Crossover from diffusive to strongly localized regime in two-dimensional systems

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We have studied the conductance distribution function of two-dimensional disordered noninteracting systems in the crossover regime between the diffusive and the localized phases. The distribution is entirely determined by the mean conductance, $\langle g \rangle$, in agreement with the strong version of the single-parameter scaling hypothesis. The distribution seems to change drastically at a critical value very close to one. For conductances larger than this critical value, the distribution is roughly Gaussian while for smaller values it resembles a log-normal distribution. The two distributions match at the critical point with an often appreciable change in behavior. This matching implies a jump in the first derivative of the distribution which does not seem to disappear as system size increases. We have also studied $1/\langle g \rangle$ corrections to the skewness to quantify the deviation of the distribution from a Gaussian function in the diffusive regime.

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I. INTRODUCTION

The distribution function P(g) of the conductance of disordered systems is quite well understood in the metallic diffusive regime. It has a Gaussian shape¹ and so its first and second moments are sufficient to describe it. The second cumulant (irreducible moment) is a universal constant² of order e^2/h for a diffusive system of any dimensionality which explains the term *universal-conductance fluctuations*.

On the other hand, the distribution function P(g) in the localized phase is known to be log normal in one-dimensional (1D) systems,³ where the metallic regime does not exist and recently has been found to be a Tracey-Widom distribution for the strongly localized phase in two-dimensional (2D) systems.⁴

The crossover between the diffusive and localized regimes is possible both in quasi-1D and in 2D systems. Extensive studies^{5,6} of quasi-1D systems have shown the distribution function to be independent of the system details with the average conductance being the only scaling parameter. This agrees with the one-parameter scaling hypothesis formulated for the mean conductance⁷ and later extended to the entire conductance-distribution function.⁸ On the insulating side of the quasi-1D crossover, P(g) has been found to be essentially a "one-sided" log-normal distribution⁵ in agreement with analytical studies of strictly 1D systems.³

The validity of the one-parameter scaling hypothesis for the conductance-distribution function has also been studied in the localized phase of 2D systems^{4,9,10} where P(g) is now understood almost as well as in the diffusive phase. However, the crossover regime between the diffusive and the localized phases, where the localization length is of the order of the system size, is poorly understood in 2D systems. The numerical investigation of this regime is the focus of this Brief Report.

The conductance distribution can be described by its cumulants, which have been found in the diffusive regime to have the form¹

$$\langle g^n \rangle_C \propto \langle g \rangle^{2-n}, \quad n < g_0, \quad \langle g \rangle \gg 1.$$
 (1)

Here g is the dimensionless conductance (measured in units of e^2/h), the brackets $\langle \ldots \rangle$ stand for the ensemble averaging over disorder, $\langle \ldots \rangle_c$ denotes a cumulant, and g_0 is the mean conductance at the scale of the elastic mean-free path ℓ . It has been shown that there are no perturbative corrections to the second cumulant (variance). Therefore, in the absence of nonperturbative corrections it would remain universal (of order 1) for any value of $\langle g \rangle$. Since in the regime of strong localization, $\langle g \rangle \ll 1$, the variance should eventually decrease and the nonperturbative corrections must exist.

In the absence of a sharp transition between localized and delocalized states in 2D systems, it is possible that such non-perturbative contribution to the variance can be numerically traced already at the threshold between the diffusive and localized regimes where $\langle g \rangle \sim 1$. As for the higher cumulants, in the metallic and crossover regime one can assess numerically only the third cumulant of the distribution, which represents the leading deviation from the Gaussian. Equation (1) shows that it is proportional to $1/\langle g \rangle$. The constant of proportionality has been calculated diagrammatically 11 and the result for quasi-2D systems is

$$\langle g^3 \rangle_c = -0.0020 \langle g \rangle^{-1}. \tag{2}$$

On the other hand, one can study numerically how the distribution function changes through the crossover regime from the almost Gaussian for $\langle g \rangle > 1$ to almost log normal for $\langle g \rangle < 1$. Analytical studies predict also the appearance of the log-normal tails in the crossover regime¹ which signify the emergence of prelocalized states. However, their statistical weight might be rather small in order to trace them numerically.

Thus the aim of this paper is twofold. First, we want to study systematically the full distribution function P(g) in the crossover regime and check if the scaling hypothesis extended to the full distribution applies in this region. Second, we want to obtain the corrections to the variance and the

leading contribution to the third cumulant as a function of $1/\langle g \rangle$ as we move away from the deep metallic regime into the crossover region.

In the next section, we describe the model and the numerical procedure. In Sec. III, we obtain the conductance distribution function for a wide variety of values of the disorder and the system size and present the results on the applicability of single-parameter scaling in the crossover region. In Sec. IV, we calculate the second and third cumulants of the conductance distribution and analyze their $1/\langle g \rangle$ corrections. In the last section we summarize our findings.

II. MODEL

We have studied numerically the zero temperature conductance of the 2D Anderson model, described by the Hamiltonian

$$H = \sum_{i} \epsilon_{i} a_{i}^{\dagger} a_{i} + t \sum_{i,j} a_{j}^{\dagger} a_{i} + \text{H.c.},$$
 (3)

where the operator $a_i^{\dagger}(a_i)$ creates (destroys) an electron at site i of an square lattice and ϵ_i is the energy of this site chosen randomly between (-W/2, W/2) with uniform probability. The double sum runs over nearest neighbors. The hopping-matrix element t is taken equal to -1, which set the energy scale and the lattice constant equal to 1, setting the length scale. We have considered square samples of size $L \times L$. All calculations are done at an energy equal to -1, to avoid possible specific effects associated with the center of the band.

The zero-temperature conductance g is proportional to the transmission coefficient T between two semi-infinite leads attached at the opposite sides of the sample

$$g = \frac{2e^2}{h}T,\tag{4}$$

where the factor of 2 comes from spin. From now on, we will measure the conductance in units of $2e^2/h$. We have calculated the transmission coefficient from the Green's function, which was obtained propagating layer by layer with the recursive Green's function method. 13 This drastically reduced the computational effort and we can easily solve samples with lateral dimension up to 250 for the calculation of the distribution function, which requires a huge number of independent runs to get good statistics in the tails. The number of different realizations employed is of 10⁶ for most values of the parameters. We have considered wide leads with the same section as the samples, which are represented by the same Hamiltonian as the system, Eq. (3) but without diagonal disorder. The leads serve to obtain the conductivity from the transmission formula in a way well-controlled theoretically and close to the experimental situation. In the study of the distribution function, we use cyclic periodic boundary conditions in the direction perpendicular to the leads. In the calculation of the corrections to the variance and the skewness (Sk), we have also considered hard-wall boundary conditions to make sure that they do not drastically change the results. The main conclusions are similar and we will present

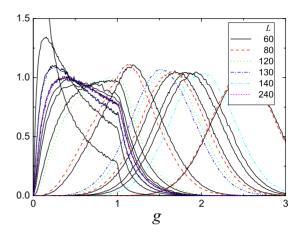


FIG. 1. (Color online) Conductance-distribution function in the crossover between the diffusive and the localized regime for the values of L size indicated in the legend and for W ranging between 3 and 6.

results for periodic boundary conditions, for which we have better statistics.

III. CONDUCTANCE DISTRIBUTION

We have obtained the conductance-distribution function for many values of the disorder and the system size, chosen in such a way that the system is in the crossover region, i.e., its mean value of the conductance is close to one. In Fig. 1 we represent many of these distributions as a function of the conductance for the values of the system size given in the legend. The disorder varies between W=3 and 6. When the mean conductance is larger than one the distribution is basically a Gaussian with an approximately constant standard deviation, given by the value of the universal conductance fluctuations. As we approach the crossover, the shape of the high-conductance tail remains close to a Gaussian function but there is a drastic change in behavior of the distribution at the value g = 1. An important conclusion that can be extracted from Fig. 1 is that the entire conductance distribution is uniquely determined by the mean conductance along the crossover region. This support the strong version of the single-parameter scaling hypothesis. In several cases, we have adjusted the value of the disorder in such a way that the mean conductance is the same for different system sizes. In all these cases, the agreement between the different distribution functions is quite remarkable. For example, the distribution function for W=4.2 and L=60, whose mean conductance is equal 0.6677, is very similar to the distribution for W=4.75 and L=240, whose mean is 0.6686.

For some distributions, we can appreciate a marked discontinuity in the first derivative of the distribution at $g \approx 1$. This drastic change in behavior has been reported in different contexts but it has never been analyzed in depth for 2D systems. It appeared in the critical conductance distribution at the metal-insulator transition in three-dimensional systems¹⁴ at the quantum-Hall transition,¹⁵ in the 2D symplectic ensemble¹⁶ and in quasi-one-dimensional systems.^{5,6} In order to check if this apparent discontinuity in the fist derivative of

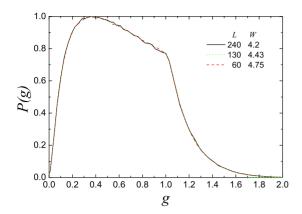


FIG. 2. (Color online) Conductance-distribution function for three different pairs of values of the disorder and the system size chosen so that the mean conductance is the same for all of them, equal to 0.67 ± 0.01 .

P(g) is a finite-size effect or not, we have run extensively three different systems with the same mean conductance, equal to 0.67 ± 0.01 , and with sizes equal to 60, 120, and 240 (the values of the disorder are 4.75, 4.43, and 4.2, respectively). In Fig. 2 we plot the conductance-distribution functions of these three systems. We first note the excellent agreement between the three of them, showing again that the distribution is entirely determined by a single parameter. Second, we appreciate that the possible discontinuity in the first derivative of the distribution does not seem to vanish away as the size increases.

IV. 1/g CONTRIBUTIONS TO THE SKEWNESS

The large amount of data gathered in our simulation allows us to study with enough precision how the conductance distribution deviates from a Gaussian in the diffusive regime as a result of 1/g corrections. We have quantified this deviation through the Sk of the conductance. As we expect a leading contribution to Sk proportional to $1/\langle g \rangle$, we have plotted in Fig. 3 Sk $\langle g \rangle$ as a function of $1/\langle g \rangle$ for periodic boundary conditions. The data corresponding to the ballistic regime have not been drawn. The criteria to consider a data in the

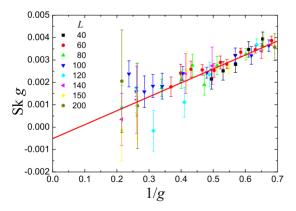


FIG. 3. (Color online) Skewness multiplied by $\langle g \rangle$ as a function of $1/\langle g \rangle$ for periodic boundary conditions. Each symbol corresponds to a different system size.

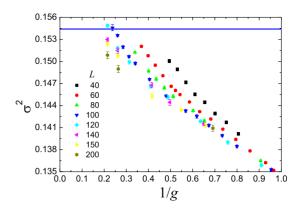


FIG. 4. (Color online) Variance as a function of $1/\langle g \rangle$ for periodic boundary conditions. Each symbol corresponds to a different system size. The horizontal line represents the value of the universal conductance fluctuations.

ballistic regime was the ratio of system size to elastic meanfree path, L/l, to be smaller than 20. We will discuss this criterion later on when analyzing the behavior of the variance. The elastic mean-free path can be obtained through the dependence of the mean conductance with the system shape. ¹⁷ For our model, we define l through the equation

$$\langle g \rangle = \frac{L_x l}{L_y} - \frac{1}{3},\tag{5}$$

where L_x and L_y are the transversal and longitudinal dimensions, respectively. We have fitted the data in Fig. 3 by an expression of the form

$$\operatorname{Sk}\langle g \rangle = a + \frac{b}{\langle g \rangle} + \frac{c}{L},$$
 (6)

where the last term corresponds to a finite-size contribution. The straight line in Fig. 3 is the extrapolation to infinite size of Eq. (6) and intersects the vertical axis at -0.0005 ± 0.0004 . This value is in reasonable agreement with the prediction of van Rossum $et~al.^{11}$ of -0.002, if we take into account that this estimate does not considered an specific set of boundary conditions and so we are not comparing exactly the same quantities. We note that in the region studied, the contribution to the skewness proportional to $1/\langle g \rangle^2$ is large and soon dominates over the negative linear contribution.

We have also calculated the variance of the conductance, $\sigma^2 = \langle g^2 \rangle_c$. In Fig. 4 we plot the variance of the data that we consider to be in the diffusive regime as a function of the inverse of the mean conductivity $1/\langle g \rangle$. The horizontal line corresponds to the value of universal conductance fluctuations for periodic boundary conditions, which is equal to $\sigma_0^2 = 0.1544$. We note that the range of the vertical axis is small. There is a region in the ballistic regime where the variance presents a peak (not shown) whose magnitude depends on system size and is larger than the value of the universal conductance fluctuations. In Figs. 3 and 4 we have only included data with L/l > 20, our criteria to be in the diffusive regime. We have calculated the eigenvalues of the transmission matrix and for L/l < 20 there are many with

transmission close to one, i.e., there are many ballistic channels contributing to the current. As *g* increases the variance gets closer to the universal value.

We note in Fig. 4 that there is a systematic size dependence of the variance, breaking the strong version of single-parameter scaling in this regime. This is probably due to the ballistic regime whose influence is much larger than expected. The existence of these finite-size effects together with the strong criteria needed to be in the diffusive regime, makes difficult a precise numerical determination of the universal conductance fluctuations.

V. DISCUSSION

We have found numerically the behavior of the variance and the skewness in the crossover regime is compatible with analytical predictions.¹ However, our results do not constitute a clear check since more precise numerical study of $1/\langle g \rangle$ corrections to the variance requires, on one hand, a very large number of realizations and on the other hand rather large sizes in order to avoid the ballistic regime.

We have also observed the change in shape of the distribution function when from diffusive through crossover regime. It can hardly be attributed, though, to the existence of prelocalized states ^{1,12} which cannot be numerically checked for available system sizes at present time. This implies that the pre-exponential factor for these states should be relatively small.

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