Chaos in Fermionic Many-Body Systems and the Metal-Insulator Transition

Z. Pluhař,[1] H. A. Weidenmüller,[2] T. Papenbrock,[3,4] and J. Tithof[3]

[1]Institute of Particle and Nuclear Physics, Faculty of Mathematics and Physics, Charles University, 18000 Praha 8, Czech Republic
[2]Max-Planck-Institut für Kernphysik, D-69029 Heidelberg, Germany
[3]Department of Physics and Astronomy, University of Tennessee, Knoxville, TN 37996, USA
[4]Physics Division, Oak Ridge National Laboratory, Oak Ridge, TN 37831, USA

We show that finite Fermi systems governed by a mean field and a few-body interaction generically possess spectral fluctuations of the Wigner-Dyson type and are thus chaotic. Our proof is based on an analogy to the metal-insulator transition. We construct a sparse random-matrix ensemble $H^{\rm cr}$ that mimicks that transition. Our claim then follows from the fact that the generic random-matrix ensemble modeling a fermionic interacting many-body is much less sparse than $H^{\rm cr}$.

PACS numbers: 05.45.Mt, 71.30.+h, 21.60.Cs

Purpose. Finite fermionic many-body systems (atoms, molecules, nuclei) often display spectral fluctuation properties that agree with predictions of random-matrix theory (RMT), more precisely, with those of the Gaussian Orthogonal Ensemble (GOE) [1]. This fact is commonly taken as evidence for chaotic motion [2]. In RMT, all pairs of states are coupled by independent matrix elements. In a many-body system, that situation arises only in the presence of many-body interactions. But atoms, molecules, and nuclei are governed by a mean field with residual interactions that are predominantly of a two-body nature. Therefore, an important question is: Does a two-body interaction (or, more generally, a k-body interaction with k integer ≥ 2 but smaller than the number m of fermions) generically give rise to chaotic motion? The question has received much attention (see the review [3]), without a definitive answer. In condensed-matter physics it has recently been addressed as the problem of many-body localization [4].

We answer the question for a generic random-matrix model that simulates a fermionic many-body system, the Embedded Gaussian Unitary Ensemble (EGUE) [5] defined below. (Our arguments apply likewise to the cases of orthogonal and symplectic symmetry.) For $k < m$ that ensemble has withstood all attempts at a direct analytical treatment [3]. The difficulty is that the matrix representation of EGUE in terms of Slater determinants becomes infinitely sparse in the limit of large matrix dimension. Thus, the analytical results of Ref. [6] do not apply. And numerical simulations for small matrix dimensions (see [3]) while showing Wigner-Dyson statistics for the eigenvalues do not reach the sparse limit. In solving the problem we use an analogy to the Anderson localization problem. Specifically, we are guided by a random band matrix model for the metal-insulator transition (MIT) [7]. We construct two versions of a random-matrix ensemble, both even more sparse than EGUE. Numerical simulations show that the sparser version of the two displays the critical behavior characteristic for the metal-insulator transition, while analytic work shows that the less sparse version possesses the same spectral fluctuation properties as the Gaussian Unitary Ensemble (GUE). The EGUE being less sparse than both versions, we can then show that EGUE possesses GUE spectral fluctuation properties for all $k \geq 2$. (The case $k = 1$ is special.) These statements imply that the eigenfunctions of EGUE are delocalized for all $k \geq 2$.

Critical Ensemble and Scaffolding Ensemble. We define both ensembles in terms of a real and symmetric scaffolding matrix $A^{(n)}$ that has dimension $N = 2^n$ with n positive integer. We recall that for matrices of dimension N, the auxiliary diagonal has matrix elements with indices $(\mu, N+1-\mu)$ and $\mu = 1, \ldots, N$. We construct the matrix $A^{(n)}$ by induction: For $n = 1$, $A^{(1)}$ has dimension 2, zero diagonal elements, and unit entries in the auxiliary diagonal. Given $A^{(n-1)}$, the two diagonal blocks (dimension $2^{(n-1)}$) of the matrix $A^{(n)}$ are each occupied by $A^{(n-1)}$. The elements in the two off-diagonal blocks are all zero except for the auxiliary diagonal for which all elements have the value unity. By construction, the matrices $A^{(n)}$ have the important property $\sum_{\nu=1}^{N} A^{(n)}_{\mu\nu} = n$ for all $\mu = 1, \ldots, N$. Thus, in every row and column of $A^{(n)}$, the number of non-zero non-diagonal elements is $n = \ln N$. Hence, with increasing distance $|\mu - \nu|$ from the main diagonal, the average density of non-diagonal elements of $A^{(n)}$ falls off like $1/|\mu - \nu|$.

With the help of the matrices $A^{(n)}$, we define the critical ensemble $H^{{\rm cr};n}$ and the scaffolding ensemble $H^{{\rm sc};n}$. In both, the matrix elements are complex random variables with bivariate Gaussian distributions and zero mean values but possess different variances. With x = cr or x = sc and with angular brackets denoting the ensemble average, we define

$$\langle H^{{\rm x};n}_{\mu\nu} H^{{\rm x};n}_{\rho\sigma} \rangle = \delta_{\mu\sigma}\delta_{\nu\rho} \left(\alpha\sqrt{n}\delta_{\mu\nu} + \frac{1}{|\mu-\nu|^{i({\rm x})}} A^{(n)}_{\mu\nu} \right) . \quad (1)$$

Here $i({\rm cr}) = 1$ and $i({\rm sc}) = 0$. Eq. (1) shows that the non-zero non-diagonal matrix elements of both ensembles reside on the unit entries of $A^{(n)}$; hence the name "scaffolding matrix". To explain the first term in round brackets on the right-hand side (where α is a real positive numerical coefficient of order unity), we observe that Trace $A^{(n)} = 0$ and $(1/N)$Trace $[A^{(n)}]^2 = n$. This suggests that the spectrum of $A^{(n)}$ is symmetric about zero and has width $\approx \sqrt{n}$. It is possible that an eigenvalue of $A^{(n)}$ vanishes. The term $\alpha\sqrt{n}\delta_{\mu\nu}$ shifts the spectrum and, with a suitable choice of α, guarantees for $i = 0$ that none of the eigenvalues of the matrix $B^{(n)}_{\mu\nu} = \alpha\sqrt{n}\delta_{\mu\nu} + A^n_{\mu\nu}$ vanishes. For reasons of symmetry we use the diagonal term $\alpha\sqrt{n}\delta_{\mu\nu}$ also for $i = 1$. To motivate Eq. (1) we note that with increasing distance $|\mu - \nu|$ from the main diagonal, the variance of $H^{\mathrm{cr};n}_{\mu\nu}$ (of $H^{\mathrm{sc};n}_{\mu\nu}$) falls off on average like $1/|\mu - \nu|^2$ (like $1/|\mu - \nu|$, respectively). Thus, $H^{\mathrm{cr};n}$ is the sparse-matrix analogue of a power-law random band matrix with exponent unity which models [7] the Anderson transition. We expect that for $n \to \infty$ the eigenfunctions and eigenvalues of $H^{\mathrm{cr};n}$ display critical behavior while those of $H^{\mathrm{sc};n}$ are GUE-like.

Spectral fluctuation properties of the two ensembles. We first study the spectral properties of $H^{\mathrm{sc};n}$ for $n \to \infty$. The average level density is $\rho(E) = -(1/\pi)\Im\langle G(E)\rangle$. Here E is the energy and $G(E) = 1/(E^+ - H^{\mathrm{sc};n})$ the retarded Green's function. To calculate $\langle G(E)\rangle$ we expand $G(E)$ in powers of $H^{\mathrm{sc};n}$ and use Wick contraction in each term of the sum [5]. We denote Wick-contracted pairs of matrix elements by the same letter and distinguish nested and cross-linked contributions. Among the sixth-order contributions, for instance, $ABCCBA$ and $ABBACC$ are nested while $ABCABC$ and $ABABCC$ are cross-linked. For $n \gg 1$, only nested contributions contribute to $\langle G(E)\rangle$. Resummation gives the Pastur equation $\langle G(E)\rangle = (1/E) + (1/E)\langle H^{\mathrm{sc};n}\langle G(E)\rangle H^{\mathrm{sc};n}\rangle\langle G(E)\rangle$. We use Eq. (1) for $i = 0$, use the definition of B, and find

$$[E - \sum_\rho B^{(n)}_{\mu\rho}\langle G(E)\rangle_{\rho\rho}]\langle G(E)\rangle_{\mu\nu} = \delta_{\mu\nu} \ . \qquad (2)$$

To solve Eq. (2) we observe that $\langle G(E)\rangle$ is expected to be an analytic function in E with a finite number of branch points but without singularity at $E = \infty$. Therefore, we expand $\langle G(E)\rangle$ for $|E| \gg 1$ in a Laurent series, $\langle G(E)\rangle_{\mu\nu} = \sum_{p=0}^\infty E^{j-p} g^{(p)}_{\mu\nu}$. Inserting that into Eq. (2) and comparing powers of E, we find that non-vanishing solutions exist only for $j = \pm 1$. For both solutions we find that the coefficients $g^{(p)}_{\mu\nu}$ are proportional to the unit matrix for all p. That conclusion hinges in an essential way on the fact that

$$\sum_\rho B^{(n)}_{\mu\rho} = n + \alpha\sqrt{n} \text{ for all } , \ \mu \qquad (3)$$

which follows from $\sum_\nu A^{(n)}_{\mu\nu} = n$ for all μ. We conclude that $\langle G(E)\rangle_{\mu\nu} = \delta_{\mu\nu} g(E)$. To determine $g(E)$ we use Eq. (2) and find with $\lambda^{\mathrm{sc}} = (n + \alpha\sqrt{n})^{1/2}$ that $\lambda^{\mathrm{sc}} g(E) = (E/(2\lambda^{\mathrm{sc}})) \pm i\sqrt{1 - (E/(2\lambda^{\mathrm{sc}}))^2}$. The two solutions with $j = \pm 1$ correspond to the two sign choices in front of the square root. We conclude that the average spectrum has the shape of Wigner's semicircle, the GUE radius $\lambda^{\mathrm{GUE}} \propto \sqrt{N}$ being replaced by $\lambda^{\mathrm{sc}} \propto \sqrt{n}$.

To determine the spectral fluctuation properties of the scaffolding ensemble, we use the supersymmetry approach [8, 9]. Averaging the generating functional and using Eq. (1), we find that removal of the quartic term in the original integration variables by means of a Hubbard-Stratonovich transformation is possible only if a separate dimensionless supermatrix σ_μ, $\mu = 1, 2, \ldots, N$ is introduced for every pair Ψ_μ, $\Psi^\dagger_\mu$ of the original integration variables.The dimension of σ_μ depends on the particular observable under consideration. We use the saddle-point approximation for $n \gg 1$ and find for the supermatrices σ_μ a set of equations that has the same form as Eqs. (2), with the replacement $\lambda^{\mathrm{sc}}\langle G_{\mu\nu}(E)\rangle \to \delta_{\mu\nu}\sigma_\mu$. The saddle-point equations admit only a single diagonal solution σ^{d} with $\sigma_\mu = \sigma^{\mathrm{d}}$ for all μ. The arguments are the same as in the last paragraph. Thus σ^{d} obeys the same equation as for the GUE, except for the replacement $\lambda^{\mathrm{GUE}} \to \lambda^{\mathrm{sc}}$. The general solution σ of the saddle-point equation then has the form $\sigma = T^{-1}\sigma^{\mathrm{d}}T$ with T in the proper coset space. Inserting that solution into the effective Lagrangean and expanding the logarithmic term to first order in the advanced-retarded-symmetry breaking term, we obtain a term proportional to trg $[T^{-1}\sigma^{\mathrm{d}}TL]$. Here trg denotes the supertrace and the diagonal matrix L breaks the retarded-advanced symmetry [9]. That term guarantees that the spectral fluctuation properties of H^{sc} coincide with those of the GUE, except for the replacement $\lambda^{\mathrm{GUE}} \to \lambda^{\mathrm{sc}}$. Expanding the effective Lagrangean around the saddle-point solution, we find that the masses of the massive modes are proportional to n. That justifies the use of the saddle-point approximation. Thus, we have proved that in the limit $n \to \infty$ and with $\lambda^{\mathrm{GUE}} \to \lambda^{\mathrm{sc}}$, all spectral properties of the scaffolding ensemble coincide with those of the GUE. By implication we conclude that the eigenfunctions are completely mixed and have Gaussian statistics. Our proof applies if α in Eq. (1) is chosen sufficiently large. However, it is physically obvious that by reducing the strength of the diagonal elements of a random-matrix ensemble, level repulsion cannot be diminished. We therefore expect that our results apply likewise for $\alpha = 0$ (barring effects due to a special symmetry of $A^{(n)}$).

We have not been able to establish the spectral properties of the critical ensemble analytically and therefore resort to numerical studies. At the MIT, the distribution of the inverse participation ratio IPR $= \sum_j |\psi_j|^4$ of an eigenstate ψ with components ψ_j has a scale-invariant form [10]. Fig. 1 (top panel) shows the distribution of IPR for the critical ensembles with $n = 10, 11, 12, 13$. For this analysis, we employed the central 20% of the eigenstates, and the ensemble size is as indicated. The distribution function is scale invariant as its form is independent of the dimension $N = 2^n$ of the ensemble. Following Ref. [10], we determine the fractal dimension D_2 from the shift of the IPR distribution function with doubling of the dimension as $D_2 \approx 0.6$. The IPR distributions exhibit a power-law tail with exponent $x_2 \approx 1$. We turn to the spectral statistics displayed in the bottom panels of Fig. 1. We find that the nearest-neighbor spacing distribution $P(s)$ increases linearly for small spacings s and falls off exponentially for large spacings. The long-ranged $\Sigma^2(L)$ statistics exhibit a logarithmic increase for small L and a linear increase for large L. Thus, the spectra of the critical ensemble exhibit short-range level repulsion while distant levels are only weakly correlated. This is in agreement with expectations for the MIT.

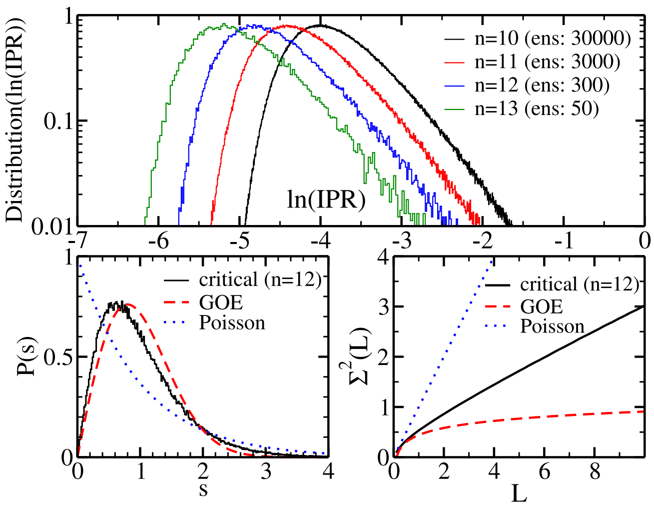

FIG. 1: (Color online) Top: distribution of $\ln \mathrm{IPR}$ for critical ensembles with dimensions 2^n, $n = 10, 11, 12, 13$. Bottom: Nearest-neighbor spacing distribution $P(s)$ (left) and Σ^2 statistics (right) of the critical ensemble compared to the GOE and Poisson.

Embedded Ensembles. To define EGUE(k) we use positive integers k, m, l with $k \leq m < l$ and consider m spinless Fermions in l degenerate single-particle states labelled $j = 1, \ldots, l$ with associated creation and annihilation operators $a^\dagger_j$ and a_j, respecively. The states carry no further quantum numbers. The k-body Hamiltonian is

$$H^{(k)} = \frac{1}{(k!)^2} \sum_{j_1 \ldots j_k; j'_1 \ldots j'_k} v^{j_1 \ldots j_k}_{j'_1 \ldots j'_k} a^\dagger_{j_1} \ldots a^\dagger_{j_k} a_{j'_k} \ldots a_{j'_1} \ . \quad (4)$$

The matrix v is Hermitian; the matrix elements are antisymmetric under the exchange of any pair of primed or unprimed indices and are uncorrelated random variables with a bivariate Gaussian probability distribution with zero mean value and a common second moment, which, without loss of generality, is taken to be unity. The matrix representation of $H^{(k)}$ in the space of m-body Slater determinants labeled μ or ν with m-body matrix elements $\langle \nu | H^{(k)} | \mu \rangle$ defines an ensemble of random matrices of dimension $N = \binom{l}{m}$ referred to as EGUE(k). We study the spectral fluctuation properties of EGUE(k) in the limit $N \gg 1$. For fixed k, that limit is reached by letting $l, m \to \infty$. Without distinction we consider both the dilute limit ($m/l \to 0$) and the dense limit ($m/l \to$ constant $\neq 0$).

EGUE(k) differs from the scaffolding ensemble in three important ways. (i) For all $k = 1, \ldots, m$, the number of non-vanishing non-diagonal elements, although equal in every row and every column, is given by $\sum_{p=1}^{k} \binom{m}{p} \binom{l-m}{p}$ and, thus, for $l, m \gg 1$ much larger than $\ln N \approx m \ln l$. Hence, for all k EGUE(k) is less sparse than the scaffolding ensemble. (ii) The number of k-body matrix elements contributing to a fixed m-body matrix element may be bigger than one. For $k = 2$, for instance, the m-body matrix element of two Slater determinants differing in the occupation numbers of orbitals 1 and 2 but both with occupied orbitals $3, 4, \ldots, (m-1)$ equals $\sum_{j=3}^{m-1} v^{1j}_{2j}$. (iii) m-body matrix elements occuring in different rows and columns may be correlated. For $k = 2$, for instance, the matrix element v^{12}_{34} contributes to all m-body matrix elements of pairs of Slater determinants for which the occupation numbers of orbitals (1 and 2) and (3 and 4) differ while all other occupation numbers agree. Correlations occur only among m-body matrix elements in different rows and columns because the same k-body matrix element cannot connect a given Slater determinant with two different ones.

Without property (iii), i.e., under neglect of all correlations, we could conclude immediately that for all k and for $N \to \infty$, the spectral properties of EGUE(k) are the same as for GUE. The proof proceeds as for $H^{\rm sc}$. It uses properties (i) and (ii) and the fact that EGUE(k) shares with the scaffolding ensemble the important property Eq. (3) (except for a suitable replacement of n and α). Under the assumption that k-body matrix elements appearing in different m-body matrix elements are uncorrelated, we conclude that the spectral fluctuation properties of EGUE(k) are the same as for GUE, except for the replacement $\lambda^{\rm GUE} \to \lambda^{{\rm EGUE}(k)} = \binom{m}{k} + \sum_{p=1}^{k} \binom{m}{k-p} \binom{m}{p} \binom{l-m}{p}$. The first term comes from the diagonal elements and the sum differs from the number of non-vanishing, non-diagonal elements by the factor $\binom{m}{k-p}$ which accounts for property (ii). Expanding the effective Lagrangean around the saddle-point solution, we confirm the stability of that solution.

For a complete understanding of the spectral properties of EGUE(k), it is thus vital to understand the influence of correlations among m-body matrix elements. We discuss these separately for $\rho(E)$ and for the spectral correlations. For $\rho(E)$, correlations cause deviations from the semicircular shape and drive $\rho(E)$ towards a Gaussian. To see this we recall the distinction introduced above Eq. (2) between nested and cross-linked contributions. Without correlations, cross-linked contributions are negligible for $N \gg 1$, the Pastur equation holds, and $\rho(E)$ has the shape of a semicircle. Conversely, non-vanishing correlations cause cross-linked contributions to be as important as nested ones. Mon and French [5], calculating even moments of the EGUE(k) in a basis of Slater determinants, have shown that such contributions drive $\rho(E)$ towards a Gaussian shape. The contributions, negligible for $k = m$, become increasingly important as k decreases.

Intuitively, one would expect that the spectral fluctuations are not affected by correlations among matrix elements in different rows and columns. That expectation is borne out by our analytical calculations. For lack of space, we can only sketch these here. While we have not been able to resum the series expansion of $\langle G(E)\rangle$ after Wick contraction, the supersymmetry approach still works. Because of the correlations, the quartic term is now much more involved than before. Removal of that term by a Hubbard-Stratonovich transformation is still possible, however. In addition to the supermatrices σ_μ introduced above, we must now define supermatrices $\sigma^\beta_{\mu\nu}$. The lower indices μ and ν stand for a pair of correlated matrix elements. The upper index β distinguishes families of such pairs. If the resulting saddle-point equations possess a unique solution (or, at least, only a single solution with a non-vanishing imaginary part), then we can conclude as before that for all $k \geq 2$ the spectral fluctuations of EGUE(k) are of GUE type. Because of the complexity of the saddle-point equations, we are not able to construct that solution, however. Therefore, we also cannot estimate the stability of the saddle-point approximation.

EGUE(1) *as a special case.* The uniqueness of the solution of the saddle-point equations, essential for our argument, does not hold for $k = 1$. The Hermitian matrix $v^j_{j'}$ can be diagonalized; the eigenvalues follow Wigner-Dyson statistics. The m-body matrix is then diagonal, too, each diagonal element being given by a sum of m such eigenvalues. For $m \gg 1$ such sums are uncorrelated, and the spectrum is Poissonian. That symmetry of EGUE(1), not obvious in the m-body matrix representation, must cause the saddle-point equations to have more than one solution. In excluding such a hidden symmetry for $k \geq 2$, we appeal to the results of numerical diagonalizations. Although done for matrices of small dimensions, such calculations should have revealed the existence of a symmetry.

EGUE(1) illustrates some of our arguments and conclusions very nicely. We compare three ensembles. (i) For EGUE(1) the average spectrum is (nearly) Gaussian and the eigenvalues have Poisson statistics. (ii) For an ensemble with the same scaffolding matrix as EGUE(1), but with uncorrelated Gaussian-distributed random variables, we have shown above that $\rho(E)$ is semicircular and that the eigenvalues obey Wigner-Dyson statistics. (iii) By randomly redistributing the single-particle matrix elements $v^j_{j'}$ over the scaffolding matrix of EGUE(1), we destroy the symmetry but keep the correlations. For that ensemble we expect a (nearly) Gaussian form for $\rho(E)$ but Wigner-Dyson statistics for the eigenvalues. That is confirmed by numerical calculations.

Conclusions. We have constructed two random-matrix ensembles, $H^{\rm cr}$ and $H^{\rm sc}$, both more sparse than EGUE(k) for all k. We have shown that $H^{\rm cr}$ mimicks the metal-insulator transition and that $H^{\rm sc}$ possesses the same spectral properties as the GUE. Generalizing our proof, we have shown that the spectral fluctuations of the embedded k-body random matrix ensemble EGUE(k) (which for $k \ll m$ is endowed with a Gaussian spectral shape) also coincide with those of the GUE, provided there are no hidden symmetries. We conclude that spectra in finite many-body systems governed by few-body interactions generically display Wigner-Dyson level statistics. Chaos may be reduced if the degeneracy of the single-particle states assumed in EGUE is lifted. These conclusions hold for all three symmetry classes (orthogonal, unitary, symplectic). The analytical results were obtained by an extension of the supersymmetry approach that might be useful also in other applications.

ZP acknowledges support by the Czech Science Foundation under Grant No. 202/09/0084. He thanks J. Kvasil and P. Cejnar for valuable comments. TP and HW thank O. Bohigas for stimulating discussions, and thank the Institute for Nuclear Theory for its hospitality during the completion of this work. This work was partially supported by the U.S. Department of Energy under contract No. DE-AC05-00OR22725 with UT-Battelle, LLC (Oak Ridge National Laboratory), and under grant No. DE-FG02-96ER40963 (University of Tennessee).

[1] T. Guhr, A. Müller-Groeling, and H. A. Weidenmüller, Phys. Rep. **299** (1998) 189.
[2] O. Bohigas, M. J. Giannoni, and C. Schmit, Phys. Rev. Lett. **52** (1984) 1.
[3] L. Benet and H. A. Weidenmüller, L. Phys. A: Math. Gen. **36** (2003) 3569.
[4] D. M. Basko, I. L. Aleiner, and B. L. Altshuler, *On the problem of many-body localization*, in: Problems of Condensed-Matter Physics, Eds.: A. L. Ivanov and S. G. Tikhodeev, Oxford University Press, Oxford 2008.
[5] K. F. Mon and J. B. French, Ann. Phys. (N.Y.) **95** (1975) 90.
[6] Y. V. Fyodorov and A. D. Mirlin, Phys. Rev. Lett. **67** (1991) 2049.
[7] A. D. Mirlin, Y. V. Fyodorov, F.-M. Dittes, J. Quezada, and T. H. Seligman, Phys. Rev. E **54** (1996) 3221.
[8] K. B. Efetov, Adv. Phys. **32** (1983) 53.
[9] J. J. M. Verbaarschot, H. A. Weidenmüller, and M. R. Zirnbauer, Phys. Rep. **129** (1985) 367.
[10] F. Evers and A. D. Mirlin, Phys. Rev. Lett. **84**, 3690 (2000).