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LETTER TO THE EDITOR

Dependence of critical level statistics on the sample shape

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Abstract. The level-spacing distribution of consecutive energy eigenvalues is calculated numerically at the metal–insulator transition for 3D systems with different cuboid shapes. It is found that the scale independent critical $P_c(s)$ changes as a function of the aspect ratio of the samples, while the critical disorder $W_c/V = 16.4$ remains the same. We use our data to test whether an expression for the small-s behaviour of the level statistics proposed by Kravtsov and Mirlin for the metallic regime is applicable also at the critical point. For this reason, a shape dependent dimensionless critical conductance g_c has been extracted from the small-s behaviour of the critical level statistics. Our result for a cubic sample, $g_c = 0.112 \pm 0.005$, is in good agreement with a value obtained previously from calculations using the Kubo formula.

Energy eigenvalue correlations provide general tools for the statistical description of disordered materials. Among them, the nearest neighbour level spacing distribution $P(s)$ represents one of the simplest statistics. Here, $s = |E_{i+1} - E_i|/\Delta$ is the energy difference of consecutive eigenvalues E_i divided by the mean level spacing Δ. Nevertheless, knowing $P(s)$, it is possible to tell whether a given system exhibits metallic or insulating behaviour at temperature $T = 0\,\mathrm{K}$.

Considerable attention has recently focused on the special case of critical statistics which were found at the metal–insulator transition in disordered 3D [1–9] and 2D [10–13] systems. In all cases, the numerically obtained critical level statistics were noticed to be independent of the system size L. This is different in the metallic and insulating regimes where a size dependence has been observed. In the limit $L \to \infty$, the nearest neighbour spacing distribution follows the Poissonian decay, $P(s) = \exp(-s)$, for disorder strength W larger than the critical disorder W_c. The metallic side, $W/W_c < 1$, is well described by random matrix theory (RMT) [14–17]. As in the metallic phase, the critical $P_c(s)$ depends on the symmetry of the Hamiltonian describing the system under consideration. In addition, and in contrast to the universal RMT description for the metallic phase, the critical $P_c(s)$ depends also on the spatial dimension. Up to now, the respective forms of $P_c(s)$ are known only from numerical studies.

In [7] using the Anderson model, the application of an Aharonov–Bohm-flux was shown not only to change the universality class of the level statistics due to breaking of time reversal symmetry. It has also been demonstrated that, depending on the strength of the flux, there exists a set of scale independent critical spacing distributions. These are associated with a continuous crossover from orthogonal to unitary symmetry [7, 18]. It is well known that the corresponding Hamilton matrix can be transformed such that the AB-flux is completely absorbed into the boundary conditions. So the question arises, whether or not $P_c(s)$ does in general depend on the boundary conditions applied. Recently, it has been shown [19]

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that $P_c(s)$ is in fact sensitive to a change of the periodic boundary conditions, which were always applied previously, to Dirichlet boundary conditions in one, two and three directions.

In this letter we show that $P_c(s)$ is sensitive to the shape of the sample, too. We present results of a numerical investigation on various finite size cuboids with square base L_0^2 and height L_z, characterized by the aspect ratio $q = L_z/L_0$. Assuming that a formula for the small-s behaviour of $P(s)$, proposed by Kravtsov and Mirlin [20] for the metallic regime, may approximately be used at the metal–insulator transition, a dimensionless critical conductance g_c can be extracted from the small-s behaviour of the calculated $P_c(s)$. We find that g_c also depends on the sample shape and that the value obtained for the cubic system is in close agreement with a result achieved previously by a different method.

We investigate the conventional 3D Anderson model which is described by the Hamiltonian

$$H = \sum_m \varepsilon_m c_m^\dagger c_m + V \sum_{\langle m \neq n \rangle} (c_m^\dagger c_n + c_n^\dagger c_m). \tag{1}$$

The creation, $c_m^\dagger$, and annihilation, c_m, operators act on the states of non-interacting electrons at the sites $\{m, n\}$ of a 3D simple cubic lattice. The disorder energies ε_m are chosen to be a set of independent random numbers distributed in the interval $[-W/2, W/2]$ with probability $1/W$, where W denotes the disorder strength measured in units of V. We consider only transfer between nearest neighbour sites. Periodic boundary conditions are applied in all directions. The sizes of the different systems investigated are described by a quadratic base L_0^2 and a height L_z ranging from 8 to 200 lattice constants a. The shape of the system is conveniently denoted by the dimensionless aspect ratio $q = L_z/L_0$. For all shapes, a size independent metal–insulator transition is found at a critical disorder of $W_c/V = 16.4$.

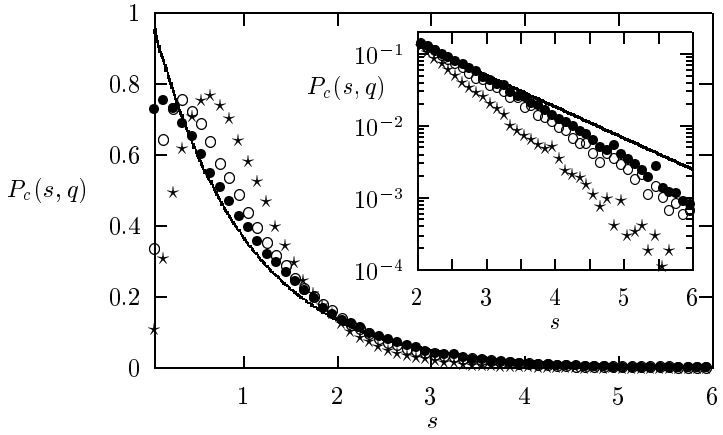

Figure 1. The critical level spacing distribution $P_c(s, q)$ versus the level spacing s for aspect ratios $q = 1$ ($\star$, $L_0 = L_z = 30\,a$), $q = 1/7$ ($\circ$, $L_0 = 56\,a, L_z = 8\,a$) and $q = 20$ ($\bullet$, $L_0 = 10\,a, L_z = 200\,a$). The solid line is the Poissonian decay $\exp(-s)$. The inset displays the semi-logarithmic plot of the large-s behaviour.

The eigenvalues used in our study have been taken from an interval $[-0.5\,V, 0.5\,V]$ around the band centre. They are obtained by direct diagonalization using a Lanczos algorithm. For each aspect ratio, several system sizes are computed with a large number of different realizations of the disorder potentials so that for each particular case the number of eigenvalues exceeded 10^5.

In figure 1 the size independent critical level spacing distribution $P_c(s, q)$ is shown for different aspect ratios: a flat quasi-2D sample ($q = 1/7$), a cube ($q = 1$) and a long narrow bar ($q = 20$). Deviations of the aspect ratio from $q = 1$ result in critical spacing distributions that seem to approach the Poissonian decay, $P(s) = \exp(-s)$, as $q \to 0$ (quasi-2D sample) or $q \to \infty$ (quasi-1D sample).

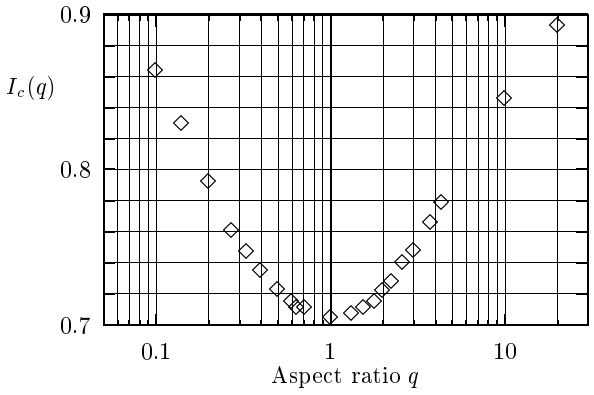

Figure 2. The second moment of the critical level spacings, $I_c(q)$, versus the aspect ratio $q = L_z/L_0$. The corresponding system sizes are in the range from ($L_0/a = 80$, $L_z/a = 8$) to ($L_0/a = 10$, $L_z/a = 200$).

To give a more quantitative description, we have calculated the second moment $I_c(q)$ of the critical level spacings

$$I_c(q) = \tfrac{1}{2}\langle s^2 \rangle = \tfrac{1}{2}\int_0^\infty s^2 P_c(s, q)\,\mathrm{d}s \tag{2}$$

which is shown in figure 2 as a function of the aspect ratio $q = L_z/L_0$. The cube ($q = 1$) represents the minimum value of the second moment, $I_c(1) = 0.705 \pm 0.005$, whereas $I_c(q) \to 1$ for aspect ratios that strongly deviate from the cube. Our value of $I_c(q = 1)$ is in accord with the result of [6]. From the symmetric appearance of the semi-logarithmic plot in figure 2 it becomes apparent that $I_c(q) \to I_c(1/q)$ when crossing $q = 1$.

At present, there exists no complete analytical theory which describes the critical energy level correlations. To compare our results, we therefore have to make do with a formula proposed recently [20] for the metallic regime. The two-level correlation function is defined as

$$R(s) = \frac{1}{\langle \rho \rangle^2}\langle \rho(E)\rho(E + \omega)\rangle \tag{3}$$

where $\rho(E)$ is the density of states at energy E, $s = \omega/\Delta$ and $\langle ... \rangle$ denotes averaging over realizations of the disorder potential. In the metallic regime and for small s, $R(s)$ becomes [20]

$$R(s) = \frac{\pi^2}{6}\left(1 + \frac{3b}{\pi^6 g^2}\right)s. \tag{4}$$

This expression contains corrections to the usual Wigner–Dyson form in the region $\omega \sim \Delta \ll E_c$, where E_c is the Thouless energy. Equation (4) depends on the dimensionless conductance $g \gg 1$, the spatial dimensions, the boundary conditions and also on the shape

of the system via the diffusive modes [20]. For cuboids $L_0^2 \times L_z$ and periodic boundary conditions one gets

$$b = \frac{9/16}{(2+q^2)^2} \sum_{\substack{n_x,n_y,n_z=-\infty \\ n_x^2+n_y^2+n_z^2\neq 0}}^{\infty} \frac{1}{(n_x^2+n_y^2+n_z^2 q^{-2})^2}. \tag{5}$$

At the critical point, where $g = g_c \lesssim 1$, the result of the expansion made in [20] is expected to give only qualitatively correct behaviour. In order to test this expectation, we tentatively assume here that equation (4) actually holds at the metal–insulator transition. Therewith, we are able to extract a shape dependence of the size independent critical conductance g_c from the small-s part of the calculated $P_c(s,q)$, because for small s, $R(s) = \sum_k P(k,s) + \delta(s) \simeq P(0,s)$, where $P(k,s)$ is the probability density of finding exactly k eigenvalues within the interval s.

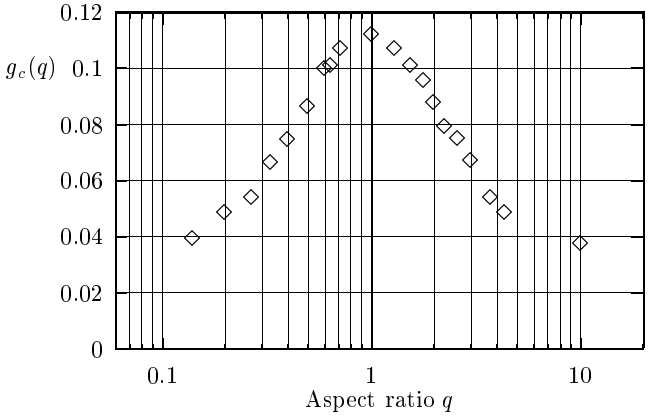

Figure 3. The shape dependent critical conductance $g_c(q)$ as a function of the aspect ratio q.

The critical conductance as a function of the sample shape is shown in figure 3. Here, the values for $q = 0.1$ and $q = 20$ have been omitted, because it was not possible to accurately extract the small-s gradient from the data. Again, the already noticed symmetry in replacing $q \to 1/q$ when crossing $q = 1$ becomes evident.

Our result for the cubic system, $g_c(1) = 0.112 \pm 0.005$, agrees very well with the value $g_c = 0.10 \pm 0.01$ obtained from the numerical calculation of the Kubo conductivity [21]. Since the two methods for determining the critical conductance are completely different, the perfect agreement of the numerical values is remarkable. If this accordance is not merely accidental, it has to be understood why the result of the expansion in [20] holds also quantitatively at the critical point. For Dirichlet boundary conditions, we obtain a numerical value $g_c = 0.079 \pm 0.002$ for the cubic system.

In mesoscopic systems, the decay of $g_c(q)$ accompanied with deviations from the cubic shape may explain some of the different values (0.03–0.2) [22] reported for measurements on various samples. However, the question remains to be answered, whether or not the expression for the small-s behaviour proposed by Kravtsov and Mirlin [20] for the metallic regime is really applicable at the metal–insulator transition.

In conclusion, a dependence of the scale independent critical level statistics on the shape of the samples has been detected at the Anderson transition in 3D systems. Using a formula which has been proposed for the metallic regime [20] to fit our data obtained at the critical

point, we find a shape dependence of the scale independent conductance g_c. Provided that this method of extracting the conductance is justified also at the critical point, the various experimentally obtained critical conductances reported in the literature can possibly be attributed to different shapes of the samples investigated.

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