the neighboring spacings $P(s)$ exhibits finite-size scaling and also becomes scale-invariant exactly at the transition point for both the orthogonal and the unitary symmetry. Interestingly, our results demonstrate that there is a essential difference between the spectral correlations for critical orthogonal ensemble (COE) and for the Gaussian orthogonal ensemble (GOE) [4]. The same is observed for the deviations between critical unitary (CUE) and Gaussian unitary ensembles (GUE).

Critical orthogonal ensemble

For the orthogonal case, which corresponds to the system without magnetic field and with spinless particles, the level statistics at non-vanishing disorder of random potential exhibits critical behaviour starting from the three dimensions. As an example, we have numerically calculated the level statistics of a

sample with time-reversal symmetry (φ= 0) for L = 6 for different disorders. Figure 1 demonstrates how the distribution $P(s)$ changes from the GOE-result to the Poisson distribution, when the disorder W increases. One observes a continuous change of the data between the two limits, the slope at small s being always linear for arbitrary disorder W in agreement with the time-invariant symmetry:

$$P^o(s) = B^o s^\beta, \qquad (1)$$

with β = 1. In the metallic regime ($W < W_c$) it diminishes towards $B^o = \pi^2/6$ with decreasing disorder or/and increasing the size, i.e. with increasing the conductance g, unless the system is in the ballistic regime. In the insulating regime the slope B^o increases to infinity when both the disorder W and the linear size of the system L tend to infinity.

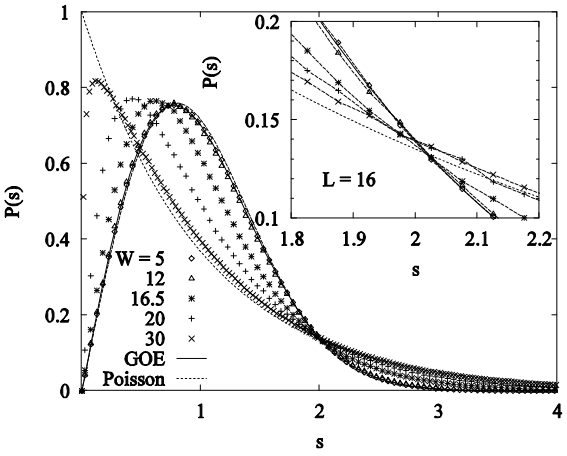

Fig.1.The level spacing distribution $P(s)$ for a cubic nanosystem with orthogonal symmetry for various disorder strength W=5, 16.5, 30 и 100 (box distribution). Taken is a nanocube of linear size L=16. Solid line is the GOE result and dashed line is Wigner surmise. Dotted line: Poisson distribution $P_p(s) = \exp(-s)$. Inset shows an enlarged area near $s = s_0 \approx 2.0$, the crossing point of the Poisson and the Wigner distributions. The number of spacings is about 10^8.

At the transition point $W = W_c$ = 16.5 of the `box' model the level spacing distribution function corresponds to the *critical orthogonal probability function* $P^o_c(s)$, which is not sensitive to the change of the system size L. The prefactor is found to be B^o_c = 2.12± 0.06, i.e. $B^o_c \approx 1.29\ B^o$, according to the Eq. (1). The scale-invariance of the critical level statistics has been justified in many works [5-8]. We analyze here the overall functional form of the critical $P^o_c(s)$, in more detail using results of large-scale computations, particularly concentrating on the asymptotic behaviour for large s.

We have computed also the level spacing distribution function (in form of a histogram) for the critical disorder W_c = 20.9 of the Gaussian distribution of the on-site energies. The eigenvalues were taken from the interval centred at E = 0 containing approximately 10% of the spectrum. Within the numerical error-bars the data of $P(s)$ are the same for different L and coincide with those of $P^o_c(s)$ for the box distribution, justifying the independence on the model of diagonal disorder. By other words, it is proved that the critical statistics are universal irrespective of the microscopic details of the system.

Of particular interest is the region of spacings around s_0 = 2.002, where the Wigner surmise $P_W(s)=\pi^2/2\ \exp(-\pi^2 s^2/4)$, and $P_P(s) = \exp(-s)$, intersect. It has been suggested by Shklovskii [5] that independently of the disorder degree W, all empirical curves $P(s)$ including the critical one, $P^o_c(s)$ should intersect at the same point s_0, which would then play the role of a universal energy. The existence of such a universal point would mean that the system possess a hidden symmetry. The underlying reason for this symmetry, however, is not known yet at present.

Focusing on a region close to s_0, we have performed detailed calculations with the large number of realizations. One should again take into account that, in fact, the Wigner surmise only approximates the exact RMT result for $P(s)$, albeit quite well (within 5%). Thus $P_{GOE}(s) \neq P_W(s)$. The true intersection of $P_P(s)$, and $P_{GOE}(s)$, lies at s_0 = 2.019. Careful analysis of our data does not, however, show any common crossing point for various disorder degrees W (see inset of Fig. 1). The computed value of $P(s_0)$ for disorder W = 16.5 (also for W = 30 and 100) differs from $P_P(s_0)$ by a magnitude which exceeds the numerical errors. No unique point so has been observed also for the unitary case.

In the vicinity of the transition point W_c the level spacing distribution exhibits critical behaviour similar to that of the level number variance, discussed in papers [6-8]. Using the finite-size scaling analysis for the distribution of neighbouring spacings one can construct the disorder dependence of the localization length $\xi(W)$ and extract the critical exponent ν. The one-parameter scaling scenario for the function *P(s)* has been corroborated in a large number of computer simulations [8-10]. Therefore we provide here only the summary of numerical results available on calculations of the critical exponent for various physical situations and do not further focus on this topic.

One can show that the critical exponent as a characteristic of the symmetry class, is almost the same within statistical uncertainty for different models of the diagonal disorder (for the uniform and the Gaussian distributions of on-cite energies ε_n) and of the quantum percolation. As expected, it is also not sensitive to the anisotropy of the system. Generally, all the data for the critical exponent of the localization length are centred about the value $\nu = 1.45 \pm 0.1$, as an acceptable estimate for the orthogonal case. It turns out that the value of the critical exponent evaluated from the level number variance is consistent with that obtained from the analysis of *P(s)*. Notably this value is somewhat smaller than that found by the high-precision transfer-matrix calculations $\nu_{TM} = 1.57 \pm 0.02$. The reason of such a slight, but resolvable discrepancy is not known yet.

Critical unitary ensemble

We now consider the level statistics for systems with broken time reversal symmetry. Such a situation can be realized by applying an external Aharonov-Bohm (AB) magnetic flux through a system forming a ring geometry. In order to achieve the maximal effect of the change of the symmetry, the AB-fluxes of the equal magnitude are applied along all three perpendicular directions in a three-dimensional cubic lattice (the three-component flux). Performing diagonalization for different magnitudes of the flux ranging from $\varphi = 0$ to $\varphi = 1/4$, we found the critical statistics to be sensitive to the flux. As a function of φ, the distribution *P(s)* at the critical point $W_c = 16.5$ changes smoothly from the critical orthogonal $P^o_c(s)$ to the critical unitary form $P^u_c(s)$ at $\varphi = 1/4$, which is known as the COE-CUE crossover [8] (see figure 2).

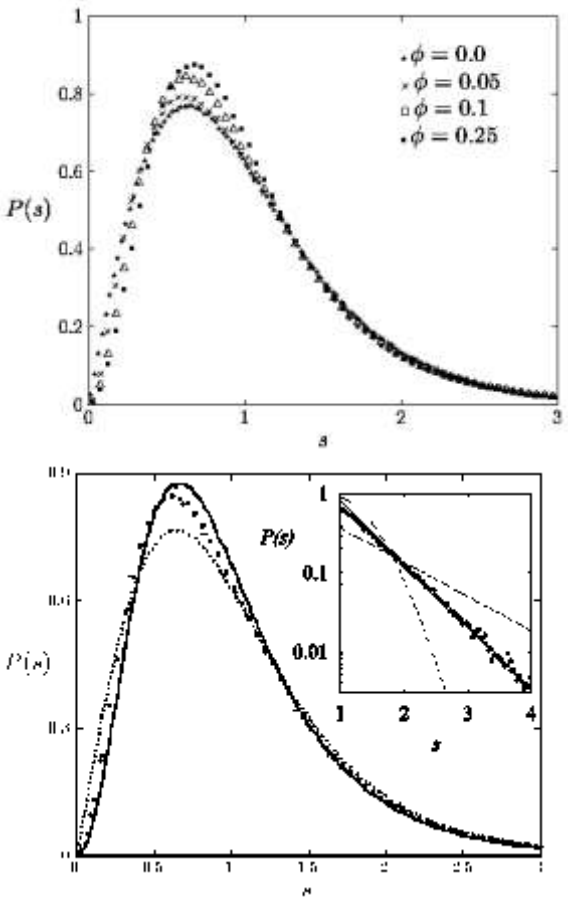

Fig.2.The level spacing distribution *P(s)* for the unitary case at the critical disorder *W*=16.5. Upper panel: at different values of the Aharonov-Bohm flux φ for a system with fixed linear size $L = 5$. Lower panel: at the fixed flux $\varphi = 0.2$ for different sizes $L = 5$ (+); 10 (□); 20 (●). Solid and dashed lines are the critical *P(s)* for two limiting phases $\varphi = 1/4$ and $\varphi = 0$, respectively. Inset: asymptotic behaviour of *P(s)* at the limiting AB-phase $\varphi = 1/4$ for linear sizes $L = 5$ (+) and 20 (●). Solid line – $P^u_c(s)$ [Eq. (3)], dashed line - $P_P(s)$ and dotted line – $P^u_W(s)$ all correspond to critical, insulating and metallic regimes, respectively.

This flux-controlled crossover of the critical level statistics repeats periodically, resuming the orthogonal form at φ=0.5, since a half of the flux quantum corresponds to the real Hamiltonian defined with antiperiodic boundary conditions

(`false' T-invariance). For fixed flux, all *P(s)* at W_c proved to be insensitive to variations of the size of the system L = 5, 10 and 20, as shown in figure 2 (left panel) for φ = 0.2. The same L-independent behaviour has been observed for other values of flux φ = 0.05, 0.1 and 0.25. As expected for the T-symmetry broken, we observe a quadratic behaviour $P_u(s) \sim s^2$ for small s at all W, as soon as L is finite. It has recently been suggested that the flux-driven crossover of the critical unitary statistics can be explained on the basis of the analogy to the semi-classical limit. For n = 0 both the Mehta parameter [9] for the unitary critical statistics $J^c_u = 0.685 \pm 0.003$ and, consequently, the spacing variance $var\ s = 2J^c_u - 1 \approx 0.344$ are larger than those for the GUE, where J_u for RMT is equal to 0.590.

The extreme form of the unitary critical $P^u_c(s)$ corresponding to the AB-phase φ = 1/4 coincides with that found in the presence of the strong magnetic field, as has been shown in Ref. [10]. In the latter case, the COE-to-CUE crossover is discontinuous, unlike to the application of an AB-flux. The behaviour of $P^u_c(s)$ for small spacings s is described by the power-law

$$P^u_c(s) = B^u_c s^\beta, \quad B^u_c = 8.5 \pm 0.1, \qquad (2)$$

with the `repulsion parameter' β=2. This result is in direct contradiction to another numerical work [11], which has claimed the linear growth of $P^u_c(s)$ at small s, i.e. β = 1, similar to the critical orthogonal case.

The asymptotic form of the size-invariant $P^u_c(s)$ for large s can be well approximated by the simple exponential decay [11]

$$P^u_c(s) = D^u_c \exp(-A^u_c s),\ A^u_c = 1.85 \pm 0.1, \qquad (3)$$

that is slower compared to the Gaussian tail characteristic of the RMT-result. On the other hand, it is similar to the Poisson decay valid in the strongly localized regime, although the decay rate A^u_c is certainly larger than unity. Note that the critical prefactor $B^u_c = 2.59\ B^u_{RMT}$ is also markedly larger than that of the GUE. In fact, the value $A^u_c \approx 1.85$ should be considered as a lower bound for the exponential decrease of $P^u_c(s)$ because obtained range of s is not sufficiently large. It was demonstrated in [12] that the similar asymptotic behaviour holds also for systems with time-reversal symmetry.

Discussions

Thus we demonstrated the symmetry dependence of the critical spectral fluctuations and the existence of a new class of critical statistical ensembles COE and CUE, which are ascribed to the disorder-induced metal-insulator transition. It would be interesting to ask: what happens with these critical statistics for lower dimensions?

For instance, in two-dimensional systems the probability density of neighbouring spacing *P(s)* in the absence of spin-orbit coupling changes towards the Poisson distribution, as the size of the system grows, with no critical behaviour [8] in contrast to the higher dimensions. This is consistent with the scaling argument that all electron states in two dimensions are localized in the thermodynamical limit. Switching on the strong spin-orbit interaction drives the open system towards a metal-insulator transition in 2D at non-zero disorder. As a result, the one-parameter scaling scenario and the critical peculiarities of the spectral fluctuations are recovered again. Indeed, with increasing the system size the two-level spectral correlation function and the distribution *P(s)* above the mobility edge tend to those which correspond to the symplectic symmetry class of the random Hamiltonians. In the insulating regime, i.e. below the mobility edge, the eigenvalues are chaotically distributed as completely uncorrelated variables. Exactly at the critical point of the transition the level statistics possess universal critical forms [11] as distinct from both the spinless situation and the Gaussian symplectic ensemble. As to asymptotic of large spacing, the logarithm of *P(s)* decays linearly similar to the two above critical symmetries of COE and CUE, however

the decay rate is almost twice faster. This is related to the fact that the quantum nanosystem has less number of degrees of freedom.

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КРИТИЧЕСКИЕ СТАТИСТИЧЕСКИЕ АНСАМБЛИ В ЭЛЕКТРОННЫХ НАНОСИТЕМАХ НА ЛОКАЛИЗАЦИОННОМ ПЕРЕХОДЕ

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Изучаются статистические свойства спектров в электронных наностуктурах с и без магнитного поля. Показано, что спектральные корреляции проявляют универсальное масштабно-независимое поведение, характерное для критических статистических ансамблей.

ЛОКАЛИЗАЦИЯЛАНҒАН АУЫСУДЫҢ ЭЛЕКТРОНДЫҚ НАНОСИСТЕМАЛАРДЫҢ КРИТИКАЛЫҚ СТАТИСТИКАЛЫҚ АНСАМБЛДЕРІ

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Біз электрондық наноструктуралардың спектрлерінің статистикалық қасиеттерін магниттік өріспен және өріссіз зерттедік. Спектралдық корреляциялардың әртүрлі масштабты-тәуелсіз сипаттамаларын критикалық статитикалық ансамблдер ретінде анық көрсетті.