Fidelity susceptibility in Gaussian random ensembles

Piotr Sierant,1,* Artur Maksymov,1 Marek Kuś,2,† and Jakub Zakrzewski1,3,‡

1Instytut Fizyki im. Mariana Smoluchowskiego, Uniwersytet Jagielloński, Łojasiewicza 11, 30-348 Kraków, Poland
2Centrum Fizyki Teoretycznej PAN, Aleja Lotników 32/46, 02-668 Warszawa, Poland
3Mark Kac Complex Systems Research Center, Uniwersytet Jagielloński, Kraków, Poland

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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.

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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 \( \lambda \). In the Pechukas-Yukawa formulation [13,14] energy levels are the positions of fictitious gas particles, derivatives with respect to the fictitious time \( \lambda \) 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 \( F \) [24]. It compares two close (possibly mixed) quantum states \( \hat{\rho}(\lambda_1) \) and \( \hat{\rho}(\lambda_2) \) for different values of the parameter \( \lambda \). For pure states, as considered below, and for \( \lambda_1 = 0 \) we adopt the following definition, \( F = |\langle \psi(0)|\psi(\lambda) \rangle| \) [25] (note that sometimes fidelity is defined as a square of \( F \); 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 \( \lambda \) it is customary to introduce a fidelity susceptibility \( \chi \) via a Taylor series expansion,

\[
\mathcal{F}(\hat{\rho}(0), \hat{\rho}(\lambda)) = 1 - \frac{1}{2} \chi \lambda^2 + O(\lambda^3)
\]

(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 \( \lambda \) [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 \( \chi \) [25,28,30–35]. All of these studies were restricted to ground-state properties while MBL considers the bulk of excited states, as considered below, for \( \lambda_1 = 0 \).

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
susceptibility of the $n$th eigenstate of $H_0$ is given by

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

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

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

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

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

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

$$P(\chi) \sim \int_{-\infty}^{\infty} d\omega e^{-i\omega \chi} \left[ \frac{\det \tilde{H}^2}{\det (\tilde{H}^2 - 2iO^2/\beta^2)} \right]^{\beta_{\text{av}}} \chi_{N-1},$$

where the averaging is now over the $(N-1) \times (N-1)$ matrix $\tilde{H}$ 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 vector $z \in \mathbb{R}^{N-1}$ for $\beta = 1$ or $z \in \mathbb{C}^{N-1}$ for $\beta = 2$. Employing the invariance of GRE with respect to an adequate class (orthogonal or unitary) of transformations allows us to choose $z = r[1,0,\ldots,0]^T$, and hence we arrive at

$$P(\chi) \sim \int_{0}^{\infty} dr r^\beta \delta(\chi - 2J^2 r^2/\beta) \langle \det \tilde{H}^2 e^{-r^2X} \rangle_{N-1},$$

where $X = \sum_{j=1}^{N-1} |\tilde{H}_{1j}|^2$ depends on the first row of $\tilde{H}$ only, and $s = \beta(N-1) - 1$. After calculating the ensuing Gaussian integrals over $\tilde{H}_{1j}$ we can reduce the averaging to one over the $(N-2) \times (N-2)$ block of $\tilde{H}$, $V_{ij} = \tilde{H}_{i+1,j+1}$ for $1 \leq i, j \leq N-2$, using the expression

$$\det \tilde{H} = \langle \det \tilde{H}_{11} - \sum_{j,k=2}^{N-1} \tilde{H}_{1j} V_{jk}^{-1} \tilde{H}_{jk} \rangle$$

for a determinant of a block matrix.

Integrating (6) over $r$ we find (details described in Ref. [42]) that the desired fidelity susceptibility distribution $P_N^0(\chi)$ for GOE reads

$$P_N^0(\chi) = \frac{C_N^0}{\sqrt{\chi}} \left( \frac{\chi}{1 + \chi} \right)^{\frac{N-1}{2}} \left( \frac{1}{1 + 2\chi} \right)^{\frac{1}{2}},$$

Fig. 1. Fidelity susceptibility $P_N^0(\chi)$ distribution for GOE matrices of small size $N$. Numerical data denoted by markers. Solid lines correspond to (7) with $T_N^{O,2}$ given by (10).

where $C_N^0$ is a normalization constant and

$$T_N^{O,2} = \langle \det V^2(2 \operatorname{Tr} V^{-2} + (\operatorname{Tr} V^{-1})^2) \rangle_N / \langle \det V^2 \rangle_N.$$

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

$$\langle \det \tilde{H}^2 e^{-r^2X} \rangle_{N-1} = J^2 \langle \det V^2 \rangle_{N-2} (T_N^{O,2} + 2),$$

showing that $T_N^{O,2}$ 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

$$T_N^{O,2} = \begin{cases} \frac{N}{N+2}, & N \text{ even}, \\ \frac{N+1}{N+2}, & N \text{ odd}. \end{cases}$$

The formula (10) is exact for arbitrary $N \geq 0$. Inserting appropriate values of $T_N^{O,2}$ into (7) we obtain an exact formula for the fidelity susceptibility distribution $P_N^0(\chi)$ for a GOE matrix of arbitrary size $N$. A comparison of the resulting distribution $P_N^0(\chi)$ with numerically generated fidelity susceptibility distributions for small matrix sizes $N \leq 20$ 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 $T_N^{O,2}$ increases linearly $T_N^{O,2} \approx N$ with the matrix size $N$. This, together with the form of $P_N^0(\chi)$, implies that $P_N^{0}(\chi) \approx P_N^{0}(\chi)$. Indeed, the distribution $P(\chi)$ scales linearly with $N$, as visible in Fig. 2. The linear in $N$ scaling of $\chi$ suggests to introduce the scaled fidelity susceptibility $x = \chi/N$. Inserting it into (7) and taking the $N \to \infty$ limit, one obtains

$$P^0(x) = \frac{1}{6x^2} \left( 1 + \frac{1}{x} \right) \exp \left( -\frac{1}{2x} \right),$$

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 $P^0(x)$ at $x = 0$ in (11). Observe also that the mean scaled fidelity susceptibility

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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 algorithms, showing the importance of the heavy tail of the distribution. Expression (11) was also obtained in the study of algorithms, showing the importance of the heavy tail of the distribution.

Starting from (6) for GUE (β = 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,

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

(12)

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

They take the form [42]

$$T_{N}^{U,K} = \int dZ_{K,N} \left( \sum_{j,k} z_j H_{jk}^{-1} z_k^* \right)^K, \quad (13)$$

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

$$T_{N}^{U,2} = J^2 (det H^4 (Tr H^{-2}) + (Tr H^{-2})^3) / (det H^4)_N. \quad (14)$$

Introducing the following generating function

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

we immediately verify that

$$T_{N}^{U,2} = \frac{J^2}{Z_N(0,0)} \left( 2 \frac{\partial^2}{\partial j_1 \partial j_2} Z_N(0,0) - \frac{\partial^2}{\partial j_1^2} Z_N(0,0) \right). \quad (16)$$

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

$$Z_N(j_1, j_2) = C_{N+2} \lim_{\lambda \rightarrow 0} \frac{\partial}{\partial \mu} \left[ W_{N-2}(j_1, \mu) W_{N-2}(j_2, \mu) \right], \quad (17)$$

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

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

The Hermite polynomials $H_N(\lambda)$ are orthogonal with respect to the measure $e^{-\pi x^2} dx$ and normalized in such a way that the coefficient in front of $\lambda^N$ 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 $j_1 \rightarrow 0$ and $j_2 \rightarrow 0$, we obtain

$$T_{N}^{U,2} = \begin{cases} \frac{3}{4} N, & N \text{ even}, \\ \frac{1}{4} (N + 1), & N \text{ odd}. \end{cases} \quad (19)$$

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 $T_{N}^{U,2}$ (9). Employing formulas for the fourth moment of the determinant of the GUE matrix [50,51] and taking into account
account the expression for $\mathcal{X}^U_2$, we obtain
\begin{equation}
\mathcal{X}^U_4 \equiv \left\{ \begin{array}{ll}
N^2 + 2N, & N \text{ even}, \\
N^2 + 4N + 3, & N \text{ odd}.
\end{array} \right. \tag{20}
\end{equation}

The distribution (12), together with expressions (19) and (20) for $\mathcal{X}^U_2$ and $\mathcal{X}^U_4$, 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 $P^U_N(\chi)$ with numerically generated data is obtained for small $N \geq 2$ (data not shown). Moreover, similarly to the GOE case, $P^U_N(\chi)$ scales linearly with increasing $N$. Therefore, considering again the scaled fidelity susceptibility $x = \chi/N$, we arrive at the large $N$ limit of the simple form
\begin{equation}
P^U(\chi) = \frac{1}{3\sqrt{\pi} x^{3/2}} \left( \frac{3}{4} + \frac{1}{x} + \frac{1}{x^2} \right) \exp\left( -\frac{1}{x} \right), \tag{21}
\end{equation}

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 $N \geq 2$. This is an unusual situation, even for GRE—for instance, the simple analytic form of the level spacing distribution $P(s)$ for $(\chi = s)$ 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 $\chi$ (2) is dominated by a single term with a small energy denominator. The algebraic decay $s^{-2} (s^{-5/2})$ 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.

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