Periodic Band Random Matrices, Curvature, and Conductance in Disordered Media

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Changes in the boundary conditions enforce variations of the eigenvalues of periodic band random matrices. We investigate the statistics of the corresponding curvatures and discuss connections with conductance fluctuations. In particular we show with numerical data that mean curvatures obey a scaling law quite similar to the one expected for mean conductance, and that a distribution law predicted for curvatures of Gaussian orthogonal ensemble matrices also holds for band matrices in the metallic regime.

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Since its birth, random matrix theory has been dealing mainly with statistical properties of "full" random matrices, which yield a faithful description of "local" spectral properties in spite of their unphysical attribution of equal statistical strength to all possible transitions. Random matrices with elements decaying away from the diagonal appear to provide more realistic models for Hamiltonians of "complex" quantum systems; in particular, random matrices whose elements vanish outside a band of half-width b centered on the main diagonal have attracted interest in various fields [1]. Much less is known about such "band random matrices" (BRM), which lack the statistical rotational invariance so useful in the mathematical analysis of full random matrices. In quantum chaology and in solid state physics global properties of BRM related to localization of eigenvectors are as important as local ones. It is known that in the limit $N \to \infty$ of infinite and homogeneous BRM all eigenstates are exponentially localized with localization length proportional to b^2; moreover, numerical investigations have shown that for finite but large matrices with $N \gg b \gg 1$ the scaling parameter $x = b^2/N$ determines statistical properties of the spectrum [2] and eigenvectors [3–6]. In particular the localization length l_N scales as $Nf(x)$ [3,7,8].

In solid state physics periodic BRMs provide good models for conduction in quasi-one-dimensional disordered solids [7]. In this connection, central objects of interest are conductance and various statistics thereof. The definition of conductance based on the Thouless formula [9] establishes a link between average conductance and level curvature; the latter is a quantity measuring the sensitivity of levels to changes in the boundary conditions, which is also of general relevance in the analysis of the energy spectra of classically chaotic systems [10–12]. The definition of conductance based on curvature is abstract enough to be applicable to BRM, thus making possible a quite general analysis. This is the subject of the present paper, in which we study statistical properties of periodic band random matrices with special emphasis on the statistics of curvatures.

By a periodic BRM we mean a real symmetric random matrix M of rank N such that $M_{ij} \neq 0$ only if $|i-j| \leq b$ or if $|i-j| \geq N-b$. All nonzero matrix elements belong to three regions: a band of half-width b along the main diagonal, the upper right corner, and the lower left one. Such a matrix may be thought to describe motion along a discrete ring of N sites, with nonzero hopping amplitudes only for transitions between sites which lie no more than b sites apart along the circle. Alternatively, it may describe motion in a finite set of N sites on the line, with periodic boundary conditions: when the particle "hops" out through either end point, it reenters through the other, with unchanged phase. Different boundary conditions can also be set, by prescribing a fixed change φ in phase at every reentering. In this case the matrix elements in the right upper corner must be multiplied by $e^{i\varphi}$ and those in the left lower one by $e^{-i\varphi}$. The matrix M_φ thus obtained is still self-adjoint, but it is not real any more and has therefore a different symmetry than the original matrix $M \equiv M_0$. This symmetry breaking can be thought of as the result of switching on a magnetic flux φ through the ring. On mathematical grounds, the matrices M_φ $(0 \leq \varphi \leq 2\pi)$ can be interpreted as fibers in the Bloch decomposition on an infinite periodic BRM of period N, and the phase φ is the corresponding Bloch number. The infinite matrix has a band spectrum, and the curvature defined below can be interpreted as an effective mass.

The eigenvalues of the matrix M_φ depend on φ, and their sensitivity to changes of the latter phase from 0 to small values nearby is a measure of the degree of localization of the eigenfunctions of the matrix M_0. The dimensionless residual average conductance $\tilde{G}$ is connected to the level shift by the famous Thouless formula:

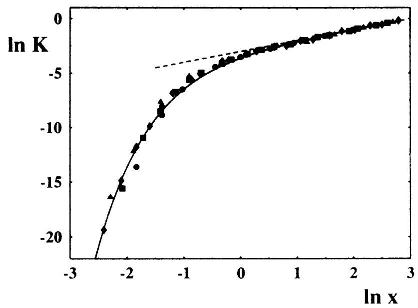

FIG. 1. Mean logarithm of mean curvature versus the logarithm of the scaling variable $x = b^2/N$, for matrix size 100 (●), 200 (■), 400 (♦), 800 (▲). The solid line corresponds to $\tilde{K} = (0.05x + 0.07)\exp(-1.5x^{-1})$ and the dashed line to the asymptote $\tilde{K} = 0.05x$.

$$\tilde{G} = \frac{1}{\Delta}\left\langle \left(\frac{d^2E}{d\varphi^2}\right)^2_{|\varphi=0} \right\rangle^{\frac{1}{2}}, \qquad (1)$$

where brackets denote averages over disorder and Δ is the mean level spacing. This formula holds in the delocalized metallic regime [13] and establishes a relation between conductance and curvature $K = |E''(0)|$. The latter quantity and its statistics were the object of our numerical analysis. We have numerically diagonalized matrices of rank 100–800 for different values of φ; the eigenvalues thus obtained were subjected to spectral unfolding, yielding a sequence of unit density.

In order to improve statistics, our statistical averages (also denoted by $\langle\ \rangle$ in the following) were taken over disorder *and* over a selected set of eigenvalues, namely, the 50% lying closer to the center of the spectrum. For each of these we have estimated $E''(0)$ as $2[E(\Delta\varphi) - E(0)]/\Delta\varphi^2$ [the "level velocity" $E'(\varphi) = 0$ at $\varphi = 0$]; special care had to be taken in the choice of the optimal step $\Delta\varphi$, which varied from $\sim 10^{-1}$ in the localized regime, where small level shifts are recorded on changing φ, to $\sim 10^{-4}$ in the delocalized regime. The curvatures of unfolded levels computed in this way coincide with the scaled curvatures entering the Thouless formula, apart from a small correction (due to variations in the level density) which is negligible in the part of the spectrum we considered. This process was repeated for a number of different realizations of the random matrix, so as to get in all cases 2000 data for statistical processing.

First we have investigated the scaling properties of the geometric average $\tilde{K} = \exp(\langle \ln K\rangle)$. For large matrices $\tilde{K}$ turned out to depend on b and N only through the localization parameter $x = b^2/N$; apart from a proportionality factor, this parameter gives the ratio of the localization length to the sample size N. As shown in Fig. 1, for $x \gg 1$, i.e., in the delocalized regime, this dependence has the form $\tilde{K} \approx c_1 x \propto N^{-1}$, that is, the dependence of mean curvature on length has the "Ohmic" character expected of mean conductance. In the localized regime $x \ll 1$, Fig. 1 indicates a dependence $\tilde{K} \approx c_2\exp(-c_3/x)$; here, too, mean curvature behaves like mean conductance and exponentially decreases on increasing length. A possible interpolating law valid in all regimes, including the crossover region, is

$$\tilde{K} = (c_1 x + c_2)\exp(-c_3/x). \qquad (2)$$

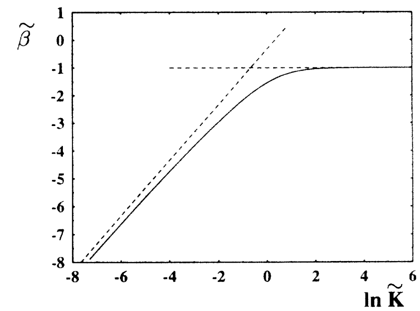

FIG. 2. Scaling function $\beta(\tilde{K})$, as computed from the fitting law (2), versus $\ln\tilde{K}$.

Comparison with numerical data in the regions $x \gg 1$, $x \ll 1$ yields $c_1 \approx 0.05$, $c_3 \approx 1.5$; adjusting the last parameter c_2 so as to fit numerical data in the intermediate region yields $c_2 \approx 0.07$. The resulting analytical formula nicely fits the numerical results in all regions and provides therefore a compact summary of our empirical data. This formula enabled us to implement a construction, which is well known in the scaling theory of localization, where the scaling properties of the mean conductance $\tilde{G}$ are efficiently studied by means of the function $\beta(\tilde{G})$ defined by [14]

$$\beta(\tilde{G}) = d\ln\tilde{G}/d\ln N. \qquad (3)$$

Using formula (2) we have computed an analogous function $\beta(\tilde{K})$, which is shown in Fig. 2. This function has two asymptotes: $\beta \approx -1 - 0.1/\tilde{K}$ for $\tilde{K} \gg 1$, and $\beta \approx -0.34 + \ln\tilde{K}$ for $\tilde{K} \ll 1$. This behavior closely corresponds to the predictions of the scaling theory of localization about the function $\beta(\tilde{G})$. Therefore Figs. 1 and 2 indicate that the scaling behavior of mean curvature is very similar to that of mean conductance not only in the metallic regime [where this is expected on the grounds of Eq. (1)], but even in the localized one.

We have also studied the statistical distribution $P(K)$ of curvatures in the various regimes. We have found that the shape of this distribution is also controlled by the same scaling parameter x. In the localized region $x \ll 1$ this distribution is approximately log-normal (Fig. 3), i.e., of the same type as the distribution of conductance. Small deviations from the log-normal distribution appearing in Fig. 3 are due to the relatively small rank $N = 100$ of the matrices. The variance of $\ln K$ decreases on increasing x and in the localized regime satisfies an approximate relation $\mathrm{var}(\ln K) \approx -\mu\langle\ln K\rangle + \gamma$, with $\gamma \approx 3.0$ and $\mu \approx 1$ (Fig. 4). This is at variance with what is known about conductance of quasi-1D solids [15], for,

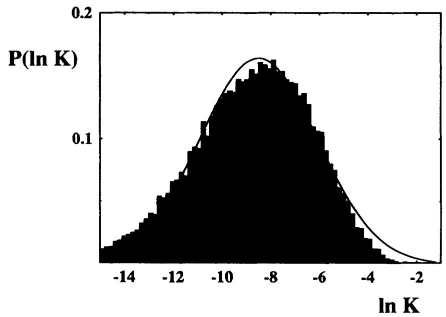

FIG. 3. Distribution of curvatures $P(\ln K)$ for a localized case $N = 100$, $b = 5$, $\ln(x) = -1.39$. The solid line is a log-normal curve (represented by a Gaussian in a logarithmic scale) with the given mean and variance.

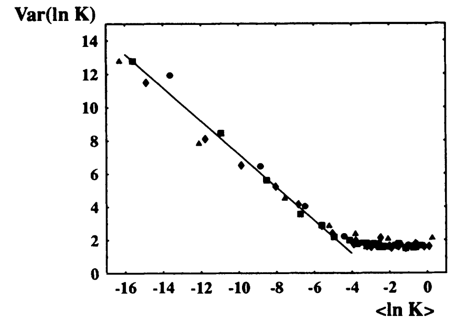

FIG. 4. Variance of $\ln K$ versus $\langle \ln K\rangle$ for values of $x = b^2/N$ in the range −2.5–3.0. Symbols have the same meaning as in Fig. 1. The straight line corresponds to $\mathrm{var}(\ln K) = -\langle \ln K\rangle + 3$.

in that case, $\mu = 2$. Thus the fluctuation properties of conductance and curvature appear to be different: further differences will emerge in the following.

On moving towards the delocalized region the shape of the distribution $P(K)$ becomes different. However, in the region corresponding to the linear part of Fig. 1, the distributions of $\ln K$ corresponding to different values of x have *the same* shape and differ from one another merely by a horizontal shift. This suggests that a fixed distribution may be obtained on suitably rescaling the curvature K. This very behavior was recently predicted for full random matrices by Zakrzewski and Delande [12] who have argued that the distribution of an appropriately scaled curvature κ could be approximated by the universal law

$$P(\kappa) = A_\beta/(1+\kappa^2)^{\beta/2+1}, \tag{4}$$

where β is the "repulsion parameter," equal to 1, 2, 4 for the Gaussian orthogonal, unitary (GUE), and symplectic (GSE) ensembles, respectively, and A_β is a normalization constant equal to 1/2 for $\beta = 1$. The relevant scaling of curvature was introduced by Gaspard *et al.* [10],

$$\kappa = K/\pi\beta\rho\alpha, \tag{5}$$

where ρ is the density of eigenvalues and α is the "mean kinetic energy" of moving eigenvalues,

$$\alpha = \overline{\left\langle \left(\frac{dE}{d\varphi}\right)^2 \right\rangle}, \tag{6}$$

where the bar denotes an average over φ in the range of the parameter controlling the level dynamics. This behavior of curvatures appears as a particular instance of a recently suggested universality in rescaled level dynamics for quantum "chaotic" systems [16].

Even in the delocalized regime, BRMs need not have a GOE structure; in particular, in the diffusive regime $b \ll N \ll b^2$ they are definitely different. Nevertheless, according to our numerical data (Fig. 5) the corresponding curvatures obey a scaling law of the type (5) remarkably well. We rescaled curvatures according to (5) with $\beta = 1$ and as a characterization of the kinetic energy $\alpha(\varphi)$ we took the value $\alpha_m = \langle \alpha(\pi/2)\rangle$ [since $\alpha(0) = 0$]. The empirical distribution of curvatures scaled in this way agrees with (4) with $\beta = 1$ to a good accuracy. A nontrivial point connected with our choice of $\beta = 1$ is that while it corresponds to the symmetry of our unperturbed matrix, the perturbation responsible for curvatures is in our case a symmetry-breaking one, which was not the case in the mentioned theoretical work leading to (4).

The generalized Cauchy distribution (4) is quite different from a log-normal distribution, which in the cases investigated by us could at best fit the empirical distribution near the central peak but strongly deviated in the tail, which appears to follow the law $\sim \kappa^{-3}$ instead. Remarkably, the latter law entails a diverging second moment of curvature, with implications to be discussed below.

The existence of the scaling law (4),(5) obviously entails a relation between mean curvature and mean kinetic energy. Simple integration of the distribution (4) with $\beta = 1$ gives $\langle\kappa\rangle = 1$, that leads to

$$\langle K\rangle = \rho\pi\alpha_m. \tag{7}$$

This relation is somewhat similar to the Thouless relation derived up to a proportionality constant a in Refs. [13,17]:

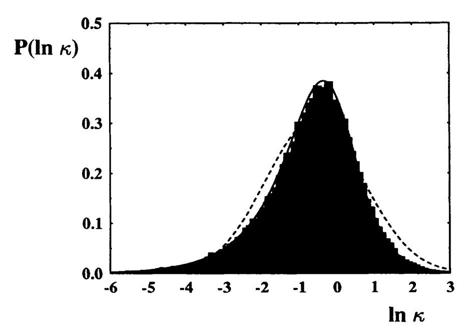

FIG. 5. Distribution of curvatures $P(\ln\kappa)$ for a delocalized case $N = 100$, $b = 27$, $\ln(x) \approx 2.0$. The solid line is the Zakrzewski–Delande distribution (4) and the dashed line is the log-normal distribution with given mean and variance.

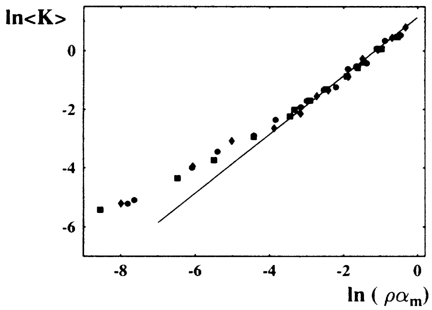

FIG. 6. The Thouless relation $\langle K\rangle = \pi\rho\alpha_m$ between mean curvature and mean kinetic energy of levels. Localization increases on moving to the left.

$$\overline{\left\langle\left(\frac{dE}{d\varphi}\right)^2\right\rangle} = \frac{a\pi^2}{\rho}\left\langle\left(\frac{d^2E}{d\varphi^2}\right)^2_{\varphi=0}\right\rangle^{1/2}, \qquad (8)$$

where the bar denotes the average over $\varphi \in (0, \pi/2)$. We have checked the relation (4) over a wide range (Fig. 6), and it turned out to hold in the delocalized region, as expected. However, in the localized region strong deviations appear.

We have thus studied the statistics of curvatures for periodic BRM for parameter values ranging from the localized regime to the delocalized one. The main conclusions that can be drawn from our results are the following. Over all the inspected parameter range the mean curvature exhibits a scaling behavior which is quite similar to the one expected of the average conductance; this result could be anticipated from theoretical predictions [13] in the delocalized regime, but not in the localized one. The interesting question can then be raised, whether a theoretical connection between mean curvature and mean conductance may be established even in the localized regime, where the theoretical assumptions used to derive (1) are not valid any more. On the other hand, our results about the distribution of curvatures imply that this similarity between curvature and conductance can hardly be extended beyond the coincidence of their respective mean values. In fact we have found evidence that the distribution of curvatures is given by the Zakrzewski-Delande distribution (4), which was theoretically predicted for GOE matrices. Thus in the metallic regime the curvature has a diverging second moment, in contrast to conductance, which has a finite variance. Besides that, the very existence of the scaling (5) excludes that a range of lengths may exist, in which the variance of K is a constant; for, in such a range, $\tilde{K}$ itself ought to be a constant. In contrast, such a range is known to exist for the variance of conductance, which is a constant in the metallic diffusive regime (defined for BRM by $b \ll N \ll b^2$). The divergence of the second moment of curvature also suggests that in formula (1) the mean of the absolute curvature K should appear instead of its divergent rms value. A similar correspondence between the mean curvatures of energy levels and the mean conductance has recently been found in the 3D Anderson model [18].

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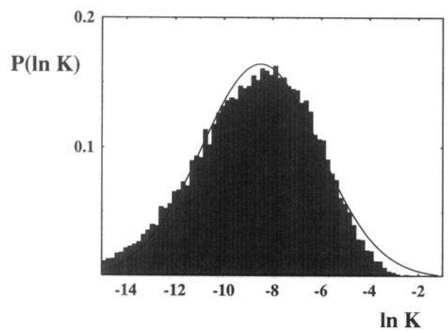

FIG. 3. Distribution of curvatures $P(\ln K)$ for a localized case $N = 100$, $b = 5$, $\ln(x) = -1.39$. The solid line is a log-normal curve (represented by a Gaussian in a logarithmic scale) with the given mean and variance.

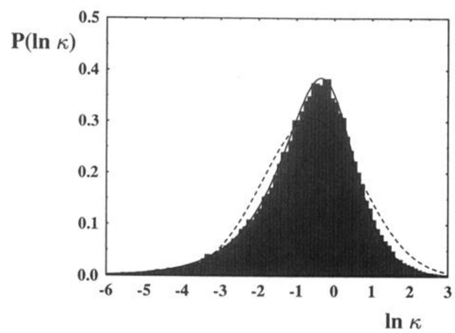

FIG. 5. Distribution of curvatures $P(\ln\,\kappa)$ for a delocalized case $N = 100$, $b = 27$, $\ln(x) \approx 2.0$. The solid line is the Zakrzewski–Delande distribution (4) and the dashed line is the log-normal distribution with given mean and variance.