Rapid Communications

Fidelity susceptibility in Gaussian random ensembles

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(Received 18 December 2018; published 20 May 2019)

The fidelity susceptibility measures the sensitivity of eigenstates to a change of an external parameter. It has been fruitfully used to pin down quantum phase transitions when applied to ground states (with extensions to thermal states). Here, we propose to use the fidelity susceptibility as a useful dimensionless measure for complex quantum systems. We find analytically the fidelity susceptibility distributions for Gaussian orthogonal and unitary universality classes for arbitrary system sizes. The results are verified by a comparison with numerical data.

DOI: 10.1103/PhysRevE.99.050102

The discovery of the many-body localization (MBL) phenomenon resulting in nonergodicity of the dynamics in many-body systems [1] restored also interest in purely ergodic phenomena modeled by Gaussian random ensembles (GREs) [2] and in possible measures to characterize them. The gap ratio between adjacent level spacings [3] was introduced precisely for that purpose as it does not involve the so-called unfolding [4] necessary for meaningful studies of level spacing distributions and yet often leading to spurious results [5]. Still, the level spacing distribution belongs to the most popular statistical measures used for single-particle quantum chaos studies [6–9] and also in the transition to MBL [10–12]. A particular place among different measures was taken by those characterizing level dynamics for a Hamiltonian $H(\lambda)$ dependent on some parameter λ. In the Pechukas-Yukawa formulation [13,14] energy levels are the positions of fictitious gas particles, derivatives with respect to the fictitious time λ are velocities (level slopes), and the second derivatives describe curvatures of the levels (accelerations). Simons and Altschuler [15] put forward a proposition that the variance of velocity distribution is an important parameter characterizing the universality of level dynamics. This led to predictions for distributions of avoided crossings [16] and, importantly, curvature distributions postulated first on the basis of numerical data for GRE [17] and then derived analytically via the supersymmetric method by von Oppen [18,19] (for alternative techniques, see Refs. [20,21]). Curvature distributions were recently addressed in MBL studies [22,23].

Apart from quantum chaos studies in the 1980's and 1990's, another "level dynamics" tool has been introduced in the quantum information area, i.e., the fidelity $\mathcal{F}$ [24]. It compares two close (possibly mixed) quantum states $\rho(\lambda_1)$ and $\rho(\lambda_2)$ for different values of the parameter λ. For pure states, as considered below, and for $\lambda_1 = 0$ we adopt the following definition, $\mathcal{F} = |\langle\psi(0)|\psi(\lambda)\rangle|$ [25] (note that sometimes fidelity is defined as a square of $\mathcal{F}$; such an overlap was considered in the context of the parametric dynamics of eigenvectors in Ref. [26]). For a sufficiently small difference of parameter values λ it is customary to introduce a fidelity susceptibility χ via a Taylor series expansion,

$$\mathcal{F}(\hat{\rho}(0), \hat{\rho}(\lambda)) = 1 - \tfrac{1}{2}\chi\lambda^2 + O(\lambda^3) \qquad (1)$$

(with the linear term vanishing due to the wave-function normalization condition). Fidelity susceptibility is directly related to the quantum Fisher information (QFI) G being directly proportional to the Bures distance between density matrices at slightly differing values of λ [27–29], with $G(\lambda) = 4\chi$.

Fidelity susceptibility emerged as a useful tool to study quantum phase transitions as at the transition point the ground state changes rapidly, leading to the enhancement of χ [25,28,30–35]. All of these studies were restricted to ground-state properties while MBL considers the bulk of excited states (for a discussion of thermal states, see Refs. [36–39]). In the context of MBL we are aware of a single study which considered the mean fidelity susceptibility across the MBL transition [40]. In particular, the issue of the fidelity susceptibility behavior for GRE still needs to be addressed. The aim of this Rapid Communication is to fill this gap and to provide analytic results for the fidelity susceptibility distributions for the physically most important orthogonal and unitary ensembles. This provides different characteristics of GRE as well as a starting point for the study of fidelity susceptibility in the transition to and within the MBL domain [41].

Consider $H = H_0 + \lambda H_1$ with H_0, H_1 corresponding to the orthogonal (unitary) class of GRE, i.e., Gaussian orthogonal ensemble (GOE) corresponding to the level repulsion parameter $\beta = 1$ or Gaussian unitary ensemble (GUE) with $\beta = 2$. For such a Hamiltonian one may easily prove that fidelity

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susceptibility of the nth eigenstate of H_0 is given by

$$\chi_n = \sum_{m\neq n} \frac{|H_{1,nm}|^2}{(E_n - E_m)^2}, \tag{2}$$

with E_n being the nth eigenvalue of H_0. We aim at calculating the probability distribution of the fidelity susceptibility

$$P(\chi, E) = \frac{1}{N\rho(E)} \left\langle \sum_{n=1}^{N} \delta(\chi - \chi_n)\delta(E - E_n) \right\rangle \tag{3}$$

at the energy E. The averaging is over two, independent GREs ($\beta = 1, 2$),

$$P(H_a) \sim \exp\left(-\frac{\beta}{4J^2}\,\mathrm{Tr}\, H_a^2\right), \quad H_a = [H_{a,nm}], \tag{4}$$

with $a = 0, 1$. Using a Fourier representation for $\delta(\chi - \chi_n)$, the average over H_1 reduces to a calculation of Gaussian integrals. Since formula (2) involves only the eigenvalues of H_0, the averaging over H_0 can be expressed as an average over the well-known joint probability density of eigenvalues [4] for a suitable GRE. At the center of the spectrum ($E = 0$), after straightforward algebraic manipulations (see Ref. [42] for details), we get

$$P(\chi) \sim \int_{-\infty}^{\infty} d\omega e^{-i\omega\chi} \left\langle \left[\frac{\det \bar{H}^2}{\det\left(\bar{H}^2 - \frac{2i\omega J^2}{\beta}\right)^{\frac{1}{2}}} \right]^{\beta} \right\rangle_{N-1}, \tag{5}$$

where the averaging is now over the $(N-1)\times(N-1)$ matrix $\bar{H}$ from an appropriate Gaussian ensemble. Similar averages have been considered in studies of curvature distributions [18–20], nonorthogonality effects in weakly open systems [43,44], and considered in a more general fashion for the GOE case in Ref. [45].

To perform the average in (5) we employ a technique developed in Ref. [20] and express the denominator as a Gaussian integral over a vector $\mathbf{z} \in \mathbb{R}^{N-1}$ for $\beta = 1$ or $\mathbf{z} \in \mathbb{C}^{N-1}$ for $\beta = 2$. Employing the invariance of GRE with respect to an adequate class (orthogonal or unitary) of transformations allows us to choose $\mathbf{z} = r[1, 0, \dots, 0]^T$, and hence we arrive at

$$P(\chi) \sim \int_0^{\infty} dr r^s \delta(\chi - 2J^2 r^2/\beta) \langle \det \bar{H}^{2\beta} e^{-r^2 X} \rangle_{N-1}, \tag{6}$$

where $X = \sum_{j=1}^{N-1} |\bar{H}_{1j}|^2$ depends on the first row of $\bar{H}$ only, and $s = \beta(N-1) - 1$. After calculating the ensuing Gaussian integrals over $\bar{H}_{1j}$ we can reduce the averaging to one over the $(N-2)\times(N-2)$ block of $\bar{H}$, $V_{ij} = \bar{H}_{i+1,j+1}$ for $1 \leqslant i, j \leqslant N-2$, using the expression $\det \bar{H} = \det V \left(\bar{H}_{11} - \sum_{j,k=2}^{N-1} \bar{H}_{1j} V^{-1}_{jk} \bar{H}^*_{1k}\right)$ for a determinant of a block matrix.

Integrating (6) over r we find (details described in Ref. [42]) that the desired fidelity susceptibility distribution $P_N^O(\chi)$ for GOE reads

$$P_N^O(\chi) = \frac{C_N^O}{\sqrt{\chi}} \left(\frac{\chi}{1+\chi}\right)^{\frac{N-2}{2}} \left(\frac{1}{1+2\chi}\right)^{\frac{1}{2}}$$

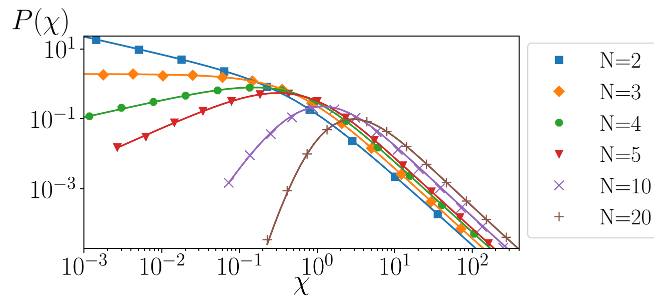

FIG. 1. Fidelity susceptibility $P_N^O(\chi)$ distribution for GOE matrices of small size N. Numerical data denoted by markers. Solid lines correspond to (7) with $\mathcal{I}_N^{O,2}$ given by (10).

$$\times \left[\frac{1}{1+2\chi} + \frac{1}{2}\left(\frac{1}{1+\chi}\right)^2 \mathcal{I}_{N-2}^{O,2} \right], \tag{7}$$

where C_N^O is a normalization constant and

$$\mathcal{I}_N^{O,2} = \langle \det V^2 (2\,\mathrm{Tr}\, V^{-2} + (\mathrm{Tr}\, V^{-1})^2) \rangle_N / \langle \det V^2 \rangle_N. \tag{8}$$

The form of (8) is suited for a random matrix theory calculation of $\mathcal{I}_N^{O,2}$. However, to obtain $\mathcal{I}_N^{O,2}$ it suffices to note that our calculation implies that

$$\langle \det \bar{H}^2 e^{-r^2 X} \rangle_{N-1}|_{r=0} = J^2 \langle \det \bar{V}^2 \rangle_{N-2} \left(\mathcal{I}_{N-2}^{O,2} + 2\right), \tag{9}$$

showing that $\mathcal{I}_N^{O,2}$ is actually determined by the second moments of determinants of matrices of appropriate sizes from GOE. Moments as well as the full probability distribution of the determinant of GOE matrices were obtained in Ref. [46] for arbitrary N. Using the expression for the second moment in (9), we get

$$\mathcal{I}_N^{O,2} = \begin{cases} N\frac{N+2}{N+3/2}, & N \text{ even}, \\ N + 1/2, & N \text{ odd}. \end{cases} \tag{10}$$

The formula (10) is exact for arbitrary $N \geqslant 0$. Inserting appropriate values of $\mathcal{I}_N^{O,2}$ into (7) we obtain an exact formula for the fidelity susceptibility distribution $P_N^O(\chi)$ for a GOE matrix of arbitrary size N. A comparison of the resulting distribution $P_N^O(\chi)$ with numerically generated fidelity susceptibility distributions for small matrix sizes $N \leqslant 20$ is shown in Fig. 1. However, it is the large N regime which is interesting from the point of view of potential applications. For $N \gg 1$ the $\mathcal{I}^{O,2}$ increases linearly $\mathcal{I}_N^{O,2} = N$ with the matrix size N. This, together with the form of $P_N^O(\chi)$, implies that $P_{\alpha N}^O(\alpha\chi) \approx P_N^O(\chi)$. Indeed, the distribution $P(\chi)$ scales linearly with N, as visible in Fig. 2. The linear in N scaling of χ suggests to introduce the scaled fidelity susceptibility $x = \chi/N$. Inserting it into (7) and taking the $N \to \infty$ limit, one obtains

$$P^O(x) = \frac{1}{6}\frac{1}{x^2}\left(1 + \frac{1}{x}\right)\exp\left(-\frac{1}{2x}\right), \tag{11}$$

which is the final, simple, analytic result for a large size GOE matrix. It performs remarkably well also for modest size matrices, e.g., $N = 200$—compare Fig. 3. For smaller matrices, for instance, for $N = 20$, the rescaled distribution $P(x)$ has a correct large x tail and a nonzero slope at $x = 0$ as compared to nonanalytic behavior of $P^O(x)$ at $x = 0$ in (11). Observe also that the mean scaled fidelity susceptibility

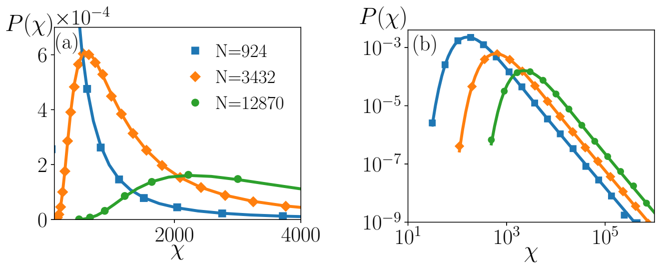

FIG. 2. Fidelity susceptibility $P_N^O(\chi)$ distribution for GOE matrices of different sizes as indicated in the figure. (a) and (b) correspond to lin-lin and log-log scales allowing for a detailed test of accuracy both for the bulk and for the tails of the distribution. Solid lines correspond to (7) with $\mathcal{I}_N^{O,2}$ given by (10).

does not exist as the corresponding integral diverges logarithmically, showing the importance of the heavy tail of the distribution. Expression (11) was also obtained in the study of the so-called complexness parameter [43].

Starting from (6) for GUE ($\beta = 2$), after a few technical steps (described in detail in Ref. [42]), we obtain the following, exact for arbitrary N, expression for the fidelity susceptibility distribution,

$$P_N^U(\chi) = C_N^U \left(\frac{\chi}{1+\chi}\right)^{N-2} \left(\frac{1}{1+2\chi}\right)^{\frac{1}{2}} \left[\frac{3}{4}\left(\frac{1}{1+2\chi}\right)^2 + \frac{3}{2}\frac{1}{1+2\chi}\left(\frac{1}{1+\chi}\right)^2 \mathcal{I}_{N-2}^{U,2} + \frac{1}{4}\left(\frac{1}{1+\chi}\right)^4 \mathcal{I}_{N-2}^{U,4}\right], \tag{12}$$

where C_N^U is a normalization constant. $P_U(\chi)$ for GUE depends on two N-dependent factors $\mathcal{I}_{N-2}^{U,2}$ and $\mathcal{I}_{N-2}^{U,4}$ that remain to be determined.

They take the form [42]

$$\mathcal{I}_N^{U,K} = \int dZ_{K,N} \left\langle \det H^4 \left(\sum_{j,k} z_j H_{jk}^{-1} z_k^*\right)^K \right\rangle_N, \tag{13}$$

where $dZ_{K,N} = (\pi J)^K \int \prod_j d^2 z_j e^{-\pi \sum_j |z_j|^2} / \langle \det H^4 \rangle_N$, $K{=}2, 4$ and H is an $N \times N$ GUE matrix. Performing the integration in (13) we find that $\mathcal{I}_N^{U,2}$ can be expressed in the following way,

$$\mathcal{I}_N^{U,2} = J^2 \frac{\langle \det H^4 (\mathrm{Tr}(H^{-2}) + (\mathrm{Tr}\, H)^{-2}) \rangle_N}{\langle \det H^4 \rangle_N}. \tag{14}$$

Introducing the following generating function

$$Z_N(j_1, j_2) = \langle \det H^2 \det(H - j_1) \det(H - j_2) \rangle_N, \tag{15}$$

we immediately verify that

$$\mathcal{I}_N^{U,2} = \frac{J^2}{Z_N(0,0)} \left(2 \frac{\partial^2}{\partial j_1 \partial j_2} Z_N(0,0) - \frac{\partial^2}{\partial j_1^2} Z_N(0,0)\right). \tag{16}$$

The generating function $Z_N(j_1, j_2)$ is actually a correlation function of a characteristic polynomial of the H matrix. It was shown in Refs. [47,48] that such quantities can be calculated exactly as determinants of appropriate orthogonal polynomials. A kernel structure of those expressions has been identified in Ref. [49], leading to formulas most convenient in our calculation of $Z_N(j_1, j_2)$. The generating function $Z(j_1, j_2)$ is given by

$$Z_N(j_1, j_2) = \frac{C_{N,2}}{(j_1 - j_2)} \lim_{\mu_2 \to 0} \frac{\partial}{\partial \mu_2} \times \det \begin{bmatrix} W_{N+2}(j_1, 0) & W_{N+2}(j_2, 0) \\ W_{N+2}(j_1, \mu_2) & W_{N+2}(j_2, \mu_2) \end{bmatrix}, \tag{17}$$

with the kernel $W_{N+2}(\lambda, \mu)$ defined as

$$W_{N+2}(\lambda, \mu) = \frac{H_{N+2}(\lambda) H_{N+1}(\mu) - H_{N+2}(\mu) H_{N+1}(\lambda)}{\lambda - \mu}. \tag{18}$$

The Hermite polynomials $H_N(\lambda)$ are orthogonal with respect to the measure $e^{-\frac{1}{2J^2}x^2}dx$ and normalized in such a way that the coefficient in front of λ^N is equal to unity. We have found a closed formula for the generating function $Z_N(j_1, j_2)$ (see Ref. [42] for details). Calculating the derivatives in (16) and taking the limits $j_1 \to 0$ and $j_2 \to 0$, we obtain

$$\mathcal{I}_N^{U,2} = \begin{cases} \frac{1}{3}N, & N \text{ even}, \\ \frac{1}{3}(N+1), & N \text{ odd}. \end{cases} \tag{19}$$

The next step is to use the idea analogous to the argument with the ratio of second moments of the determinants of GOE matrices which allowed us to obtain the exact expression for $\mathcal{I}_N^{O,2}$ (9). Employing formulas for the fourth moment of the determinant of the GUE matrix [50,51] and taking into

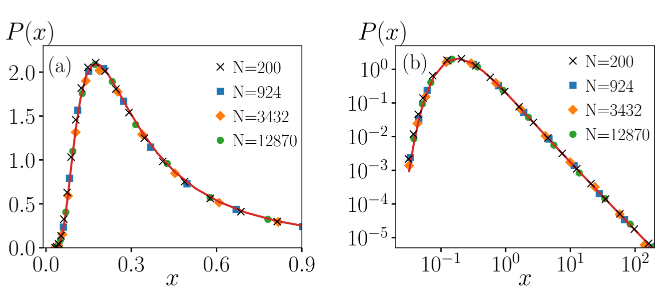

FIG. 3. Distribution of rescaled fidelity susceptibility $P^O(x)$ for GOE; numerical data denoted by markers, and solid lines are formula (11).

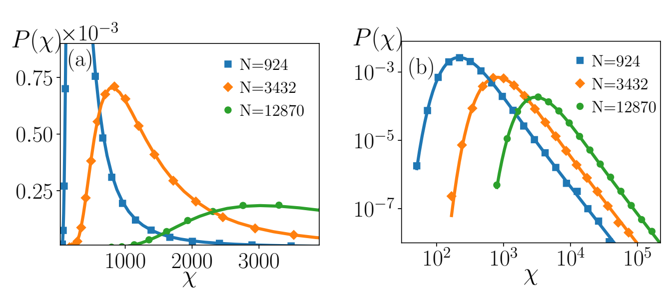

FIG. 4. Fidelity susceptibility distribution $P_N^U(\chi)$ for GUE; numerically generated data denoted by markers, and solid lines are formula (12) with $\mathcal{I}_N^{U,2}$ and $\mathcal{I}_N^{U,4}$ given by (19) and (20), respectively.

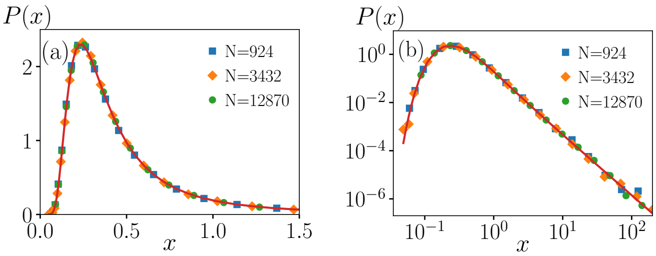

FIG. 5. Distribution of rescaled fidelity susceptibility $P_U(x)$ for GUE; numerical data denoted by markers, and solid lines are formula (21).

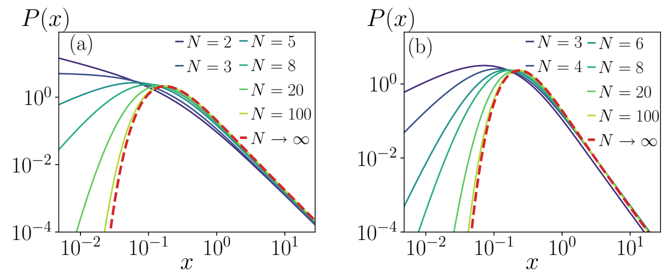

FIG. 6. Distributions of rescaled fidelity susceptibility $P(x)$ for (a) GOE and (b) GUE for matrix size N. Red dashed lines correspond to the universal $N \to \infty$ GOE/GUE limits.

account the expression for $\mathcal{I}_N^{U,2}$, we obtain

$$\mathcal{I}_N^{U,4} = \begin{cases} N^2 + 2N, & N \text{ even}, \\ N^2 + 4N + 3, & N \text{ odd}. \end{cases} \tag{20}$$

The distribution (12), together with expressions (19) and (20) for $\mathcal{I}_N^{U,4}$ and $\mathcal{I}_N^{U,2}$, is the exact fidelity susceptibility distribution for GUE for arbitrary N. As shown in Fig. 4, expression (12) is confirmed by numerical data for different system sizes $N \gg 1$. Similar, perfect agreement of our formula $P_N^U(\chi)$ with numerically generated data is obtained for small $N \geqslant 2$ (data not shown). Moreover, similarly to the GOE case, $P_N^U(\chi)$ scales linearly with increasing N. Therefore, considering again the distribution of scaled fidelity susceptibility $x = \chi/N$, we arrive at the large N limit of the simple form

$$P^U(x) = \frac{1}{3\sqrt{\pi}}\frac{1}{x^{5/2}}\left(\frac{3}{4} + \frac{1}{x} + \frac{1}{x^2}\right)\exp\left(-\frac{1}{x}\right), \tag{21}$$

which works well for GUE data as shown in Fig. 5.

Remarkably, the obtained distributions of fidelity susceptibility both for GOE (7) and GUE (12) are exact for arbitrary $N \geqslant 2$. This is an unusual situation, even for GRE—for instance, the simple analytic form of the level spacing distribution $P(s)$ for $N = 2$ becomes more complicated for larger N [2]. We study thus the onset of universal large N behavior of the rescaled fidelity susceptibility distribution $P(x)$. The results are shown in Fig. 6. Clearly, the power-law tail of the distributions for GOE (GUE) is observed for all N. This power-law tail arises in instances when the sum for χ_n (2) is dominated by a single term with a small energy denominator. The algebraic decay x^{-2} ($x^{-5/2}$) for GOE (GUE) can be derived from the small s behavior of the level spacing distribution $P(s)$ [23,52]. The approach to the limiting $N \to \infty$ distributions $P^{O,U}(x)$ is associated with a decreasing number of instances of very small fidelity susceptibility.

To conclude, we have derived closed formulas for fidelity susceptibility distributions corresponding to level dynamics for both the orthogonal and the unitary class of Gaussian random ensembles. Particularly simple analytic expressions are found in the large N limit. The fidelity susceptibility distributions obtained for quantally chaotic systems may be compared with the results found for GOE (GUE) in order to characterize the degree to which a given system is faithful to random matrix predictions. The obtained distributions also open a way to address level dynamics in the transition between ergodic and many-body localized regimes [41].

As a last touch let us mention that fidelity susceptibility is experimentally accessible by Bragg spectroscopy [53], e.g., in ultracold atomic systems [54,55], or by a direct measurement of many-body wave functions overlapping either in a NMR setting [56] or a system of ultracold bosons [57]. That paves a way for comparing experimental measurements with universal features of the fidelity susceptibility distribution provided in this work.

We thank Dominique Delande for a careful reading of this manuscript. P.S. and J.Z. acknowledge support by PL-Grid Infrastructure and EU project the EU H2020-FETPROACT-2014 Project QUIC No. 641122. This research has been supported by National Science Centre (Poland) under Projects No. 2015/19/B/ST2/01028 (P.S. and A.M.), No. 2018/28/T/ST2/00401 (doctoral scholarship to P.S.), No. 2017/25/Z/ST2/03029 (J.Z.), and No. 2017/27/B/ST2/0295 (M.K.).

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