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Level curvature and metal–insulator transition in 3d Anderson model

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Abstract. — The level curvature in the Anderson model on a cubic lattice is numerically investigated as an indicator of the metallic–insulator transition. It is shown that the mean curvature obeys a scaling law in the whole range of the disorder parameter. In the metallic regime, the distribution of rescaled curvatures is found to be well described by a formula proposed by Zakrzewski and Delande [1] for random matrices, implying a relation similar to that by Thouless. In the localized regime the distribution of curvatures is approximated by a log-normal distribution.

Introduction.

The numerical investigation of transport properties of disordered 3D systems is severely limited by the problem of diagonalizing large matrices. This occurs for example in the identification and the study of the metal–insulator transition, which shows in a structural change of the eigenfunctions from extended to localized. It is therefore desirable to devise appropriate indicators that capture the structure of eigenfunctions with the minimal computational effort.

One such quantity is level curvature, which measures the response of energy levels to variations of boundary conditions, and obviously relates to the tails of eigenfunctions, responsible for conduction. This quantity was first proposed and investigated by Edwards and Thouless [2, 3]. The parametric dependence of boundary conditions can be introduced by replicating the cubic sample in a periodic sequence, so that each eigenvalue becomes a function of a Bloch phase. An equivalent procedure is to connect two opposite faces of the cube and allow a magnetic flux through the ring, involving a phase change of the wave function across the cut that affects the eigenvalues.

To probe the bulk properties of eigenfunctions, it is possible to resort on first order perturbation theory, by applying external weak fields [4]. The response of levels to a uniform electric field provides the average position $\langle \mathbf{n} \rangle$ in the lattice. This, and the response to a linear field,

provide the variance in space of the probability distribution of a single eigenvector: a measure of its localization [5].

An interesting feature of the metallic-insulator transition is the change of the level spacing statistics from the Wigner distribution, characteristic of the Gaussian orthogonal ensemble (GOE), to the Poisson distribution. Shklovskii *et al.* [6] investigated the Anderson transition by looking at a parameter γ which weights the tail of the spacing distribution $P(s)$, being Gaussian or exponential, respectively for GOE (delocalized states, small disorder) and Poisson statistics (localized states, large disorder). In the large sample size limit the quantity γ , as a function of the disorder parameter W , is expected to approach a step function centered on the critical value W_c of the Anderson transition. Even for cubes with side lengths $L = 10-16$ the transition is evidenced by a nodal structure in the superposition of the curves $\gamma(W, L)$. In computing the tail of $P(s)$, the central half of the energy spectrum was used.

In this paper we investigate numerically the properties of the distribution of level curvatures in the 3D cubic Anderson model. Curvature of energy levels appears to be a good indicator for the metal-insulator transition, even with relatively small sizes of the samples. The mean curvature satisfies a scaling law in the same parameter that describes the scaling of localization lengths, numerically investigated by MacKinnon and Kramer [7]. In the metallic regime a simple rescaling of curvatures allowed us to reproduce the universal curvature distribution proposed by Zakrzewski and Delande [1] for GOE. The form of the rescaling and the existence of a universal curve imply a relation which has the same content as the famous Thouless formula. In the localized regime the distribution of curvatures is well described by a log-normal distribution.

Level curvature.

The 3D Anderson model on a cubic lattice is described by an ensemble of tight binding Hamiltonians, which are the sum of a kinetic term accounting for the hopping among nearest neighbour sites, and a random potential. Labelling a site with a triple of integers: $\mathbf{n} = (n_1, n_2, n_3)$ the Hamiltonian is

$$\hat{H} = \sum_{\langle \mathbf{n}, \mathbf{m} \rangle} |\mathbf{n}\rangle \langle \mathbf{m}| + W \sum_{\mathbf{n}} V(\mathbf{n}) |\mathbf{n}\rangle \langle \mathbf{n}| \quad (1)$$

where $\langle \mathbf{n}, \mathbf{m} \rangle$ are nearest neighbours, $W \geq 0$ is the disorder parameter and $\{V(\mathbf{n})\}_{\mathbf{n}}$ is a set of values of independent random variables with uniform distribution in $[-1/2, 1/2]$. In the free situation ($W = 0$), the eigenfunctions are plane waves with energies in a band $-6 < E < 6$. The metallic-insulator transition takes place at a critical value $W_c \approx 16.5$, where for $|E|$ below a mobility edge E_c the eigenfunctions are exponentially localized [7].

When dealing with finite samples of size L^3 , one has to specify boundary conditions for the eigenfunctions $\psi(\mathbf{n})$. We have chosen periodic conditions along the x and y directions, and introduced a flux parameter in the z direction, so that

$$\begin{cases} \psi(L+1, n_2, n_3) = \psi(1, n_2, n_3) \\ \psi(n_1, L+1, n_3) = \psi(n_1, 1, n_3) \\ \psi(n_1, n_2, L+1) = e^{i\phi} \psi(n_1, n_2, 1) \end{cases} \quad (2)$$

Introducing an ordering of sites through the integer $a(\mathbf{n}) = n_1 + (n_2 - 1)L + (n_3 - 1)L^2$ and defining $\psi_a = \psi(\mathbf{n})$, the eigenvalue equation $\hat{H}\psi^{(r)} = E_r \psi^{(r)}$, $r = 1 \dots L^3$, can be put in matrix form, with the matrix H_{ab} incorporating the boundary conditions. The Hamiltonian matrix takes the form

$$H(\phi) = H^{(0)} + e^{i\phi} V + e^{-i\phi} V^T \quad (3)$$

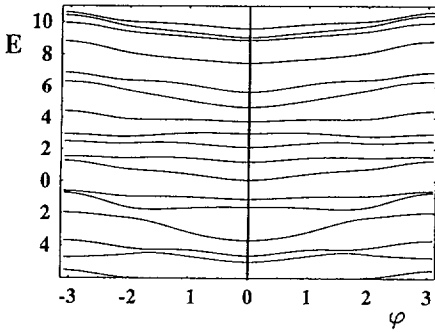


Fig. 1

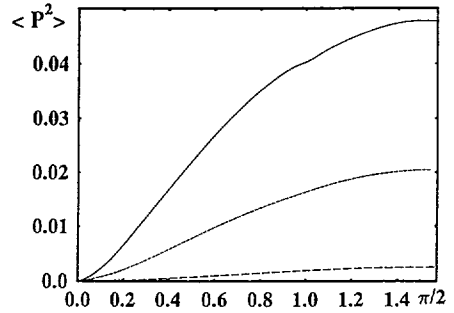


Fig. 2

Fig. 1. — Level motion in a sequence of eigenvalues, changing the phase from $-\pi$ to π . The eigenvalues are rescaled to have a unitary average spacing at $\phi = 0$. The value of the disorder parameter is $W = 10$, with extended states sensitive to the boundary.

Fig. 2. — Mean kinetic energy $\langle P^2 \rangle$ versus the phase parameter ϕ , for different values of disorder. From above: $W = 12, 16, 20, 24$. Inspection of the curves indicates that $\langle P^2 \rangle$ at $\phi = \pi/2$ is, up to a constant, a good measure of the ϕ -averaged value of the mean kinetic energy.

where $H^{(0)}$ is a real symmetric $L^3 \times L^3$ matrix, V is a real matrix with nonzero entries $V_{ab} = 1$ for $a = 1 \dots L^2$, $b = a + L^3 - L^2$, and V^T is its transpose. The V matrices describe the couplings between the $n_3 = 1$ and the $n_3 = L$ faces of the cube.

The eigenvalues of the matrix are functions of the external parameter ϕ . In figure 1 we display the motion of a few levels in the metallic phase, where states are extended and sensitive to boundary changes. Note the symmetry $E(\phi) = E(-\phi)$. The dynamics involves the definition for each eigenvalue of a momentum and a curvature

$$p_r(\phi) = \frac{\partial E_r(\phi)}{\partial \phi} \quad , \quad k_r(\phi) = \frac{\partial^2 E_r(\phi)}{\partial \phi^2} \tag{4}$$

Perturbation theory around $\phi = 0$ yields $p_r = 0$ and

$$\frac{1}{2} k_r = - \sum_{n_1, n_2} \psi^{(r)}(n_1, n_2, 1) \psi^{(r)}(n_1, n_2, L) + \sum_{s \neq r} \frac{|\sum_{n_1, n_2} [\psi^{(s)}(n_1, n_2, 1) \psi^{(r)}(n_1, n_2, L) - \psi^{(r)}(n_1, n_2, 1) \psi^{(s)}(n_1, n_2, L)]|^2}{E_s - E_r} \tag{5}$$

At $\phi = 0$ the response of the energy level is therefore proportional to curvature.

It is worth to recall some recent results which will be of interest in the following discussion. The introduction of a complex phase factor changes the symmetry of the random Hamiltonians from real symmetric to complex Hermitian: Dupuis and Montambaux [8] have shown that the spectral properties near the transition are functions of the scaling parameter $\langle k^2 \rangle^{1/4} \phi$. Szafer and Altshuler [9], and Beenakker [10] have shown that the correlation of momenta

$$C(\phi) = \frac{1}{2\pi} \int_0^{2\pi} \langle \frac{1}{\Delta^2} p(\phi') p(\phi + \phi') \rangle d\phi' \tag{6}$$

exhibits the universal behaviour $C(\phi) \approx \phi^{-2}$ for ϕ larger than a critical value. A simple analytical expression for the whole range of ϕ has been recently proposed by Delande and

Zakrzewski [11]. In the above formula and in the following, $\langle \dots \rangle$ denotes an average on disorder, and Δ is the local spacing between eigenvalues. The quantity $C(0)$ measures the average kinetic energy of the gas of levels, rescaled in order to have local spacing equal to one; for the Anderson model it is plotted in figure 2. Simon and Altshuler [12, 13] have then shown that defining the rescaled flux parameter $\Phi = \phi\sqrt{C(0)}$, the rescaled eigenvalues $\epsilon_r(\Phi) = \Delta^{-1}E_r(\Phi/\sqrt{C(0)})$ are random functions with universal statistical properties. This strong statement is consistent with the hypothesis of a universal distribution of curvatures that is discussed in the next section. The perturbative formula (5) and certain assumptions led Thouless to the fundamental relation that in the metallic regime the mean curvature divided by the level spacing is proportional to conductance, as given by Kubo's formula. This relation has been recently reconsidered by Akkermans and Montambaux [14], who restated Thouless' formula with greater generality and showed its equivalence with the following relation

$$\overline{\langle p^2 \rangle} = \pi^2 a \Delta \langle k^2 \rangle^{1/2} \quad (7)$$

in which a is a model dependent constant and the overbar denotes an average over the flux ϕ of squared momenta.

Numerical results.

We constructed matrices representing the 3D Anderson model for the cube size varying from 4 to 12, with various values of the disorder parameter W and the phase ϕ and diagonalized them numerically. The energy levels were then rescaled so that the average spacing at $\phi = 0$ is set to unity. We accordingly define the normalized momenta and curvatures $P = p/\Delta$ and $K = k/\Delta$.

Curvatures in $\phi = 0$ are computed for each level by fitting a parabola to three energy values obtained for $\phi = -\delta, 0, \delta$. The accuracy of computation was verified by comparing with the curvature obtained for $\phi = -2\delta, 0, 2\delta$. The optimal value of δ varies from 10^{-1} to 10^{-3} and depends on the parameters W and L .

The density of states $\rho(E)$ is displayed in figure 3 for $W > W_c$, for which localization occurs (Fig. 3b), and for $W < W_c$ (Fig. 3a), for which states are extended. It is worth to note that the mean spacing $\Delta = 1/\rho$ is practically constant over an extended energy range: this will

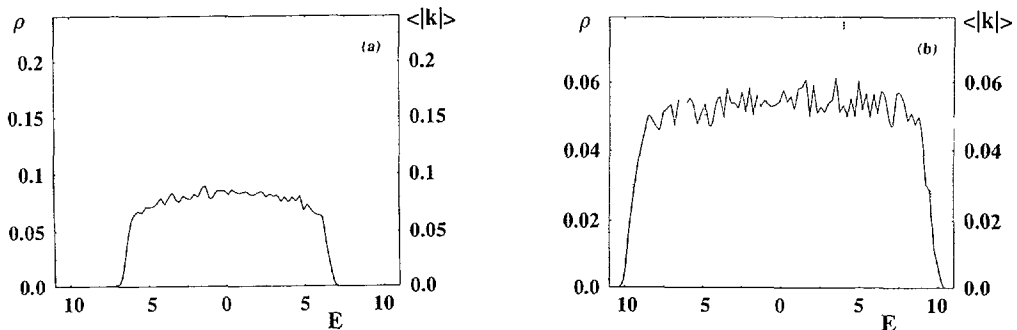


Fig. 3. — The energy density ρ (full line) and the mean absolute value of curvature (dotted line) as functions of rescaled energy. Lattice size $5 \times 5 \times 5$, disorder average on 100 samples. a) $W = 12$, b) $W = 20$.

allow to take it out from average symbols. The same graph also shows the dependence of the absolute value of curvature $\langle |K(E)| \rangle$. The observation that both distributions are almost flat in a wide range suggests to consider the whole central third fraction of eigenvalues for computing average quantities. The probability distribution $P(K)$ of curvature is shown in figures 4a, b, c; it broadens with decreasing disorder and is always symmetric around $K = 0$. An approximate number of 4000 level curvatures are computed in each hystogram.

The metallic-insulator transition is well reflected in the behaviour of average curvatures. In a truly insulator phase, occurring at $L \rightarrow \infty$, the curvature should be zero due to the exponential localization of states. For finite but increasing values of L , the shape of the curve $\log |K|$ versus W shows a more pronounced inflection at the critical value W_c . This effect is enhanced by superposing the curves, as in figure 5, where a nodal structure appears near the transition value. This pattern is very similar to that produced by Shklovskii *et al.* [6], at the cost of collecting many more data to get a reliable tail for the level spacing distribution.

The same data are shown in figure 6, as a function of the scaling ratio ξ_∞/N . The localization length for the infinite sample $\xi_\infty(W)$ has been taken from the paper by MacKinnon and Kramer [7]. As in the previous picture, a transition is evident at the value $(\log K) \approx -3.5$. This figure demonstrates the scaling property of the average curvature, since all points are distributed along a line. A similar behaviour was observed for the quantity γ by Shklovskii *et al.* [6]. Next we exhibit other interesting properties, which concern the distribution of curvatures in the two regimes of the Anderson model.

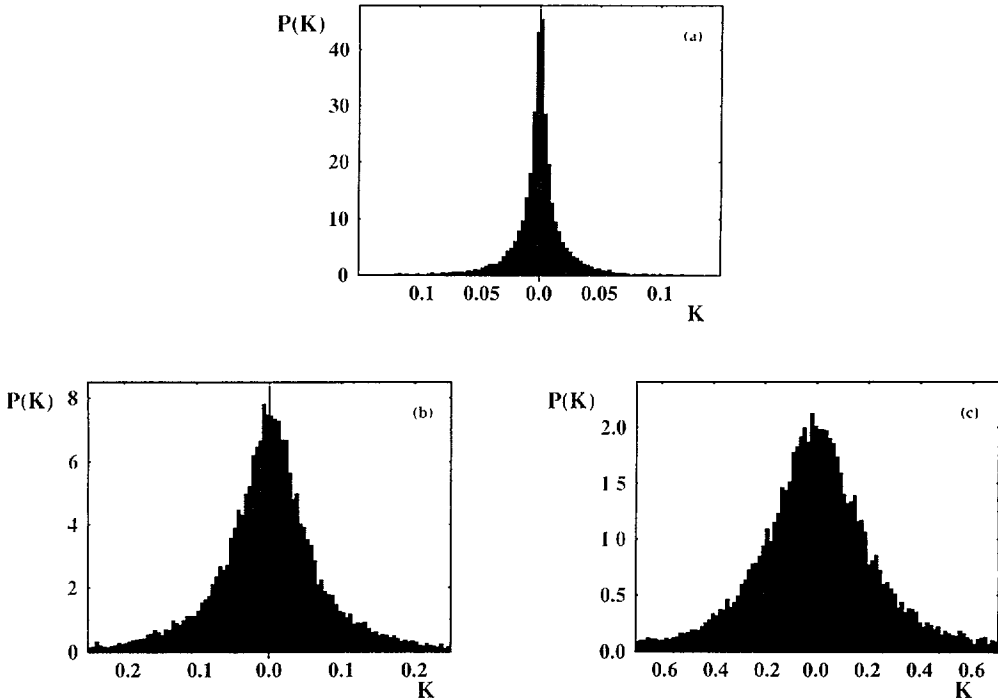


Fig. 4. — Distribution of curvature for decreasing disorder. The curves are symmetric about $K = 0$. Only the middle third of the energy spectrum is considered hereafter. The lattice size is $5 \times 5 \times 5$, disorder average on 100 samples. Note the change of scales. a) $W = 26$ (localized regime), b) $W = 16.5$ (near metallic-insulator transition), c) $W = 10$ (metallic regime).

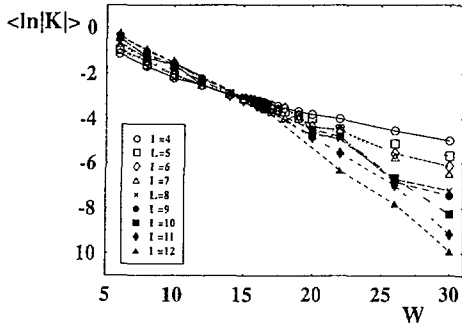


Fig. 5

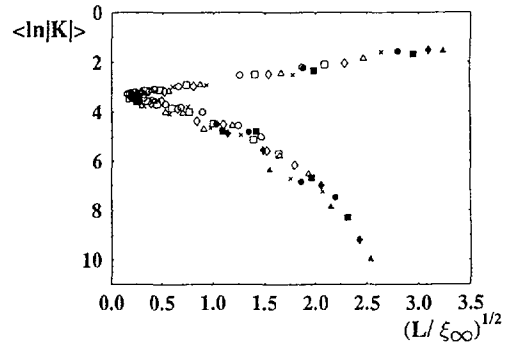


Fig. 6

Fig. 5. — The behaviour of the mean curvature $\langle \log |K| \rangle$ with disorder W , for various sizes of the cube. The lines cross at the critical value $W_c \approx 16.5$ and change their order approaching the step curve, expected in the limit of large size L .

Fig. 6. — One parameter scaling of curvatures. Data of figure 5 are plotted against the scaling parameter $(L/\xi_\infty(W))^{1/2}$, with the localization length $\xi_\infty(W)$ taken from [7].

In the recent work by Gaspard *et al.* [15] the following dimensionless curvature is defined:

$$\tilde{\kappa} = \frac{1}{\pi\nu \langle P^2 \rangle} K \tag{8}$$

where $\overline{\langle P^2 \rangle} = C(0)$ is the average kinetic energy. The factor ν is equal to 1 for the level dynamics inside the orthogonal ensemble, and $\nu = 2$ for the level dynamics inside the unitary ensemble. Note that this curvature definition coincides with the second derivative of rescaled energy with respect to rescaled flux, as defined in [12].

For the rescaled curvature $\tilde{\kappa}$ of the level dynamics inside the canonical ensembles, Zakrzewski and Delande [1] proposed the following distribution

$$P_\nu(\tilde{\kappa}) = N_\nu \frac{1}{(1 + \tilde{\kappa}^2)^{1+\nu/2}}, \tag{9}$$

which well reproduces numerical results obtained for random matrices. N_ν is a normalization constant equal to $1/2$ ($\nu = 1$) and $2/\pi$ ($\nu = 2$). The same distribution was later derived by Takami and Hasegawa [11].

The distribution implies a $|\tilde{\kappa}|^{-(\nu+2)}$ tail, already predicted by Gaspard *et al.* [15]. that excludes the existence of moments of degree higher than ν .

The universal formula for the curvature distribution in the metallic regime has been found to hold also for the level dynamics of band random matrices [16].

It is interesting to verify whether it holds for the Anderson model, which is described by band and sparse matrices. In both cases the level dynamics is driven by a complex phase, which produces a motion from real symmetric matrices, at $\phi = 0$, where curvatures are sampled, to the Hermitian ones ($0 < \phi < \pi$). We have considered a rescaling with $\nu = 1$, a choice that revealed to be correct by measuring the tail behaviour of the experimental curvature distribution.

The rescaling in equation (8) requires the evaluation of the average of the function $\langle P^2(\phi) \rangle$, shown in figure 2, over the whole range of ϕ . This evaluation is a time-consuming procedure

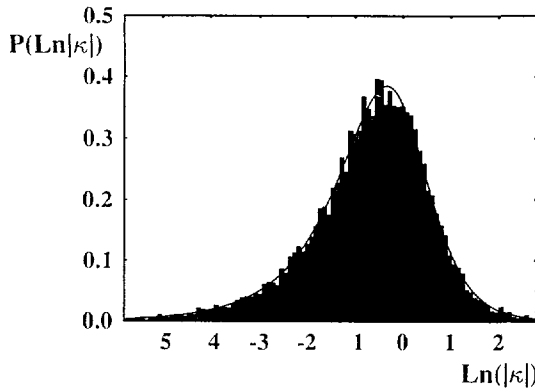


Fig. 7

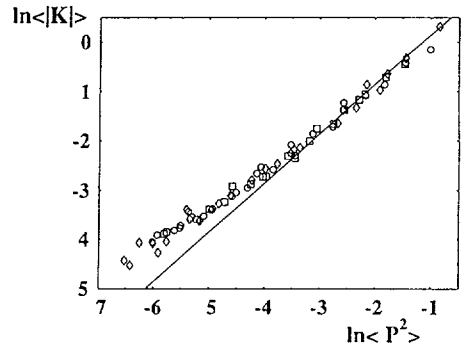


Fig. 8

Fig. 7. — Distribution of the rescaled curvature κ for $W = 10$, in the metallic regime (see also Fig. 4c). The histogram is well fitted by the universal distribution (9).

Fig. 8 — Curvature and squared momentum for sizes $L = 4$ (circle), $L = 5$ (square) and $L = 6$ (diamond). The disorder parameter ranges from 30 (left) to 5 (right). The solid line reproduces the relation (11).

in numerical computations. It turned out to be a good criterion to consider $\langle P^2(\pi/2) \rangle$ as a good representative of $\langle P^2 \rangle$, since the two values are almost in constant ratio. Therefore we introduce the rescaled curvature

$$\kappa = \frac{1}{\pi \langle P^2(\pi/2) \rangle} K, \quad (10)$$

which differs from the definition equation (8) only by a constant factor.

It turned out that the rescaling (10) actually produced a good correspondence of numerical data, in the metallic regime, with the universal distribution (9), with κ replacing $\tilde{\kappa}$.

In order to demonstrate this correspondence and to exhibit properties of curvature distribution, it is convenient to use a logarithmical scale. Figure 7 shows the distribution $P(\log |\kappa|)$ in the metallic regime ($W = 10$). Note the fine agreement with the Zakrzewski–Delande distribution. A different rescaling would manifest in a shift in figure 7. In the range $1 < \log \kappa < 2.5$ our numerical results follow the $|\kappa|^{-3}$ law. However, the statistics obtained is not sufficient to extend the validity of this statement to larger values of κ and to conclude that the second moment of the curvature distribution in the Anderson model does not exist.

The rescaling equation (10) and the assumption of the existence of a universal curve for κ in the metallic regime imply a relation similar to that by Akkermans and Montambaux (7). Taking the mean value in both sides of equation (10), and evaluating $\langle |\kappa| \rangle = 1$ by means of the distribution (9) with $\nu = 1$, we obtain

$$\langle P^2(\frac{\pi}{2}) \rangle = \frac{1}{\pi} \langle |K| \rangle. \quad (11)$$

The linear relation is shown in the logarithmic plot in figure 8, the straight line representing equation (11). The agreement with the numerical data, good in the metallic phase represented in the right side of the figure, is lost for the disorder parameter close to the critical value W_c for the Anderson transition.

The relation (11) should be compared with equation (7) with $\Delta = 1$, where the effective value of curvature is measured by the variance of the curvature distribution, and not by the

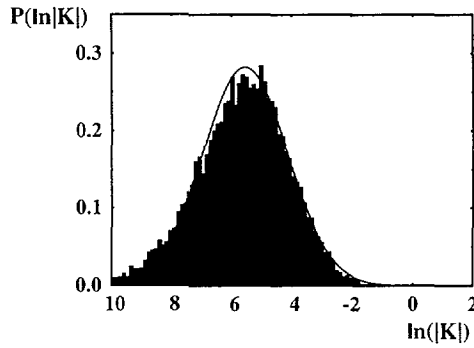


Fig. 9. — Distribution of rescaled curvatures κ for $W = 30$, in the insulating regime (see also 3a). The solid line describes a fitting with a log-normal distribution.

average value of the modulus of curvature. The validity of equation (7) would indicate that the formula (9) fails to describe correctly the large K behaviour of the curvature distribution. An investigation towards the identification of the universal curve for the metallic regime would be very interesting.

In figure 9 we show the distribution of normalized curvatures for large disorder, where states are localized. The distribution is well fitted by a log-normal distribution, shown as a Gaussian in logarithmic variables.

To summarize, we have shown that the statistical properties of curvatures may be used to study the Anderson transition. The mean absolute value of curvatures exhibits a behaviour very similar to conductance, namely scaling and a relation of the type stated by Akkermans and Montambaux, who showed its equivalence to Thouless' relation. The distribution of curvatures cannot however be associated with that of conductivity. The latter is characterized by a constant variance in the metallic regime (universal conductance fluctuations [17]), while the problem of the variance of the curvature distribution remains open. We have also shown that in the metallic regime, rescaled curvature exhibits a universal distribution. The universal distribution (9) and the related equation (11) have been verified also in a model of random matrices with a band structure [16].

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