Bivariate-*t* distribution for transition matrix elements in Breit-Wigner to Gaussian domains of interacting particle systems

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Interacting many-particle systems with a mean-field one-body part plus a chaos generating random two-body interaction having strength λ exhibit Poisson to Gaussian orthogonal ensemble and Breit-Wigner (BW) to Gaussian transitions in level fluctuations and strength functions with transition points marked by $\lambda=\lambda_c$ and $\lambda=\lambda_F$, respectively; $\lambda_F \gg \lambda_c$. For these systems a theory for the matrix elements of one-body transition operators is available, as valid in the Gaussian domain, with $\lambda > \lambda_F$, in terms of orbital occupation numbers, level densities, and an integral involving a bivariate Gaussian in the initial and final energies. Here we show that, using a bivariate-*t* distribution, the theory extends below from the Gaussian regime to the BW regime up to $\lambda=\lambda_c$. This is well tested in numerical calculations for 6 spinless fermions in 12 single-particle states.

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Two-body random matrix ensembles apply in a generic way to finite interacting many-fermion systems such as nuclei [1,2], atoms [3,4], quantum dots [5], small metallic grains [6], etc. A common feature of all these systems is that their Hamiltonian (H) consists of a mean-field one-body [$h(1)$] plus a complexity generating two-body [$V(2)$] interaction. With this, one has the embedded Gaussian orthogonal ensemble of one- plus two-body interactions [EGOE(1+2)] operating in many-particle spaces [2]; for the definition of EGOE(1+2) for m fermions in N single-particle states, see [2,7]. The most significant aspect of EGOE(1+2) is that as λ, the strength of the random (represented by the GOE) two-body interaction [in $H=h(1)+\lambda V(2)$], changes, in terms of state density, level fluctuations, strength functions, and entropy [8], the ensemble admits three chaos markers. First, it is well known that the state densities take Gaussian form, for large enough m, for all λ values [9]. With λ increasing, there is a chaos marker λ_c such that for $\lambda \geq \lambda_c$ the level fluctuations follow the GOE; i.e., λ_c marks the transition in the nearest-neighbor spacing distribution from Poisson to Wigner form [10]. As λ increases further from λ_c, the strength functions [for $h(1)$ basis states] change from Breit-Wigner (BW) to Gaussian form and the transition point is denoted by λ_F [11]. The $\lambda_c \leq \lambda \leq \lambda_F$ region is called the BW domain and the $\lambda > \lambda_F$ region is called the Gaussian domain. Thus in the BW and Gaussian domains the level fluctuations follow the GOE. It is important to remark that the BW to Gaussian transition in the nuclear shell model and related examples was first discussed by Zelevinsky and coworkers [12] and for lanthanide atoms (CeI to SmI) by Angom *et al.* [13]. As we increase λ much beyond λ_F, there is a chaos marker λ_t around which different definitions of entropy, temperature, etc., will coincide and also the strength functions in $h(1)$ and $V(2)$ bases will coincide. Thus the $\lambda \sim \lambda_t$ region is called the thermodynamic region [14,15].

With the three chaos markers λ_c, λ_F, and λ_t, the EGOE generates statistical spectroscopy: i.e., smoothed forms for state densities, orbit occupancies, strength sums [for example, Gamow-Teller (GT) sums in nuclei, electric dipole ($E1$) sums in atoms], transition strengths themselves [for example, electric quadrupole ($E2$), magnetic dipole ($M1$), and GT strengths in nuclei, $E1$ strengths in atoms and molecules, etc.], information entropy in wave functions and transition strengths, etc. The EGOE Gaussian-state densities are being used to generate a theory (valid for $\lambda > \lambda_c$—i.e., in the region where level fluctuations follow the GOE) for nuclear level densities with interactions [16]. Similarly, a theory for orbit occupancies and strength sums, as valid in the BW to Gaussian regimes (i.e., for $\lambda > \lambda_c$), has been developed [15]. However, for transition strengths (experimentally they are most important for probing the wave function structure of a quantum system), a theory valid only in the Gaussian domain is available [17–19]. Although a theory was given by Flambaum *et al.* for the BW domain [3,20,21], it is well known to underestimate the exact values by a factor of 2 [19,20]. Thus, a major gap (see the discussion in [19]) in understanding transition strengths is in extending the theory that works in the Gaussian domain, well into the BW domain. The purpose of this paper is to show that the bivariate-*t* distribution known in statistics will bridge this gap. As in Refs. [19,21], we restrict ourselves to one-body transition operators.

Given a Hamiltonian H and its m-particle eigenstates $|E\rangle$, the transition strengths generated by a one-body transition operator $\mathcal{O}$ are denoted by $|\langle E_f|\mathcal{O}|E_i\rangle|^2$; $\mathcal{O}=\Sigma_{\alpha,\beta}\epsilon_{\alpha\beta}a_\alpha^\dagger a_\beta$ where $\epsilon_{\alpha\beta}$ are single-particle matrix elements of the operator $\mathcal{O}$, $a_\alpha^\dagger$ creates a particle in the single-particle state α, and a_β destroys a particle in the state β. Note that the one-body transition operators $\mathcal{O}$ will not change m. Now the bivariate strength density $I_{biv;\mathcal{O}}^{H,m}(E_i,E_f)$ is defined by

$$
\begin{aligned}
I_{biv;\mathcal{O}}^{H,m}(E_i,E_f) &= \langle\langle \mathcal{O}^\dagger \delta(H-E_f)\mathcal{O}\delta(H-E_i)\rangle\rangle^m \\
&= I^m(E_f)|\langle E_f|\mathcal{O}|E_i\rangle|^2 I^m(E_i) \\
&= \langle\langle \mathcal{O}^\dagger\mathcal{O}\rangle\rangle^m \rho_{biv;\mathcal{O}}^{H;m}(E_i,E_f).
\end{aligned} \tag{1}
$$

In Eq. (1), $\langle\langle\cdots\rangle\rangle$ denotes trace. The $I_{biv;\mathcal{O}}$ is a square of the matrix elements of $\mathcal{O}$ in H eigenstates weighted by the state densities $I^m(E_i)$ and $I^m(E_f)$ at the initial and final energies, respectively, and the corresponding $\rho_{biv;\mathcal{O}}$ is normalized to unity. More importantly $I_{biv;\mathcal{O}}$ takes into account the degeneracies in the energies (E_i, E_f) and, as seen from Eq. (1), it can be treated as a bivariate probability density. Integrating E_f in $\rho^{H;m}_{biv;\mathcal{O}}(E_i, E_f)$ gives the marginal density $\rho_i(E_i)$ and similarly integrating E_i gives the second marginal density $\rho_f(E_f)$. Clearly $\rho_i(E_i)$ gives the strength sum originating from states with energy E_i and similarly $\rho_f(E_f)$. The bivariate moments of $\rho_{biv;\mathcal{O}}$ are defined by $M_{pq}=\langle\langle \mathcal{O}^\dagger H^q \mathcal{O} H^p\rangle\rangle^m / \langle\langle \mathcal{O}^\dagger \mathcal{O}\rangle\rangle^m$. With $M_{10}=\epsilon_i$ and $M_{01}=\epsilon_f$ defining the centroids of its two marginals $\rho_i(E_i)$ and $\rho_f(E_f)$, respectively, the bivariate central moments of $\rho_{biv;\mathcal{O}}$ are given by

$$\mu_{pq} = \langle\langle \mathcal{O}^\dagger (H-\epsilon_f)^q \mathcal{O} (H-\epsilon_i)^p \rangle\rangle^m / \langle\langle \mathcal{O}^\dagger \mathcal{O}\rangle\rangle^m. \qquad (2)$$

Most important of these are $\mu_{20}=\sigma_i^2$ and $\mu_{02}=\sigma_f^2$, the variances of the two marginals $\rho_i(E_i)$ and $\rho_f(E_f)$, respectively, and $\zeta=\mu_{11}/\sigma_i\sigma_f$, the bivariate correlation coefficient. Thus the five parameters $(\epsilon_i, \epsilon_f, \sigma_i, \sigma_f, \zeta)$ of $\rho_{biv;\mathcal{O}}$ are completely defined, in terms of traces, by the transition operator $\mathcal{O}$ and the Hamiltonian H. Also, if the operators $\mathcal{O}$ and H effectively commute (this happens with a EGOE representation), then $\zeta \to 1$. On the other hand, if they are representable by the GOE, then $\zeta \to 0$; see [17] for further details.

For EGOE(1+2), going well into the Gaussian domain [then EGOE(1+2) will be effectively EGOE(2)], it is well established that the bivariate strength densities take bivariate Gaussian form (this applies to nuclei [17,18])

$$\rho_{biv;\mathcal{O}}(E_i,E_f) \xrightarrow{\lambda \gg \lambda_F} \rho_{biv\text{-}\mathcal{G};\mathcal{O}}(E_i,E_f;\epsilon_i,\epsilon_f,\sigma_i,\sigma_f,\zeta)$$
$$= \frac{1}{2\pi\sigma_i\sigma_f\sqrt{(1-\zeta^2)}} \exp\left(-\frac{1}{2(1-\zeta^2)}\left\{\left(\frac{E_i-\epsilon_i}{\sigma_i}\right)^2 - 2\zeta\left(\frac{E_i-\epsilon_i}{\sigma_i}\right)\left(\frac{E_f-\epsilon_f}{\sigma_f}\right) + \left(\frac{E_f-\epsilon_f}{\sigma_f}\right)^2\right\}\right). \qquad (3)$$

An immediate question is how to extend this result well into the BW domain and up to λ_c (note that GOE fluctuations operate for $\lambda > \lambda_c$ and hence in this regime it is possible to consider smoothed transition strengths). In a recent work, Angom *et al.* [13] showed that strength functions covering the BW to Gaussian regimes can be well represented by a student's *t*-distribution. Following this result, here we conjecture that the bivariate strength density $\rho_{biv;\mathcal{O}}$ in Eq. (1) can be represented by the bivariate-*t* distribution

$$\rho_{biv\text{-}t;\mathcal{O}}(E_i,E_f;\epsilon_i,\epsilon_f,\sigma_1,\sigma_2,\zeta;\nu)$$
$$= \left(1/2\pi\sigma_1\sigma_2\sqrt{1-\zeta^2}\right)\Big[1+\left[1/\nu(1-\zeta^2)\right] \times\Big\{\left[(E_i-\epsilon_i)/\sigma_1\right]^2 - 2\zeta\left[(E_i-\epsilon_i)/\sigma_1\right]\left[(E_f-\epsilon_f)/\sigma_2\right] + \left[(E_f-\epsilon_f)/\sigma_2\right]^2\Big\}\Big]^{-(\nu+2)/2},$$
$$\nu \geq 1. \qquad (4)$$

The properties of $\rho_{biv\text{-}t}$ are given in [22,23]. Most important is that for $\nu=1$, $\rho_{biv\text{-}t}$ gives a bivariate Cauchy distribution [23,24], and as $\nu\to\infty$, $\rho_{biv\text{-}t}$ becomes bivariate Gaussian. Second the marginal distributions of $\rho_{biv\text{-}t}$ are easily seen to be univariate t distributions, with ν degrees of freedom, independent of ζ with a univariate Cauchy distribution for $\nu=1$ and Gaussian as $\nu\to\infty$. It is important to note that BW is called Cauchy in the statistics literature. Therefore, hereafter we call the $\rho_{biv\text{-}t}$ with $\nu=1$ bivariate BW distribution. In summary, as the parameter ν changes from 1 to ∞, $\rho_{biv\text{-}t}$ changes from bivariate BW to bivariate Gaussian. Assuming that the transition strength densities follow strength functions (they change from BW to Gaussian), it can be argued that the $\rho_{biv\text{-}t}$ defined by Eq. (4) has the correct limiting forms and the intermediate shapes (for fixed ζ) are determined by the ν parameter (thus $\rho_{biv\text{-}t}$ bridges the gap pointed out in [19]). As can be seen from Fig. 2 ahead, for λ not far from λ_c, the ν value is not far from 1 while ν is large for $\lambda \sim \lambda_t$. In Eq. (4), in general ϵ_i and ϵ_f are the centroids of the two marginals of $\rho_{biv\text{-}t}$; however, σ_1 and σ_2 will approach the marginal widths σ_i and σ_f only in the limit $\nu\to\infty$—i.e., for the bivariate Gaussian given in Eq. (3). In fact, the second central moments $\mu_{20}=\sigma_i^2$ and $\mu_{02}=\sigma_f^2$ are related to σ_1^2 and σ_2^2 by $\mu_{20}=\frac{\nu}{\nu-2}\sigma_1^2$ and $\mu_{02}=\frac{\nu}{\nu-2}\sigma_2^2$ for $\nu>2$. However, ζ remains the bivariate correlation coefficient. Exceptions to all these will occur for $\nu \leq 2$, and here (this happens only when λ is very close to λ_c) one has to use the spreading widths of the marginal densities to define σ_1, σ_2, etc.; see [22,23] for details.

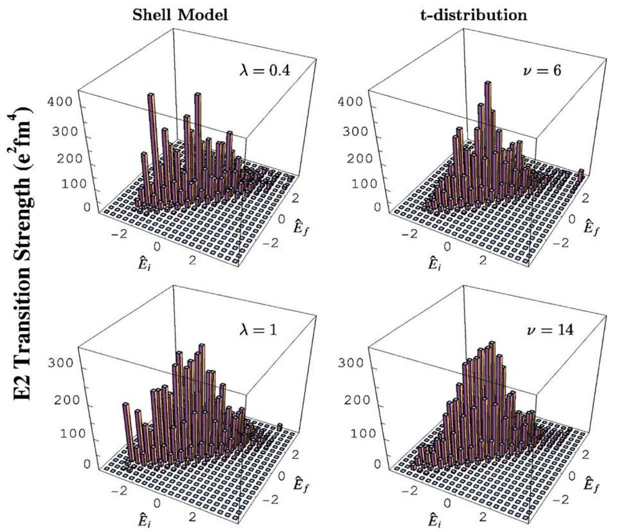

FIG. 1. (Color online) $E2$ transition strength $|\langle E_f|T^{E2}|E_i\rangle|^2$ vs $(\hat{E}_i, \hat{E}_f)$. The height of the vertical bars in the figures gives the total strength in a given bin area and a bin size of 0.3 is taken for both $\hat{E}_i$ and $\hat{E}_f$. The energies $\hat{E}_i$ and $\hat{E}_f$ are the energies of $(0^+,0)$ and $(2^+,0)$ levels, respectively (they are zero centered and scaled to unit width), for six valence nucleons in $(2s1d)$ shell with Hamiltonian matrix dimensions 71 and 307, respectively. Note that the nuclear levels are denoted by (J^π, T) where J, T, and π denote angular momentum, isospin, and parity. The Hamiltonian employed in the calculations is $H(\lambda)=h(1)+\lambda V(2)$ with the single-particle energies defining $h(1)$ and two-particle matrix elements defining $V(2)$ taken from [25] and references therein (they define the so-called Wildenthal's W interaction). The proton and neutron effective charges defining the $E2$ operator T^{E_2} are $e_p=1.29$ and $e_n=0.49$, respectively. All the calculations are carried out using the OXBASH computer code for Windows PC (2005-05 version) [26]. Although Eq. (4) is for EGOE(1+2), which is for spinless fermion systems, it can be applied directly to the shell model with good (J^π, T) states as described in [27].

In order to test the applicability of the t distribution, nuclear shell-model calculations are performed for isoscalar $E2$ transitions in ^{22}Na nucleus as shown in Fig. 1. Let us mention that smaller spaces as in the shell-model example arise for the EGOE only for $m=4$ or 5. However, for these m's the Gaussian densities are not obtained and therefore Eq. (4) will not be good. As in reality the BW and Gaussian forms are more or less universal and do not depend critically on the interaction, we are considering here a shell-model example. Figure 1 shows the results for $\lambda=0.4$ and 1 in the shell-model Hamiltonian $H=h(1)+\lambda V(2)$; $\lambda=1$ gives a realistic nuclear Hamiltonian. The parameters σ_1 and σ_2 in Eq. (4) are determined via their relation to μ_{20} and μ_{02}. The values of μ_{20}, μ_{02}, and ζ are calculated using Eq. (2) with the shell-model $E2$ strengths. They give $\zeta=0.88$, and this is used in Eq. (4) with ν determined by a fit. For $\lambda=0.4$, the deviations are large for some of the strengths connecting the states close to the ground states (for example, for $\hat{E}_i=\hat{E}_f=-1.65$ and -1.35 in the figure). Ignoring these strong collective $E2$ strengths in the low-lying states, the percentage deviation on average is $\sim 16\%$. Similarly, for $\lambda=1$, the percentage deviation on average is $\sim 20\%$. Therefore, ignoring the deviations near the ground states, as seen from Fig. 1, the t distribution gives a reasonable description of the transition strengths with $\nu=6$ for $\lambda=0.4$ and with a large ν value, as expected, for $\lambda=1$.

In larger spectroscopic spaces, instead of using a single t distribution, to represent transition strength densities, it is more appropriate to partition the space and then apply $\rho_{biv\text{-}t}$ appropriately. A simple and physically motivated decomposition of the m-particle space is into the subspaces Γ_i defined by the mean-field Hamiltonian $h(1)$, $m \rightarrow \Sigma_i \Gamma_i$ with Γ_i denoting the eigenstates of $h(1)$ with eigenvalues $\mathcal{E}_i$. Now constructing the strength distribution generated by $h(1)$ alone—i.e., $|\langle \Gamma_f | \mathcal{O} | \Gamma_i \rangle|^2$—spreading this distribution by convolution with a t distribution generated by $V(2)$ and then applying some simplifying assumptions, as described in complete detail in [19] where this procedure is applied to bivariate Gaussian spreadings, the transition strengths $|\langle E_f | \mathcal{O} | E_i \rangle|^2$ are given by

$$|\langle E_f|\mathcal{O}|E_i\rangle|^2 = \sum_{\alpha,\beta} |\epsilon_{\alpha\beta}|^2 \langle n_\beta (1-n_\alpha)\rangle^{E_i} \overline{D(E_f)} \mathcal{F}, \tag{5a}$$

$$\mathcal{F} = \int_{-\infty}^{+\infty} \rho_{biv\text{-}t;\mathcal{O}}(E_i, E_f; \mathcal{E}_i, \mathcal{E}_f = \mathcal{E}_i - \epsilon_\beta + \epsilon_\alpha, \sigma_1, \sigma_2, \zeta; \nu) d\mathcal{E}_i. \tag{5b}$$

In Eq. (5a), $\bar{D}(E_f)$ denotes the mean spacing at the energy E_f, ϵ_α (similarly ϵ_β) is the energy of the single-particle state or orbit α, and $\langle n_\beta(1-n_\alpha)\rangle^{E_i} \sim \langle n_\beta \rangle^{E_i} \langle (1-n_\alpha)\rangle^{E_i}$ with $\langle n_\alpha \rangle^{E_i}$ giving the occupation probability for the single-particle state or orbital α. Most remarkable is that the integral for $\mathcal{F}$ in Eq. (5b) can be carried out exactly for any ν and this gives

$$\mathcal{F} = \frac{\Gamma[(\nu+1)/2]}{\sqrt{\pi}\Gamma\left(\frac{\nu}{2}\right)} \frac{1}{\sqrt{\nu(\sigma_1^2+\sigma_2^2-2\zeta\sigma_1\sigma_2)}} \{1 + \Delta^2/[\nu(\sigma_1^2+\sigma_2^2 - 2\zeta\sigma_1\sigma_2)]\}^{-(\nu+1)/2}, \quad \Delta = E_f - E_i + \epsilon_\beta - \epsilon_\alpha. \tag{6}$$

Note that, for $\nu > 2$, σ_1 and σ_2 are related [as discussed after Eq. (4)] to the marginal variances μ_{20} and μ_{02}. These marginal variances and the correlation coefficient ζ in Eq. (6) are defined by Eq. (2) with H replaced by $V(2)$; then, $\zeta \sim \langle \mathcal{O}^\dagger V \mathcal{O} V\rangle / \langle \mathcal{O}^\dagger \mathcal{O}\rangle \langle VV\rangle$. More importantly, as $\nu \rightarrow \infty$, Eq. (6) goes exactly to Eq. (6) of [19] as it should be.

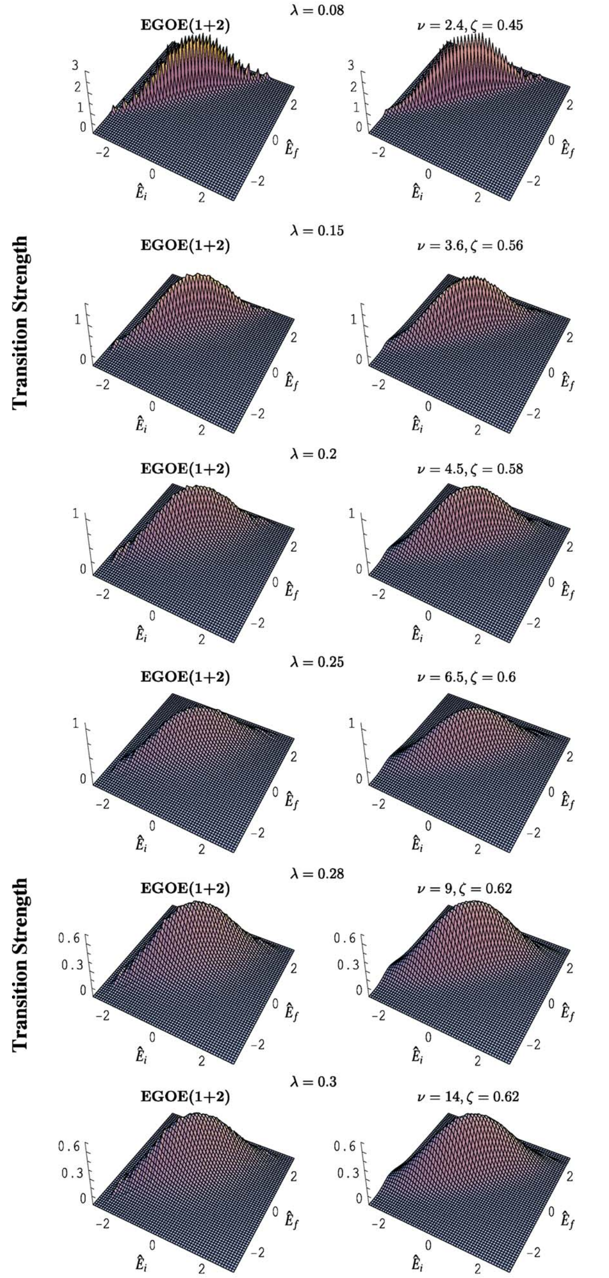

FIG. 2. (Color online) Transition strength $|\langle E_f|\mathcal{O}|E_i\rangle|^2$ vs $(\hat{E}_i, \hat{E}_f)$ for $\lambda=0.08$, 0.15, 0.2, 0.25, 0.28, and 0.3; $\hat{E}_i=(E_i-\epsilon)/\sigma$ and $\hat{E}_f=(E_f-\epsilon)/\sigma$ where ϵ and σ are the centroids and widths of the state densities. In all the figures, the ensemble-averaged strengths in the window $\hat{E}_i \pm \frac{\Delta'}{2}$ and $\hat{E}_f \pm \frac{\Delta'}{2}$ are summed and plotted at $(\hat{E}_i, \hat{E}_f)$; Δ' is chosen to be 0.1. The EGOE(1+2) system and the one-body transition operator $\mathcal{O}$ are defined in the text. For this system the total strength is 252. As λ changes from 0.08 to 0.3, the ν value changes from 2.4 to 14 and the bivariate correlation coefficient ζ changes from 0.45 to 0.62. Note the change in the scales of the vertical axes in the figures.

To test the final theory given by Eqs. (5a) and (6), numerical calculations are carried out for various λ values using a 25-member EGOE(1+2) ensemble $\{H\}=h(1)+\lambda\{V(2)\}$ in the 924-dimensional $N=12$, $m=6$ space; $h(1)$ is defined by the single-particle energies $\epsilon_i=(i)+(1/i)$, $i=1,2,\ldots,12$, and the variance of $V(2)$ matrix elements in two-particle spaces is chosen to be unity. The one-body transition operator employed in the calculations is $\mathcal{O}=a_2^\dagger a_9$ as in [19]. For the system considered, $\lambda_c\sim 0.06$, $\lambda_F\sim 0.2$, and $\lambda_t\sim 0.3$. Results for six different λ values, going from BW to Gaussian domains, are shown in Fig. 2. In these calculations ν is a free parameter determined by fits to exact results. The exact distributions give $\zeta\simeq 0.5$ but in the fits ζ is varied around the exact value (from 0.45 to 0.62 as shown in Fig. 2), and this to some extent takes into account some of the approximations that led to the simple form given by Eqs. (5a) and (6). It is seen from Fig. 2 that Eqs. (5a) and (6) obtained via the t distribution describe the exact EGOE(1+2) transition strengths as we go from the BW domain with $\lambda=0.08$ to the Gaussian domain with $\lambda=0.3$ with ν changing from 2.4 to 14: $\nu\sim 2-6$ for $\lambda_c<\lambda<\lambda_F$ and $\nu\sim 6-15$ for $\lambda_F<\lambda<\lambda_t$. Thus ν changes slowly as we go from λ_c to λ_F, and then it increases fast to a large value as we reach λ_t. In principle ν also depends on (m,N) but this has not been investigated in this work.

Results in Fig. 2 confirm that we have a good method for the calculation of transition strengths in the BW domain. A calculation is also performed for $\lambda=0.06$ by fixing σ_1 and σ_2 using the spreading widths of the marginals of the strength distribution and using the same ζ value as that obtained for $\lambda=0.08$. Then the deduced ν value is 1.5. This and the comparisons in Fig. 2 clearly emphasize the role of the bivariate correlation coefficient ζ in the BW domain, and without ζ it is not possible to get a meaningful description (it should be mentioned that the theory in the BW domain given before [19,21] uses only the marginals of the t distribution with $\nu=1$). Thus all the problems seen before [19,20] in the BW domain are cured by the bivariate-t distribution with the two parameters (ν,ζ).

In conclusion, random matrix ensembles generated by a mean-field plus a random two-body interaction generate three chaos markers. They in turn provide a basis for statistical spectroscopy. The theory for transition strengths is now extended (from Gaussian domain) to BW domain down up to the λ_c marker by employing the bivariate-t distribution. The theory given by Eqs. (5a) and (6) will be useful in the calculation of Gamow-Teller strengths (also electric quadrupole and magnetic dipole) in nuclei and dipole transition strengths in atoms in the quantum chaotic domain.

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[7] The EGOE(1+2) for spinless fermion systems is defined by $\{H\}=h(1)+\lambda\{V(2)\}$ where $\{\cdots\}$ denotes an ensemble. The mean-field one-body Hamiltonian $h(1)$ is a fixed one-body operator defined by single-particle energies ϵ_α with average spacing Δ. The $\{V(2)\}$ is EGOE(2) with unit variance for the two-body matrix elements, and λ is the strength of the two-body interaction (in units of Δ). Thus, EGOE(1+2) is defined by the four parameters (m,N,Δ,λ), and without loss of generality we put $\Delta=1$.
[8] State density $I^m(E)=\langle\langle\delta(H-E)\rangle\rangle^m$ where $\langle\cdots\rangle$ denotes trace and the corresponding normalized state density $\rho^m(E)=\langle\delta(H-E)\rangle^m$ with $\langle\cdots\rangle$ denoting the average. Given the mean-field $h(1)$ basis states $|k\rangle=\Sigma_E C_k^E|E\rangle$, the strength functions (one for each k) $F_k(E)=\Sigma_{\beta\in E}|C_k^{E,\beta}|^2$. Similarly the number of principle components NPC $(E)=\{\Sigma_k|C_k^E|^4\}^{-1}$ and the closely related information entropy $S^{info}(E)=-\Sigma_k|C_k^E|^2\ln|C_k^E|^2$.
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