Level curvatures and conductances: A numerical study of the Thouless relation

D. Braun
FB7, Universität–GHS Essen, 45 117 Essen, Germany

E. Hofstetter and A. MacKinnon
Blackett Laboratory, Imperial College, London SW7 2BZ, England

G. Montambaux
Laboratoire de Physique de Solides, associé au CNRS, Université Paris Sud, 91405 Orsay, France
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The Thouless conjecture states that the average conductance of a disordered metallic sample in the diffusive regime can be related to the sensitivity of the sample's spectrum to a change in the boundary conditions. Here we present results of a direct numerical study of the conjecture for the Anderson model. They were obtained by calculating the Landauer-Büttiker conductance g_L for a sample connected to perfect leads and the distribution of level curvatures for the same sample in an isolated ring geometry, when the ring is pierced by an Aharonov-Bohm flux. In the diffusive regime ($L \gg l_e$) the average conductance $\langle g_L \rangle$ is proportional to the mean absolute curvature $\langle |c| \rangle$, $\langle g_L \rangle = \pi \langle |c| \rangle / \Delta$, provided the system size L is large enough, so that the contact resistance can be neglected. l_e is the elastic mean free path, and Δ is the mean level spacing. When approaching the ballistic regime, the limitation of the conductance due to the contact resistance becomes essential and expresses itself in a deviation from the above proportionality. However, in both regimes and for all system sizes the same proportionality is recovered when the contact resistance is subtracted from the inverse conductance, showing that the *curvatures measure the conductance in the bulk*. In the localized regime, the mean logarithm of the absolute curvature and the mean logarithm of the Landauer-Büttiker conductance are proportional. [S0163-1829(97)03813-7]

I. INTRODUCTION

It has been shown by Thouless and Edwards in the 1970s that the conductance of a disordered diffusive system can be related to the dependence of the energy levels to a change in the boundary conditions.[1,2] A physical realization of this change in the boundary conditions is made when the sample is closed to a ring and pierced by a Aharonov-Bohm flux ϕ. In such a case the wave function must obey the condition $\psi(x+L) = \psi(x) e^{i\eta}$ where $\eta = 2\pi\phi/\phi_0$. Here $\phi_0 = h/e$ is the flux quantum. Thouless found that the average conductance is proportional to the width of the distribution of the curvatures of the energy levels when η is the perturbation parameter. This relation is based on a similar structure of the Kubo expression for the conductance and of the curvature of energy levels when the boundary conditions are changed. In the diffusive regime, the average absolute curvature of the energy levels is proportional to the diffusion coefficient and thus to the conductance. Although this conjecture was derived under oversimplified assumptions, its basic idea has proved to be very powerful and has become a keystone in our understanding of localization.

Meanwhile, other measures of the conductance in terms of the response of the system's energy spectrum to a change of the boundary conditions have been derived. These spectral measures of the conductance were all obtained for the diffusive regime. They all measure the diffusion constant in the bulk, and are in this sense equivalent to each other. Indeed, it has been shown that the Kubo conductance can be expressed as the average square of the first derivative of the energy levels with respect to flux.[3–5] The average has to be taken over both flux and disorder. The relation between these quantities and the curvature distribution was studied both numerically and analytically.[4,6,7]

However, so far very little effort has been devoted to comparing spectral measures of the conductance to the customary conductance formulas based on transport considerations, like in particular the Landauer-Büttiker formula. Exceptions are Ref. 8, where small one-dimensional (1D) systems were treated numerically, and Ref. 9 devoted to the study of random banded matrices. This is surprising, since spectral measures of the conductance have been widely used in the mesoscopic community. Yet it is well known that the conductance of a mesoscopic sample depends sensitively on the measurement geometry and on the way the leads are attached to the sample. On the other hand, the spectral measures of conductance are completely insensitive in this respect, since the sample is closed to a ring and no leads are attached. The system is then in fact a different one. Its spectrum is discrete when the system is finite, whereas the system attached to the leads always has a continuous spectrum.

How can it then be possible that the width of the curvature distribution measures the conductance obtained in a transport measurement? In this paper we find that the appropriate conductance is obtained in a situation where the system is connected to leads with the same transverse width and with maximal transmission coefficient. We refer to this situation as ''maximal coupling.'' It is analogous to the ''matching wire'' condition defined by Economou and Soukoulis[17] and also used in Ref. 9. In this case the mean absolute cur-

vature is proportional to the Landauer-Büttiker conductance. This proportionality holds if the system is large enough and the disorder strong enough such that the contact resistance can be neglected. In the ballistic regime, the contact resistance is always important and destroys the proportionality. However, after subtracting the contact resistance from the total inverse conductance, the remaining bulk conductance is proportional to the mean absolute curvature. The proportionality coefficient is the same in the diffusive and in the ballistic regime for all system sizes, as long as the samples have similar geometry. This shows that *the curvatures measure a bulk conductance*. In the localized regime, it is the mean logarithm of the absolute curvatures and the conductances that are proportional to each other.

In the next section we briefly review the different definitions of the conductance. In Sec. III we discuss our numerical method and in Sec. IV we present the results of extensive numerical simulations, in which we calculated the level curvatures from a perturbative formula and the conductances with the Landauer-Büttiker formula. The conductances extend over seven orders of magnitude and allow us to study the diffusive as well as the ballistic and localized regimes. We conclude in Sec. V.

II. KUBO, LANDAUER, AND THOULESS CONDUCTANCES

A. Kubo and Thouless conductances

Let us first recall the main line of the Thouless derivation. On the one hand, the dc Kubo conductivity can be written as[10]

$$\sigma=\frac{\pi e^2\hbar}{m^2V}\sum_{\alpha,\beta}|p_{\alpha\beta}|^2\delta(E_F-\varepsilon_\alpha)\,\delta(E_F-\varepsilon_\beta), \tag{1}$$

where ε_α are single-energy levels and $p_{\alpha\beta}=\langle\alpha|\hat{p}|\beta\rangle$ are the matrix elements of the momentum operator. $V=L^d$ is the volume and E_F the Fermi energy. Strictly speaking, this expression is zero for a finite system.[11] To get a finite σ, the δ functions must have a finite width larger than the interlevel spacing. Under this condition and assuming that the matrix elements $p_{\alpha\beta}$ are decorrelated from the ε_α,[12] the average conductivity is given by

$$\langle G_K\rangle=\langle\sigma\rangle L^{d-2}=\frac{\pi e^2\hbar L^{2d-2}}{m^2}\langle|p_{\alpha\beta}|^2\rangle\rho_0^2. \tag{2}$$

$\langle\cdots\rangle$ represents an average over the disorder. ρ_0 is the average density of states per unit volume at the Fermi energy. The dimensionless conductance $\langle g_K\rangle$ can be written as[13]

$$\langle g_K\rangle\equiv\frac{\langle G_K\rangle}{e^2/h}=2\pi\frac{E_c}{\Delta}, \tag{3}$$

where $\Delta=1/(\rho_0L^d)$ is the mean level spacing, and the Thouless energy E_c is given by $E_c=\hbar D/L^2$, D being the diffusion coefficient.[2] The second equality in formula (3) is nothing but the Einstein relation $\sigma=e^2D\rho_0$. All these quantities are defined for a given Fermi energy and will in general depend on E_F.

On the other hand, under the change in the boundary conditions $\psi(x+L)=\psi(x)e^{i\eta}$, the curvature of a given energy level ε_α at the origin ($\eta=0$) is given exactly by perturbation expansion in η:

$$c_\alpha=\left(\frac{\partial^2\varepsilon_\alpha}{\partial\eta^2}\right)_{\eta=0}=\frac{\hbar^2}{mL^2}+\frac{2\hbar^2}{m^2L^2}\sum_{\beta\neq\alpha}\frac{|p_{\alpha\beta}|^2}{\varepsilon_\alpha-\varepsilon_\beta}. \tag{4}$$

In order to relate the width of the curvature distribution to the diffusion coefficient, Thouless assumed first that the energy levels ε_α are not correlated with the matrix elements $p_{\alpha\beta}$. Replacing then $|p_{\alpha\beta}|^2$ by its average value, the distribution of the curvatures is that of $1/(\varepsilon_\alpha-\varepsilon_\beta)$. Second, assuming that the energy levels themselves are not correlated, the sum in Eq. (4) gives rise to a Levy law for the distribution of the curvatures in the limit of infinitely many levels.[1] It has the Cauchy form $P(c)=(\gamma_0/\pi)/(\gamma_0^2+c^2)$ with a width γ_0 given by

$$\gamma_0=\frac{2\pi\hbar^2}{m^2L^2}\frac{\langle|p_{\alpha\beta}|^2\rangle}{\Delta}. \tag{5}$$

Comparison between Eqs. (2) and (5) gives the relation between the dimensionless average conductance $\langle g_K\rangle=\langle G_K\rangle h/e^2$ and the width of the distribution of curvatures, known as the Thouless relation,[2] $\langle g_K\rangle=\pi(\gamma_0/\Delta)$. However, it is now known that the energy levels are strongly correlated in a metal so that the curvature distribution does not have the Cauchy form. Instead, it is given by

$$P_\beta(c)=\frac{N_\beta}{(\gamma_\beta^2+c^2)^{(\beta+2)/2}}. \tag{6}$$

Here, $\beta=1$ if there is time-reversal symmetry and $\beta=2$ if time-reversal symmetry is broken. N_β is a normalization coefficient. This form was guessed by Zakrzewski and Delande[14] to fit numerical calculations on various models exhibiting chaotic spectra. It has been proven analytically by von Oppen[15] for random matrices of the form $H(\lambda)=H+\lambda K$ where H and K are random matrices belonging to the same symmetry class [$\beta=1$ for the Gaussian orthogonal ensemble (GOE), $\beta=2$ for the Gaussian unitary ensemble (GUE)]. λ is the perturbation parameter. Recent numerical calculations have shown that this distribution is also characteristic of metallic spectra when the perturbation parameter is an AB flux ϕ.[6] In particular, in the limit where $\phi\to0$, the distribution is still the GOE distribution [$\beta=1$ in Eq. (6)].[6] This has been proven analytically by Fyodorov and Sommers who also found that there are no corrections of order Δ/E_c.[7]

The normalized distribution in zero field is thus

$$P_1(c)=\frac{1}{2}\frac{\gamma_1^2}{(\gamma_1^2+c^2)^{3/2}}. \tag{7}$$

Fyodorov and Sommers have shown that the width of this distribution can be related to the diffusion coefficient.[7] They find that the width γ_1 of this distribution for a three-dimensional ring is given by $\gamma_1=2E_c$. Using now Eq. (3), relating E_c to the Kubo conductance, one deduces $\gamma_1=\Delta\langle g_K\rangle/\pi$. To characterize this width it is convenient to

introduce the average absolute curvature $\langle|c|\rangle=\gamma_1$, so that *the Thouless conductance defined as*

$$\langle g_T\rangle \equiv \pi\frac{\langle|c|\rangle}{\Delta} \tag{8}$$

equals the Kubo conductance: $\langle g_T\rangle=\langle g_K\rangle$.

It has to be noted that, first, all conductances considered so far are average conductances, the average extending over disorder realizations. Second, the equation $\langle g_T\rangle=\langle g_K\rangle$ holds so far only for the diffusive regime, since $\gamma_1=2E_c$ was derived in Ref. 7 for the diffusive regime. We will see that the equation has to be modified in the ballistic and localized regimes.

B. Landauer-Büttiker conductances

Another way to express the conductance has been introduced by Landauer. He related this quantity to the scattering properties of the disordered system, when it is *connected* to *incoherent* reservoirs through *ideal leads*. This approach ideally suits transport through finite mesoscopic systems and shows the importance of the measurement geometry. For one dimension, Landauer derived the dimensionless conductance $\tilde{g}_L$:[16]

$$\tilde{g}_L \equiv \frac{\tilde{G}_L}{e^2/h}=\frac{T}{1-T}. \tag{9}$$

This conductance is the ratio $\tilde{G}_L=I/(\mu_A-\mu_B)$ where μ_A and μ_B are the chemical potentials of ideal leads attached to the barrier. T is the transmission coefficient through the disordered region. $\tilde{g}_L$ diverges for an ideal, clean sample. On the other hand, Economou and Soukoulis, trying to derive this formula from linear response theory (Kubo formula), found[17]

$$g_L=\frac{G_L}{e^2/h}=T \tag{10}$$

instead. In this case, $G_L=I/(\mu_1-\mu_2)$, where μ_1 and μ_2 are the chemical potentials of the reservoirs.[11] Equation (9) describes a four-terminal measurement in one dimension, that is, a measurement with separate current and voltage probes.[18] $g_L=T$ describes a two-probe measurement, where only two leads are attached to the sample and serve as current and voltage probes at the same time. The remaining finite resistance at zero disorder ($g_L=1$) is a ''contact resistance'' which has its origin in the coupling of the sample to the incoherent reservoirs.[11,19] This resistance cannot be avoided in a two-probe measurement. One may therefore think of the total resistance G_L^{-1} in such a 1D two-probe geometry as being the sum of the contact resistance h/e^2 and a ''bulk resistance'' $\tilde{G}_L^{-1}$ The latter vanishes when the disorder goes to zero and is identical with the original Landauer contribution:

$$G_L^{-1}=\tilde{G}_L^{-1}+\frac{h}{e^2}. \tag{11}$$

Fisher and Lee generalized Eq. (10) to the multichannel case:[20]

$$g_L=g_K=\sum_{i=1}^{M} T_i=\mathrm{tr}tt^{+}. \tag{12}$$

T_i is the total transmission probability in the ith channel, t the transmission matrix, and M the number of channels. When the disorder in the sample goes to zero, g_L is limited by the number of open channels. Today there is a general agreement that Eq. (12) describes a two-probe measurement in a multichannel geometry. In our numerical simulations we will focus on this situation and use Eq. (12) for the numerical evaluation of the conductance.

Comparing Eqs. (8) and (12), one gets a relation between the average Landauer-Büttiker conductance and the width of the curvature distribution:

$$\langle g_L\rangle=\pi\frac{\langle|c|\rangle}{\Delta}. \tag{13}$$

In the two-probe multichannel geometry we will consider in the following one might again decompose the total resistance into a sum of a contact resistance plus a bulk resistance, the latter being entirely due to the motion in the bulk of the sample. In straight generalization of Eq. (11), it is then natural to define the bulk conductance $\tilde{G}_L=(e^2/h)\tilde{g}_L$ by

$$G_L^{-1}=\tilde{G}_L^{-1}+R_c, \tag{14}$$

where $R_c=h/(Me^2)$ is the ''contact resistance'' for the multichannel system.[11,21] We have then

$$\tilde{g}_L=\frac{\Sigma T_i}{1-\Sigma T_i/M}. \tag{15}$$

In the diffusive regime, the effective number of conducting channels, $M_{\mathrm{eff}}=\Sigma T_i$, is much smaller than M: $M_{\mathrm{eff}}=Ml_e/L$ where l_e is the elastic mean free path.[23] Consequently, g_L and $\tilde{g}_L$ are almost identical in the diffusive regime, the relative deviations being of order l_e/L. However, in the ballistic regime they behave very differently: $\tilde{g}_L\to\infty$ and $g_L\to M$ in the limit of zero disorder.

For more than one channel $\tilde{g}_L$ has not the simple and general interpretation of the conductance measured in a four-probe measurement. Indeed, in the multichannel case not only the number of leads but also the way (e.g., under what angles) they are attached influences the measured conductance, such that a general four-probe formula might not even exist.[22] Similarly $\langle|c|\rangle$ cannot correspond to any particular four-probe conductance, since it is an intrinsic property of the disordered region. We will show that for a finite system $\langle|c|\rangle$ is proportional to $\langle\tilde{g}_L\rangle$:

$$\langle\tilde{g}_L\rangle=\pi\frac{\langle|c|\rangle}{\Delta}. \tag{16}$$

III. NUMERICAL METHOD

The starting point of our analysis is the Anderson tight-binding Hamiltonian H of a disordered system on a square lattice of $L_x\times L_y\times L_z$ sites. For the curvature calculation the system is closed to a ring and pierced by an Aharonov-Bohm flux ϕ:

$$H=\sum_i e_i|i\rangle\langle i|+u\sum_{\langle ij\rangle}|i\rangle\langle j|+u \times \sum_{\substack{\langle ij\rangle \\ i_x=L_x,j_x=1}}(e^{i\eta}|i\rangle\langle j|+\text{H.c.}). \quad (17)$$

The e_i are distributed uniformly and independently in an interval between $-w/2$ and $w/2$. Here $\langle ij\rangle$ denote next nearest neighbors, u is the hopping matrix element which we set equal to one in the following, and w is the disorder parameter. The last sum in Eq. (17) is over the set of sites on the two boundaries limiting the open sample in the x direction. Hopping between these boundary sites arises when the system is closed to a ring and includes a phase factor $e^{i\eta}$. For $\phi=0$ or entire multiples of the flux quantum, one recovers periodic boundary conditions.

For the calculation of g_L, the system is open and coupled to perfect leads. The last sum in Eq. (17) is then missing. This is the only difference between the two Hamiltonians. In particular, for the numerical implementation the same random number generator was used for the diagonal matrix elements in both situations.

A. Curvatures

In the diffusive regime, the curvatures can be evaluated by replacing differentials by small flux differences whose values are varied for control in a suitable way.[6] This procedure has the numerical advantage that only eigenvalues, not the eigenvectors, are needed. However, it is very difficult to control in the ballistic and in the localized regime. We adopted therefore a routine based on an exact perturbative formula corresponding to Eq. (4). In fact, treating η in Eq. (17) as a perturbation up to second order, one finds for the curvatures at zero flux

$$\frac{c_\alpha}{2}=\sum_{\substack{\langle ij\rangle \\ i_x=L_x,j_x=1}}\langle\epsilon_\alpha|i\rangle\langle j|\epsilon_\alpha\rangle+\sum_{\beta\neq\alpha}\frac{1}{\epsilon_\beta-\epsilon_\alpha} \times\left(\sum_{\substack{\langle ij\rangle \\ i_x=L_x,j_x=1}}\langle\epsilon_\beta|i\rangle\langle j|\epsilon_\alpha\rangle-\langle\epsilon_\beta|j\rangle\langle i|\epsilon_\alpha\rangle\right)^2, \quad (18)$$

where ϵ_α and $|\epsilon_\alpha\rangle$ denote the eigenvalues and eigenvectors of the Hamiltonian at zero flux, respectively. Higher-order terms vanish since $\eta=0$. In the two directions perpendicular to the transport direction, periodic boundary conditions were used. Formula (18) is exact as long as $\epsilon_\beta\neq\epsilon_\alpha$. Thus, for a finite system, where level repulsion is always present at sufficiently small energy scales,[25] Eq. (18) remains valid also in the localized and ballistic regimes. Besides rounding errors which can be neglected here the only remaining errors in the calculation of $\langle|c_\alpha|\rangle$ are statistical errors that can be controlled by increasing the number of disorder realizations. We used up to 1000 disorder realizations for system sizes of $6\times6\times6$ sites and still about hundred for $10\times10\times10$ sites. Relatively, the remaining statistical errors in the diffusive and ballistic regimes were of the order of 10^{-2}, which we checked by varying the number of disorder realizations. As Eq. (18) indicates, *all* eigenvalues and eigenvectors are needed for the calculation of a single curvature. Realizations where our Lanczos routine failed to find all eigenvalues and eigenvectors were therefore discarded.

B. Conductances

The conductance g_L was calculated from Eq. (12) by the Green's function recursion technique.[24] The Green's function connecting the two ends of a strip can be calculated recursively using the equations

$$\mathbf{G}^{(N)}_{N,N}=[Z-\mathbf{H}_N-\mathbf{u}^\dagger\mathbf{G}^{(N-1)}_{N-1,N-1}\mathbf{u}]^{-1}, \quad (19)$$

$$\mathbf{G}^{(N)}_{1,N}=\mathbf{G}^{(N-1)}_{1,N-1}\mathbf{u}\mathbf{G}^{(N)}_{N,N}, \quad (20)$$

where $\mathbf{G}^{(N)}_{N,N}$ represents the submatrix of the Green's function between sites on the Nth slice of a strip of length N, $\mathbf{G}^{(N)}_{1,N}$ is the corresponding submatrix between sites on the 1st and Nth slices, and $\mathbf{H}_N$ represents the Hamiltonian of the Nth slice alone. The system can be embedded in semi-infinite leads by choosing the initial values of the two Green's functions to represent the end of a semi-infinite wire and by adding a final slice for which the Hamiltonian of the slice is replaced by the self-energy matrix for another semi-infinite wire. Having the Green's functions one can derive the transmission matrix t (Ref. 24) and then the conductance g_L.

IV. RESULTS

A. Energy dependence

Without averaging over energy, both $\langle g_T\rangle$ and $\langle g_L\rangle$ are energy dependent: $\langle g_T(E)\rangle$ and $\langle g_L(E)\rangle$. The variation of $\langle g_L(E)\rangle$ is smooth and is due to the energy dependence of the density of states (DOS) and of the number of channels, M. The energy dependence of $\langle g_T(E)\rangle$ arises from the variation with energy of both $\langle|c|\rangle$ and $\Delta(E)$, where the latter quantity is the mean level spacing at a given energy (averaged over disorder only). In order to get the conductance at a given energy, we therefore rescaled the curvatures with an energy-dependent Δ: $\tilde{c}_\alpha=c_\alpha/\Delta(\epsilon_\alpha)$. The disorder-averaged DOS $1/\Delta(E)$ was obtained by the standard method of fitting the spectral staircase (integrated DOS) to a polynomial.

After averaging over 1000 disorder realizations (in the case of systems with $6\times6\times6$ sites), the fluctuations of $\langle|\tilde{c}_\alpha|\rangle=\langle|c_\alpha|\rangle/\Delta(\epsilon_\alpha)$ as a function of energy turned out to be still much more pronounced than those of $\langle g_L(E)\rangle$. This is not too surprising, as it is well known that in the diffusive regime the conductance distribution (which is a universal Gaussian distribution[26,27] with a width of the order of the conductance quantum) and the curvature distribution (see Sec. I) are very different. Thus, when using just one disorder realization, the fluctuations of the function $|\tilde{c}_\alpha(\epsilon_\alpha)|$ will be much larger than those of $g(E)$, due to the long $1/c_\alpha^3$ tails of the curvature distribution. For a finite number of realizations this difference will still persist, and only when averaging over infinitely many disorder realizations should the energy dependence of $\langle g_L\rangle$ follow that of $\langle|\tilde{c}_\alpha|\rangle$. Having in mind that even 1000 disorder realizations did not suffice to reduce the fluctuations of $\langle g_T(E)\rangle$ to a level comparable to those of $\langle g_L(E)\rangle$, it seems very difficult to check the Thouless conjecture in the stronger sense for a given energy with the current computing power available. We therefore averaged g_L and g_T not only over the realizations but over a band

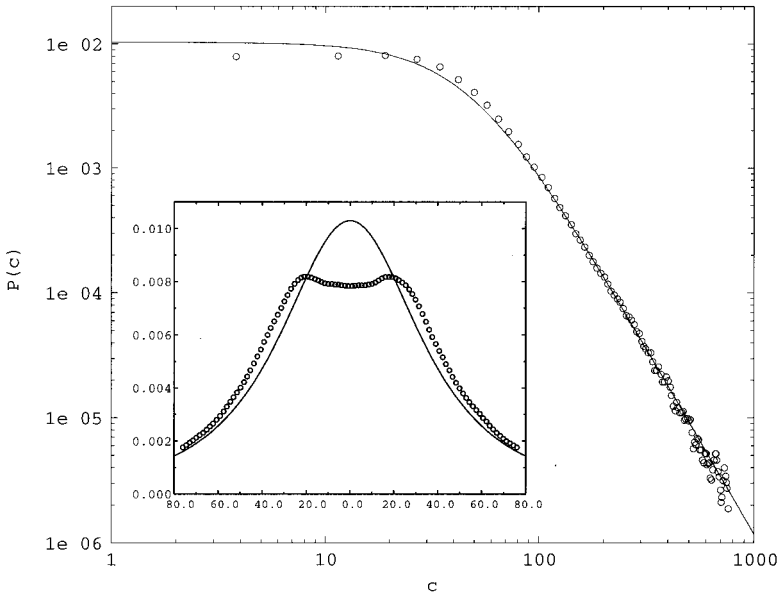

FIG. 1. The curvature distribution in the ballistic regime. The solid line is the prediction of Eq. (7) known to be valid in the diffusive regime. Deviations at small curvature are visible (see inset). $6\times6\times6$ sites, $w=1.0$, 4000 disorder realizations.

of energy ΔE comprising typically about the central half of the spectrum as well. We checked that increasing the size of the system or the number of realizations allows one to decrease ΔE to obtain the same results. This suggests that our results are independent of ΔE. In the following, $\langle\cdots\rangle$ will stand for the combined disorder and energy average. Care was taken in order to average both curvatures and conductances over exactly the same energy interval.

B. Curvature distribution

In the diffusive regime, the distribution of the curvatures is well described by Eq. (7). Thus, $\langle|c|\rangle$ is a good measure of the width of the curvature distribution.

Outside the diffusive regime the curvature distribution was not known so far, and one might wonder whether $\langle|c|\rangle$ is still well defined. We therefore calculated $P(c)$ numerically for both the ballistic and the localized regimes. Figure 1 shows $P(c)$ for a system in the ballistic regime ($6\times6\times6$ sites, $w=1.0$, 4000 disorder realizations) and the prediction of Eq. (7), where γ_1 was determined as $\gamma_1=\langle|c|\rangle$ (no fitting parameter). Equation (7) works well for large curvatures and shows that in the ballistic regime $P(c)$ has $1/c^3$ tails as in the diffusive regime. For small curvatures deviations from Eq. (7) in the form of nonuniversal features appear and the distribution develops two maxima. A relative minimum appears at zero curvature. These deviations become even more pronounced for smaller disorder. Altogether we conclude that $\langle|c|\rangle$ can still serve as a measure for the width of the curvature distribution, even in the ballistic regime.

In the localized regime at least two different numerical works favor a log-normal curvature distribution.[28,29] Analytical evidence for a log-normal distribution at least for small curvatures in 1D is given in Ref. 30. On the other hand, one might suspect that Thouless' original result of a Cauchy dis-

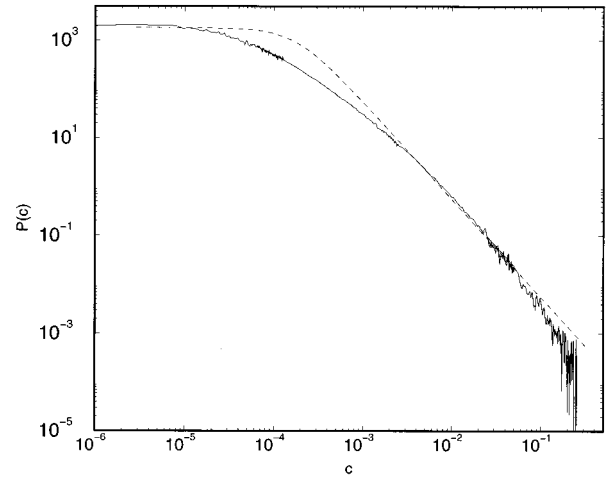

FIG. 2. The curvature distribution in the localized regime with a fit to a Cauchy distribution (dashed line). This plot shows that $P(c)$ decays faster than $1/c^2$ for large curvatures. $6\times6\times6$, $w=50$, 4000 disorder realizations.

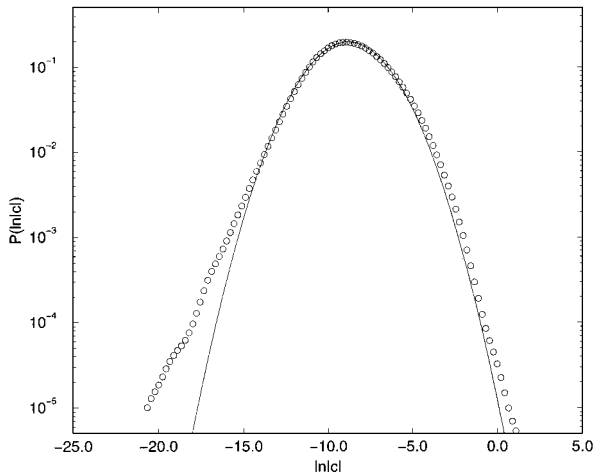

FIG. 3. Distribution of $\ln|c|$ in the localized regime with a fit to a Gaussian distribution (corresponding to a log-normal distribution for $|c|$). Same parameters as in Fig. 2.

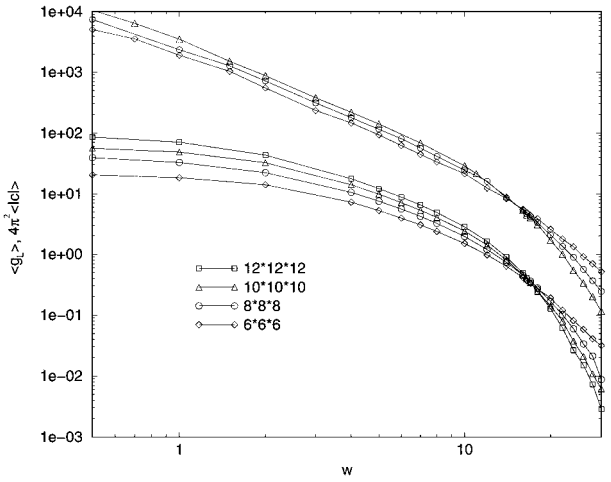

FIG. 4. The overall disorder dependence of $\langle|\tilde{c}_\alpha|\rangle$ (top) and $\langle g_L\rangle$ (bottom) for different system sizes: diamonds, $6\times6\times6$; circles, $8\times8\times8$; and triangles, $10\times10\times10$. The straight lines of $\langle|\tilde{c}_\alpha(w)|\rangle$ in the logarithmic plot correspond to a $1/w^2$ divergence for small w. Solid lines are guides to the eye only. For clarity the $\langle|\tilde{c}_\alpha(w)|\rangle$ curves were shifted by an arbitrary factor $4\pi^2$.

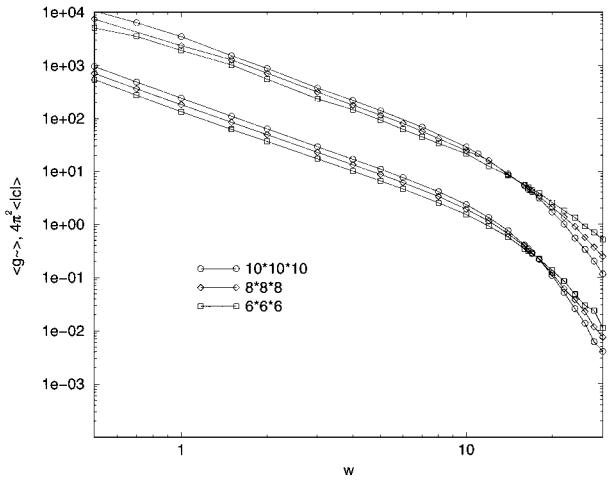

FIG. 5. The overall disorder dependence of $\langle|\tilde{c}_\alpha|\rangle$ (top) and $\langle\tilde{g}_L\rangle$ (bottom) for different system sizes (same symbols as in Fig. 4). $\langle\tilde{g}_L(w)\rangle$ diverges in the same manner as $\langle|c_\alpha(w)|\rangle$ for small w. Solid lines are guides to the eye only.

tribution due to uncorrelated eigenvalues might apply to the localized regime. Such a distribution would of course spoil the use of $\langle|c|\rangle$ as a measure of the Thouless conductance. We therefore reexamined this question numerically. As shown in Fig. 2, a Cauchy distribution can be ruled out: For large curvatures, the distribution falls off faster than $1/c^2$. This can probably be explained by the fact that the eigenvalues and the eigenvectors are strongly correlated for large disorder in contrast to what was assumed by Thouless in the derivation of his formula. On the other hand, Fig. 3 shows that a log-normal distribution does not fit perfectly either. Rather large deviations are visible for large curvatures. We will address this question in more detail in a future work. Nevertheless, we can conclude from Fig. 2 that both $\langle|c|\rangle$ and $\langle\ln|c|\rangle$ are well-defined quantities in the localized regime.[31]

C. Disorder dependence

Before discussing the disorder regimes separately, we display in Fig. 4 an overall plot of the disorder dependence of $\langle|\tilde{c}_\alpha|\rangle$ and $\langle g_L\rangle$. Several points can be observed immediately: First of all, $\langle|\tilde{c}_\alpha|\rangle$ diverges for small disorder like $1/w^2$. This is a well-known fact which can be derived from perturbation theory (first Born approximation.[32]) Also, $\langle|\tilde{c}_\alpha|\rangle$ has the right scaling behavior of a conductance. In 3D, in the ballistic and diffusive regimes, $\langle|\tilde{c}_\alpha|\rangle$ increases proportionally to the system size L within the parameter range provided ($L=6$–10). In the localized regime it decays with the system size. In 3D there is a critical value $w_c\simeq16.5$ where $\langle|\tilde{c}_\alpha|\rangle$ becomes independent of the system size, thus indicating the position of the metal-insulator transition (MIT). Within the error bars it coincides with the well-known value found by MacKinnon and Kramer, who examined the scaling behavior of the transmission through disordered samples.[33] We also checked that in 2D $\langle|\tilde{c}_\alpha|\rangle$ is independent of L in the diffusive and ballistic regimes.

1. Ballistic and diffusive regimes

Figure 4 shows that $\langle g_L\rangle$ obeys the same scaling behavior as $\langle|\tilde{c}_\alpha|\rangle$. However, the disorder dependence of $\langle g_L\rangle$ and $\langle|\tilde{c}_\alpha|\rangle$ is rather different. Even in the diffusive regime, $\langle g_L\rangle$ follows $\langle|\tilde{c}_\alpha|\rangle$ only over a small disorder interval close to the metal-insulator transition. The interval's width increases with the system size, but for all system sizes the discrepancy becomes very pronounced in the ballistic regime, where $\langle g_L\rangle$ converges to a constant value, whereas $\langle|\tilde{c}_\alpha|\rangle$ keeps diverging.

Following our discussion of Sec. II this result is not surprising. In the ballistic regime, D formally diverges, as does $\langle|\tilde{c}_\alpha|\rangle$. Any limitation of the conductance due to the coupling of the sample to the environment must then result in a deviation from the conjectured proportionality between $\langle|\tilde{c}_\alpha|\rangle$ and $\langle g_L\rangle$. Clearly, the discrepancy in the lower disorder limit of the diffusive regime is already caused by the crossover to constant $\langle g_L\rangle$ due to the boundary resistance.

In order to improve the agreement of $\langle|\tilde{c}_\alpha|\rangle$ with the conductance, the latter has to be defined such that it does not incorporate the contact resistance. We therefore also compared the disorder dependence of $\langle\tilde{g}_L\rangle$ with the one of $\langle|\tilde{c}_\alpha|\rangle$. As explained in Sec. II, $\langle\tilde{g}_L\rangle$ does not contain the contribution of the boundary resistance and should be a measure of the bulk conductance. It will therefore also diverge when the disorder vanishes. Whereas it is not clear from the beginning that this divergence will be of the same kind as the one of $\langle|\tilde{c}_\alpha|\rangle$, Fig. 5 shows that $\langle\tilde{g}_L\rangle$ diverges for small w indeed with the same power as $\langle|\tilde{c}_\alpha|\rangle$. Both curves follow each other from the diffusive regime until far into the ballistic regime.

In Fig. 6 we have plotted $\langle\tilde{g}_L\rangle$ as function of $\langle|\tilde{c}_\alpha|\rangle$. The MIT is given in this plot by the point where $4\pi^2\langle|\tilde{c}_\alpha|\rangle\simeq4.1$. The points from all sample sizes considered in 3D now fall on one straight line with slope 1 and this in the diffusive as well as in the ballistic regime.[34] A fit to a linear law gives

$$\langle\tilde{g}_L\rangle=(0.99\pm0.04)\,\pi\langle|\tilde{c}_\alpha|\rangle-0.029\pm0.008, \qquad (21)$$

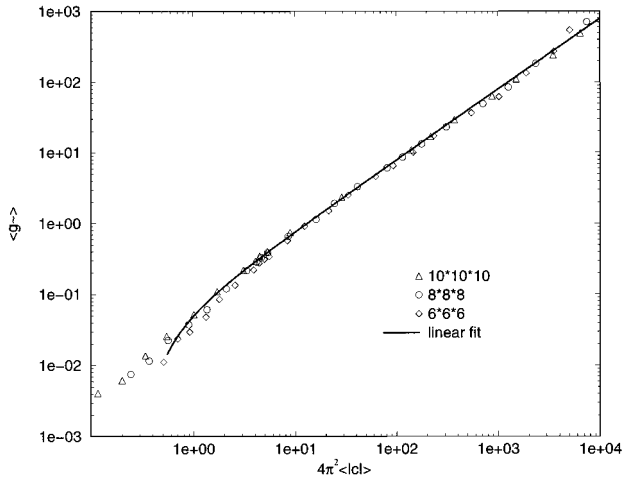

FIG. 6. The conductance $\langle\tilde{g}\rangle$ plotted against $\langle|\tilde{c}_\alpha|\rangle$ for different system sizes (same symbols as in Fig. 4). The diffusive regime starts with the critical mean curvature $4\pi^2\langle|\tilde{c}_\alpha|\rangle\simeq 4.1$. In this regime and the ballistic regime the dependence is very well fitted by the same linear law $\langle\tilde{g}_L\rangle=(0.99\pm0.04)\pi\langle|\tilde{c}_\alpha|\rangle-0.029\pm0.008$ (solid line).

in remarkable agreement with Eq. (16).[35] The error bars were obtained as standard deviations from the three system sizes considered. The conclusion is therefore that $\langle|\tilde{c}_\alpha|\rangle$ measures the bulk conductance $\langle\tilde{g}_L\rangle$ in both the diffusive and ballistic regimes.

In a recent paper, Casati *et al.* also study the relation between Landauer conductance and curvature distributions for band random matrices and they find the relation

$$\langle g_L\rangle=(7.5\pm0.4)\mathcal{K}_{\rm av}, \tag{22}$$

where they define $\mathcal{K}_{\rm av}$ as the *geometric* average $\exp\langle\ln(|c|/\Delta)\rangle$.[9] For a distribution of curvatures like Eq. (7), the geometric average is related to the arithmetic average by[36]

$$\mathcal{K}_{\rm av}=\exp\left\langle\ln\frac{|c|}{\Delta}\right\rangle=\frac{1}{2}\left\langle\frac{|c|}{\Delta}\right\rangle.$$

Using the relation (13) we get the following result:

$$\langle g_L\rangle=2\pi\mathcal{K}_{\rm av}.$$

This factor 2π has to be compared with the the numerical result [Eq. (22)] found by these authors.

2. Localized regime

Figure 6 shows that the power between $\langle|\tilde{c}_\alpha|\rangle$ and $\langle\tilde{g}_L\rangle$ changes at the MIT. We obtain approximately $\langle g_L\rangle\propto\langle|\tilde{c}_\alpha|\rangle^{1.2}$. However, in the localized regime $\langle|\tilde{c}_\alpha|\rangle$ and $\langle\tilde{g}_L\rangle$ might not be the right quantities to look at. At least from the conductance it is known that in this regime the function with the right scaling behavior is $\langle\ln g_L\rangle$,[37] not $\langle g_L\rangle$. Since the favored log-normal distribution of curvatures is due to the same reason as the log-normal distribution of the conductances, namely, the exponentially decaying wave functions with normally distributed localization length, one might suspect that a similar statement holds for the curvatures as well. We therefore also examined $\langle\ln g_L\rangle$ and $\langle\ln|c|\rangle$

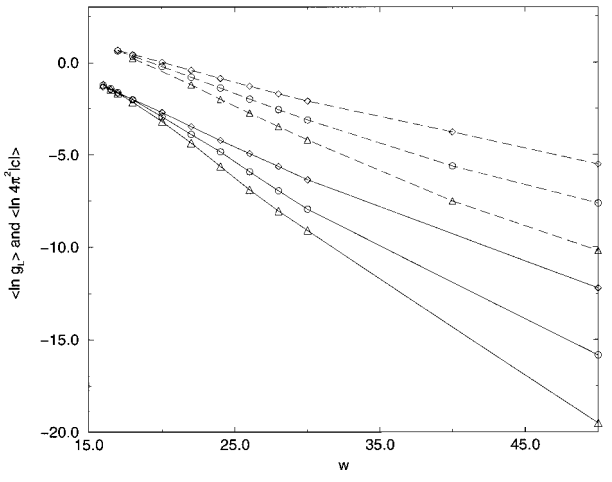

FIG. 7. $\langle\ln|c|\rangle$ (top) and $\langle\ln g_L\rangle$ (bottom) as a function of disorder for three different system sizes in the localized regime (same symbols as in Fig. 4).

as functions of disorder and system size. Figure 7 shows the result: First of all both quantities are proportional to the system size and, second, proportional to each other. Plotting $\langle\ln g_L\rangle$ versus $\langle\ln|c|\rangle$ (see Fig. 8) yields a straight line that is best approximated by the linear law

$$\langle\ln g_L\rangle\simeq 1.7\langle\ln|c|\rangle-2.5. \tag{23}$$

Again, the validity of this equation extends over several orders of magnitude of the conductance. However, the prefactor seems to decrease slightly but systematically with the system size. A law like Eq. (23) was also reported in Ref. 9 with a similar prefactor (1.73) for banded random matrices. Nevertheless, Ref. 9 also reports a prefactor 2.0 for an Anderson model. We do not have any explanation for this difference besides the fact that in contrast to our box-distributed disorder the disorder was Gaussian distributed in Ref. 9. The found behavior is *a priori* surprising. Assuming that in the localized regime the flux dependence of each en-

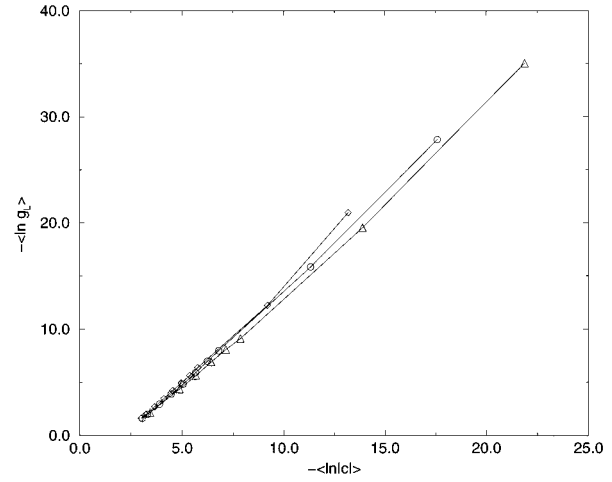

FIG. 8. $\langle\ln g_L\rangle$ as a function of $\langle\ln|c|\rangle$ in the localized regime for three different system sizes (same symbols as in Fig. 4).

ergy level is purely sinusoidal[38] one deduces that $\langle \overline{i^2(\varphi)} \rangle \propto \langle c^2 \rangle$, where $i_\alpha(\varphi) = -\partial e_\alpha / \partial \varphi$ and the overbar indicates a flux average. Since $\langle \overline{i^2(\varphi)} \rangle$ can be related to the Kubo conductance, one would expect a quadratic relation $\langle g_L \rangle \propto \langle c^2 \rangle$.[39]

V. CONCLUSION

We have examined numerically the relation between level curvatures and conductances for disordered systems. We showed that in the diffusive regime a proportionality between the dimensionless mean absolute curvature $\langle |\tilde{c}_\alpha| \rangle$ and the average Landauer-Büttiker conductance $\langle g_L \rangle$ holds if the system is large enough so that the influence of the boundary resistance can be neglected. In the ballistic regime, the boundary resistance can never be neglected and leads to a strong violation of the proportionality. In the limit of zero disorder it completely dominates the total resistance and limits $\langle g_L \rangle$ to the number of open channels, whereas $\langle |\tilde{c}_\alpha| \rangle$ diverges in the same limit. However, for all system sizes a proportionality between a properly defined bulk conductance $\langle \tilde{g}_L \rangle$ and $\langle |\tilde{c}_\alpha| \rangle$ could be established that holds in the same form in the diffusive and ballistic regimes. This shows that in these regimes level curvatures measure a conductance that is entirely due to the dynamics in the bulk of the sample and therefore not influenced by details of the measurement setup, like the number of leads and the way they are attached. In the localized regime, we found a proportionality between $\langle \ln|c| \rangle$ and $\langle \ln g_L \rangle$.

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[35] We draw attention to the fact that the prefactor π is not universal but depends on the sample geometry (Ref. 7). In our calculations all samples had the same ring geometry.
[36] The distribution of conductances is Gaussian: The arithmetic and the geometric averages are identical as long as they are large compared to the width of the distribution.
[37] In the localized regime it is irrelevant whether or not the boundary resistance is included in the conductance: $\langle g_L \rangle = \langle \tilde{g}_L \rangle$ up to exponentially small corrections.
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