Boundary conditions, the critical conductance distribution, and one-parameter scaling

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We study the influence of boundary conditions transverse to the transport direction for disordered mesoscopic conductors both at the Anderson metal-insulator transition and in the metallic regime. We show that the boundary conditions strongly influence the conductance distribution exactly at the metal-insulator transition and we discuss implications for the standard picture of one-parameter scaling. We show in particular that the scaling function that describes the change of conductance with system size depends on the boundary conditions from the metallic regime up to the metal-insulator transition. An experiment is proposed that might test the correctness of the one-parameter scaling theory.

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I. INTRODUCTION

More than 40 years after its discovery by Anderson[1] the disorder-induced metal-insulator transition is still the subject of much theoretical as well as experimental research.[2] One of the major achievements in the long history of the Anderson metal-insulator transition (MIT) is the renormalization group theory, which has also become known as the one-parameter scaling theory.[3,4] Its basic assumption is that close to the transition the change of the dimensionless conductance g with the sample size L depends only on the conductance itself and not separately on energy, disorder, the size of the sample, its shape, the elastic mean free path l_e, etc. Many predictions, like the lower critical dimension or the critical behavior,[5,6] were successfully based on this theory, as well as an enormous amount of numerical work that aimed at the direct calculation of the scaling function $\beta(g)=d\ln g/d\ln L$. Another important consequence of the one-parameter scaling theory is the prediction of a universal conductance distribution $P^*(g)$ exactly at the MIT.[7] Earlier numerical work on the three-dimensional Anderson model seemed to confirm the universality of the conductance distribution.[8] The dependence on the universality class was stressed in Ref. 9.

Recently, however, some doubts have been cast on whether the conductance distribution is universal within the *same* universality class. Two different numerical studies reported two different forms of $P^*(g)$ for the same system,[9,10] and it was found that the difference originates in the use of different boundary conditions (BC's).[11]

The idea that $P^*(g)$ might depend on the BC's indeed appears very natural after the discovery that spectral statistics, and in particular the energy level spacing distribution $P(s)$ exactly at the MIT, *do* depend on the BC's.[12] Samples with periodic boundary conditions show a much stronger level repulsion than samples with hard walls (Dirichlet boundary conditions).

In this work we show with a numerical analysis of the conductance distribution at the critical point that $P^*(g)$ does indeed depend on the BC's applied perpendicular to the transport direction. Choosing the appropriate boundary conditions, we can reproduce the results of both Refs. 9 and 10. In particular, the average critical conductance g_c depends on the BC's. This alone already implies a dependence of $\beta(g)$ on the BC's since g_c is defined as $\beta(g_c)=0$. We confirm the BC dependence of $\beta(g)$ analytically by reinvestigating its form in the metallic regime with the help of a $1/g$ expansion. Much to our surprise we find that earlier analyses overlooked the effect of the BC's by approximating a sum over diffusion modes by an integral. Evaluating the sum more carefully, we find not only a dependence on the BC's, but also a so far unknown $\ln(l_e/L)/g$ term in $\beta(g)$ in three dimensions that makes $\beta(g)$ nonuniversal in the metallic regime.

II. NUMERICAL INVESTIGATION AT THE ANDERSON TRANSITION

The model studied is the three-dimensional tight binding Anderson Hamiltonian with diagonal disorder on a simple cubic lattice,

$$H=\sum_i e_i|i\rangle\langle i|+u\sum_{\substack{\langle ij\rangle\\ \text{bulk}}}|i\rangle\langle j|+u\sum_{\substack{\langle ij\rangle\\ \sigma_y,\sigma_z}}\times c(e^{2\pi i\phi}|i\rangle\langle j|+\text{H.c.}). \quad (1)$$

The e_i are distributed uniformly and independently between $-w/2$ and $w/2$. The notation $\langle ij\rangle$ means next nearest neighbors, u is the hopping matrix element, which we set equal to unity in the following, and w is the disorder parameter. The last sum in Eq. (1) links corresponding sites on opposite sides of the cubic sample perpendicular to the y and z directions, assuming that transport occurs in the x direction. Hopping between these boundary sites arises when the system is closed to a ring ($c=1$) and includes a phase factor $e^{i2\pi\phi}$, where ϕ is the magnetic flux in units of h/e enclosed by the ring. Hard wall (Dirichlet) BC's correspond to $c=0$. The model (1) shows a MIT at the critical disorder $w_c\simeq 16.5$.[13]

The numerical calculation of the conductances uses a standard Green's function recursion technique[14] that yields

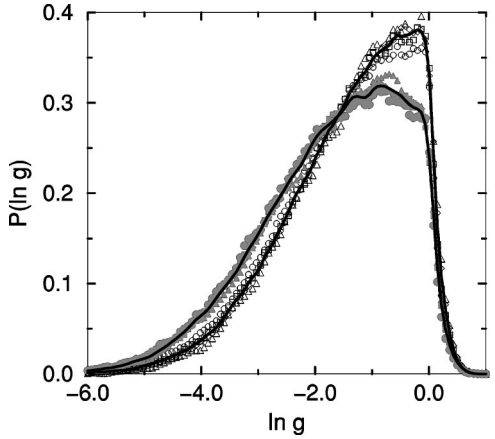

FIG. 1. Critical conductance distribution for periodic and hard wall boundary conditions, and different sample sizes. Sample sizes $L=8$, 10, 12, and 16 are denoted by circles, squares, diamonds, and triangles, respectively; open symbols indicate periodic BC's, full ones hard walls. The full lines are averages over the above system sizes.

the transmission matrix t of the sample. The latter is connected to the two-probe conductance of the sample by the Landauer-Büttiker formula

$$g=\mathrm{tr}\, tt^{+}, \tag{2}$$

where $g=G/(e^2/h)$ denotes the conductance G in units of the inverse of the von Klitzing constant h/e^2. Whether the two-probe conductance formula or the four-probe conductance formula is used is irrelevant at the metal-insulator transition, since the bulk resistance always greatly dominates over the contact resistance.[15] All conductances were calculated at energy $E\simeq 0$. The number of conductances used for each BC and system size ranged from 10^5 for $L=6$ and $L=8$ to 2×10^3 for $L=16$. All system sizes L are measured in units of the lattice constant.

Our main numerical result is shown in Fig. 1, where we have plotted the distributions of the logarithm of the conductance at the transition for periodic and hard wall (HW) BC's, and different system sizes. For the same BC the distribution is almost independent of the system size, as is to be expected from the criticality of the ensemble at $w_c=16.5$. But the distributions are clearly very different for the two BC's. The maximum of the distribution is considerably more pronounced for periodic BC's than for hard walls. A more detailed statistical analysis is presented in Table I and for the average values $\langle \ln g\rangle$ in Fig. 2.

The average is always over the disorder ensemble. Figure 2 shows that the average logarithmic conductance still depends slightly on the system size in the regime investigated. But the difference between periodic and hard wall BC's does not diminish with increasing L, and the dependence on L decreases for larger L. Where we have used the same system sizes as in Refs. 9 and 10 our values for all quantities calculated ($\langle g\rangle$, $\langle \ln g\rangle$, and the standard deviations of g and $\ln g$) coincide within 1% with the values given in these references. For comparison with Ref. 10, g should be multiplied by a factor 2, since we consider only one spin direction. Thus, the discrepancy between Refs. 9 and 10 can indeed be explained by the influence of the BC's (see also Ref. 11).

TABLE I. Statistical analysis of the critical conductance distribution for different boundary conditions (P periodic and HW hard wall). Besides the averages of g and $\ln g$ the standard deviations of these quantities, σ_g and $\sigma_{\ln g}$ are also given.

L	BC	$\langle g\rangle=g_c$	σ_g	$\langle \ln g\rangle$	$\sigma_{\ln g}$
6	P	0.356	0.314	-1.554	1.183
8	P	0.377	0.324	-1.476	1.159
10	P	0.392	0.329	-1.412	1.129
12	P	0.402	0.334	-1.378	1.118
16	P	0.413	0.336	-1.329	1.092
6	HW	0.313	0.306	-1.777	1.281
8	HW	0.326	0.310	-1.710	1.252
10	HW	0.331	0.312	-1.685	1.246
12	HW	0.338	0.311	-1.675	1.211
16	HW	0.348	0.319	-1.614	1.222

Our result has important implications for the scaling theory of the metal-insulator transition, since it shows that the scaling function $\beta(g)$ must depend on the BC's. The conductance that enters into this equation has to be understood as an average conductance,[16] and the critical conductance is given by $\beta(g_c)=0$. According to our results g_c depends on the BC's, $g_c=0.413$ for periodic BC's and $g_c=0.348$ for hard walls at $L=16$ (see Table I), and therefore the $\beta(g)$ curves must at least be shifted as a function of the BC's. In the next section we show by reexamining the weak localization corrections to the conductance that $\beta(g)$ depends on the BC's in the metallic regime also.

III. METALLIC REGIME

It is well known that in the metallic regime $g\gg 1$ the quantum interference of diffusing electrons reduces the conductance compared to the classical value $g=\sigma L$, where σ is the bulk conductivity. The weak localization correction δg is given by a sum over diffusion modes as[16]

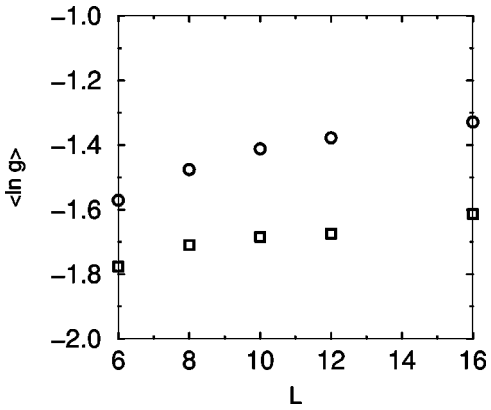

FIG. 2. As a function of system size the average $\langle \ln g\rangle$ is plotted for periodic (circles) and hard wall boundary conditions (squares).

$$\delta g = -2\sum_{\mathbf{q}} \frac{e^{-D\mathbf{q}^2\tau_e}}{\mathbf{q}^2 L^2}. \tag{3}$$

The sum is limited to the diffusive regime where $D\mathbf{q}^2 \ll 1/\tau_e$. This limitation is taken into account by the exponential cutoff; τ_e is the elastic collision time, $D=v_F^2\tau_e/3$ denotes the diffusion coefficient, and v_F is the Fermi velocity. The sum (3) depends on the BC's via the quantization condition for the diffusion modes **q**. For the transport direction the wave vector is quantized according to $q_x = n_x\pi/L$, $n_x = 1,2,\ldots$. Periodic boundary conditions in the y direction imply $q_y = n_y 2\pi/L$, $n_y = \pm 1, \pm 2, \ldots$ and correspondingly for the z direction. Hard wall BC's on the other hand, lead to $q_y = n_y\pi/L$, $n_y = 0,1,2,\ldots$ and $q_z = n_z\pi/L$, $n_z = 0,1,2,\ldots$. Consequently, we have

$$\delta g = -\frac{2}{\pi^2} S_{BC}(y) \tag{4}$$

where the index BC stands for a boundary condition and

$$S_P(y) = \sum_{\substack{n_x>0 \\ n_y,n_z\neq 0}} \frac{\exp[-\pi^2(n_x^2+4n_y^2+4n_z^2)y]}{n_x^2+4n_y^2+4n_z^2}, \tag{5}$$

$$S_{HW}(y) = \sum_{\substack{n_x>0 \\ n_y,n_z\geqslant 0}} \frac{\exp[-\pi^2(n_x^2+n_y^2+n_z^2)y]}{n_x^2+n_y^2+n_z^2}. \tag{6}$$

The argument y is defined as

$$y = \frac{D\tau_e}{L^2} = \frac{1}{3}\left(\frac{l_e}{L}\right)^2. \tag{7}$$

Previous analyses in the literature proceeded by approximating the sum by an integral,[16] whereupon all dependence on the boundary conditions is lost. While this is a good approximation for $g\to\infty$, important corrections of the order $(\ln g)/g$ arise for finite g, which we are going to derive now, assuming that to this order no further diagrams beyond the diffuson approximation contribute. In Ref. 17 it was shown by field theoretical methods combined with a renormalization group approach that the diffuson approximation gives the leading perturbative contribution to the small energy behavior of the spectral correlation function to order $1/g^2$.

In order to proceed it is convenient to differentiate $S_{BC}(y)$. The derivatives for both periodic BC's (PBC's) and HW BC's can be written with the help of the function

$$F(y) = \sum_{n=1}^{\infty} e^{-\pi^2 n^2 y} \tag{8}$$

as

$$\partial_y S_P(y) = -\pi^2 F(y)[2F(4y)]^2, \tag{9}$$

$$\partial_y S_{HW}(y) = -\pi^2 F(y)[1+F(y)]^2. \tag{10}$$

The function $F(y)$ is related to the complete elliptic integrals $K\equiv K(k)$ and $K'\equiv K(k')$ with $k'=\sqrt{1-k^2}$ by[18]

$$\frac{1}{2}\left[\left(\frac{2K}{\pi}\right)^{1/2} - 1\right] = \sum_{n=1}^{\infty} e^{-\pi n^2 K'/K}. \tag{11}$$

Since we are interested in $y \ll 1$, we need $K'/K \ll 1$ and therefore $k\to 1$ $(k'\ll 1)$. For small values of k' the elliptic integrals behave like

$$K = \ln\frac{4}{k'} + O(k'^2), \quad K' = \frac{\pi}{2} + O(k'^2), \tag{12}$$

and we therefore obtain

$$F(y) \simeq \frac{1}{2}\left[\left(\frac{1}{\pi y}\right)^{1/2} - 1\right]. \tag{13}$$

Inserting this into Eqs. (9) and (10) and integrating with respect to y yields

$$S_P = \frac{\sqrt{\pi}}{4\sqrt{y}} + \frac{5}{8}\pi\ln y - 2\pi^{3/2}\sqrt{y} + \frac{\pi^2}{2}y - \alpha_P, \tag{14}$$

$$S_{HW} = \frac{\sqrt{\pi}}{4\sqrt{y}} - \frac{1}{8}\pi\ln y + \frac{1}{4}\pi^{3/2}\sqrt{y} + \frac{\pi^2}{8}y - \alpha_{HW}, \tag{15}$$

whereas by replacing the sum (3) by an integral one would have found

$$S = \frac{\sqrt{\pi}}{4\sqrt{y}} - \alpha, \tag{16}$$

where α is an integration constant resulting from the cutoff at small $q\simeq 1/L$. Thus, the leading term for small y, $\sqrt{\pi/y}/4$, is the same for both boundary conditions. The integration constants α_P and α_{HW} can be evaluated numerically, by subtracting from the exactly calculated sums the analytical formulas (14) and (15) without the constants. At the same time this serves as a sensitive check for the correctness of these formulas. For small y the differences converge to

$$\alpha_P \simeq -6.1509, \quad \alpha_{HW} \simeq 2.3280. \tag{17}$$

We have evaluated the sum numerically down to values $y = 10^{-6}$, where in particular the logarithmic term with the prefactors given above could be clearly verified.

With Eqs. (14) and (15) the conductance as a function of the dimensionless length $\tilde{L}\equiv L/l_e$ takes the form

$$g = (\tilde{\sigma} - A)\tilde{L} - a\ln\tilde{L} + b + O(1/\tilde{L}) \tag{18}$$

for both periodic and hard wall BC's. The dimensionless bulk conductivity $\tilde{\sigma}$ is defined as $\tilde{\sigma} = \sigma l_e h/e^2$, and the constant $A=\sqrt{3}/(2\pi^{3/2})$ is the same for both BC's. The coefficients a and b, on the other hand, do depend on the boundary conditions; their values are given in Table II. Note that in the traditional approach the coefficient a vanishes.

Quite surprisingly $a<0$ for PBC's, which means that the conductance increases even slightly faster than linearly with

TABLE II. Coefficients in the $1/\tilde{L}$ expansion of g for periodic boundary conditions (PBC) and hard walls (HW).

	a	b
PBC	$-5/(2\pi)\simeq -0.7958$	$5(\ln 3)/(4\pi)-2\times 6.1509\pi^2\simeq -0.8093$
HW	$1/(2\pi)\simeq 0.1592$	$2\times 2.328/\pi^2-(\ln 3)/(4\pi)\simeq 0.3843$

the system size. This looks as if there is antilocalization, but it should be noted that the leading behavior due to weak localization is still the usual decrease of the (bulk) conductivity, i.e., the leading term is linear in the system size and with the expected negative sign. The fact that $a<0$ only for PBC's suggests a simple physical explanation for the logarithmic term: Closing the sample to a double torus by imposing PBC's allows for additional paths that interfere constructively and lead to enhanced localization for small system sizes compared to the HW case. When increasing the system size these additional localizing paths quickly stop contributing and the conductance therefore increases more rapidly than would be expected just from the volume part of the weak localization.

We are now in a position to explore the consequences of the BC dependent weak localization corrections for the scaling function $\beta(g)$. Inserting Eq. (18) into the definition

$$\beta(g)\equiv\frac{d\ln g}{d\ln\tilde{L}} \tag{19}$$

yields

$$\beta(g)=1+\frac{1}{g}[a\ln\tilde{L}-b-a+O(1/\tilde{L})]. \tag{20}$$

It remains to reexpress $\tilde{L}$ by g. To this end we invert $g(\tilde{L})$ from Eq. (18) to order $1/g$,

$$\tilde{L}=\frac{1}{\tilde{\sigma}-A}[g+a\ln g-a\ln(\tilde{\sigma}-A)+b], \tag{21}$$

and insert it in Eq. (20). We obtain the final result

$$\beta(g)=1-\frac{1}{g}\{b+a[1+\ln(\tilde{\sigma}-A)]-a\ln g\}+O(1/g^2). \tag{22}$$

It is now obvious that the scaling function does indeed depend on the BC's via the coefficients a and b, and the dependence arises at order $(\ln g)/g$. Furthermore, $\beta(g)$ depends to order $1/g$ as well on the material dependent dimensionless bulk conductivity $\tilde{\sigma}$, and is therefore *nonuniversal*. Again, the nonuniversality vanishes for $g\to\infty$ (equivalently, on the metallic side of the transition: $L\to\infty$), but is important if one is interested in $\beta(g)$ at finite values of g. This nonuniversality was already noticed by Abrahams *et al.*,[3] who where ''unable to show definitely that the mean free path does not represent a relevant scale for the problem.'' Since HW BC's lead to smaller values of $\beta(g)$ at intermediate values of g than PBC's but to a smaller critical conductance, there should be a point where the two curves cross, which would imply that at that point the change of g with the system size is independent of the BC's. Due to the dependence of $\beta(g)$ on $\tilde{\sigma}$, this point is not expected to be universal, though.

Our result implies that the relevant length scale for a correct renormalization procedure cannot be the system size as proposed in the seminal paper of Abrahams *et al.*[3] As suggested by Gorkov *et al.*, a correct procedure is scaling driven by frequency or temperature in an infinite system.[4]

The most interesting question is, of course, whether the slope of $\beta(g)$ at $g=g_c$ is also changed by the BC's and/or $\tilde{\sigma}$, as this slope determines the critical exponent ν defined by $\xi(w)\propto|g-g_c|^{-\nu}$ according to $\beta(g)=(1/\nu)(g-g_c)/g_c$. This question actually arises already from the dependence of spectral statistics on the BC's, since the scaling function can be determined also from purely spectral statistics.[19,20] Very recently it has been argued that within the same universality class ν at least does not depend on the shape of the sample.[21] Since the critical spectral statistics does depend on the shape of the sample much in the same way[22] as on the BC's (indeed, all that has been said above about the dependence on the BC's translates one to one to a dependence on the shape of the sample), one might suspect that ν is also independent of the BC's. On the other hand, considering the qualitative behavior of the two scaling curves, a critical exponent independent of the BC's would appear rather as a coincidence. However, so far it is an open question and definitely deserves attention.[23]

The scale dependence of the conductance at the MIT was predicted by Polyakov[24] to be a simple power law, $\delta g=g-g_\infty\propto 1/L^y$ with an exponent $y=3-d_2$ in three dimensions, where d_2 is the multifractal exponent of the wave functions ψ associated with $|\psi|^4$. While our results do not contradict such a power law dependence, it is difficult to establish the exponent from the present numerical data due to the limited L interval accessible to the simulation.

With the dependence of the critical conductance distribution on the BC's, an experimental test of the correctness of the one-parameter scaling picture seems within reach. Even though an accurate absolute measurement of the critical exponent is rather difficult,[25,26] one might hope to detect a *change* with the BC's. To this end it is not even necessary to open and close the sample. Rather, one can investigate the difference between periodic and *antiperiodic* boundary conditions. At least in one direction antiperiodic BC's, i.e., a phase factor -1 between two opposite sides of the sample, can easily be produced by closing the sample to a ring and introducing half a magnetic flux quantum [$\phi=1/2$ in Eq. (1)]. Note that for $\phi=1/2$ the system still belongs to the orthogonal universality class, since the Hamiltonian has a

real representation. This situation has been termed ''false time reversal symmetry breaking.''[27] An experimental search for a change of the scaling function in the metallic regime upon inclusion of half a flux quantum would also be a most welcome contribution to the long-lasting debate on the limits of validity of one-parameter scaling.

In summary, we have shown that the conductance distribution at the Anderson metal-insulator transition depends on the boundary conditions applied in the directions transverse to the transport. Furthermore, in the metallic regime the dependence of a change of the conductance on the system size does not depend solely on the conductance itself but also on the boundary conditions and the dimensionless bulk conductivity. As a consequence the scaling function $\beta(g)$ that describes the change of conductance when the size of the sample is changed is not entirely universal but depends on the boundary conditions and the amount of disorder in the sample from the metallic regime up to the metal-insulator transition.

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