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# Single-particle entropy in (1+2)-body random matrix ensembles

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Random matrix ensembles defined by a mean-field one-body plus a chaos generating random two-body interaction (called embedded Gaussian orthogonal ensembles of $(1+2)$-body interactions[EGOE$(1+2)$]) predict for the entropy defined by the occupation numbers of single-particle states, in the chaotic domain, an essentially one parameter Gaussian form for their energy dependence. Numerical embedded ensemble calculations are compared with the theory. In addition, it is shown that the single-particle entropy, thermodynamic entropy defined by the state density and information entropy defined by wave functions in the mean-field basis for EGOE$(1+2)$ describe the results known for interacting Fermi systems such as those obtained from nuclear shell model.

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Chaos vs thermalization in isolated finite interacting many-particle quantum systems, with a mean-field and a chaos generating two-body interaction, is a topic of considerable interest in the subject of quantum chaos [1–5]. Zelevinsky and co-workers [1] addressed questions in this topic for the first time by examining different definitions of entropy using the interacting nuclear shell model with 12 nucleons. They found that the thermodynamic entropy ($S^{ther}$) defined by the state density, the information entropy ($S^{info}$) in the wave functions expanded in the mean-field basis and the single-particle entropy ($S^{sp}$) defined by the mean occupation numbers of the single-particle states, all coincide for strong enough interaction but only in the presence of a mean field (a similar conclusion is reached by Casati and co-workers who examined different definitions of temperature for a smaller symmetrized coupled two-rotor model [3]). On the other hand, in the last few years it is established that the two-body random matrix ensembles and their various extended versions are good models for understanding various aspects of chaos in interacting particle systems [6] and they are applied to nuclei [6,7], atoms [8], quantum dots [9], quantum computers [4,10], etc. In particular, using the so called embedded Gaussian orthogonal ensemble of $(1+2)$-body interactions [EGOE(1+2)] defined by a mean-field one-body interaction plus a chaos generating random two-body interaction, for the first time Flambaum and Izrailev [2] showed that occupation numbers for single-particle states, in the chaotic domain of interacting Fermi systems, will be close to Fermi-Dirac distribution but with effective temperatures and chemical potentials. With this result, it can be argued that the Zelevinsky *et al.* results for various entropy definitions should have their basis in EGOE$(1+2)$. The purpose of this brief report is to establish this result. In fact the Gaussian form for exp($S^{ther}$) for EGOE$(1+2)$, essentially independent of the strength of the two-body interaction, is easily understood from the old results of Mon and French for the EGOE(2) state densities; see Refs. [11,6] and the last part of the present paper. However, only last year a complete EGOE$(1+2)$ theory for $S^{info}$ was given and it is shown to describe the results for realistic systems [12]. Therefore for a complete understanding of Zelevinsky *et al.* results, EGOE$(1+2)$ theory for $S^{sp}$ is needed. This is worked out in this Brief Report and the theoretical results are compared with numerical ensemble calculations. In the later part of the paper, EGOE$(1+2)$ results for the three entropies are compared with nuclear shell model results for eight nucleons.

Let us consider $m$ fermions in $N$ single-particle states $i$, $i=1,2,\ldots,N$. Given the Hamiltonian which is one plus two-body $[H=h(1)+V(2)]$, the nature of state densities $\rho^H(E)=\langle \delta(H-E)\rangle^m$ ($\langle\ \rangle^m$ denotes average over all $m$ particle states) generated by $H$ is understood by assuming that $H$ is representable by EGOE$(1+2)$, $H\rightarrow\{H\}=h(1)+\lambda\{V(2)\}$, where $\{\ \}$ denotes an ensemble, $h(1)$ is a fixed one-body operator (or an ensemble) generating single-particle spectrum with average spacing $\Delta=1$, the $V(2)$ matrix elements variance is chosen to be unity and $\lambda$ is the interaction strength. As $\lambda\rightarrow\infty$ EGOE$(1+2)$ behaves as EGOE(2) and it is well known that for EGOE(2) in the dilute limit ($m\rightarrow\infty$, $N\rightarrow\infty$ and $m/N\rightarrow 0$) the ensemble averaged (smoothed) state densities approach Gaussian form [11]. For EGOE$(1+2)$ one can define two "quantum chaos" markers $\lambda_c$ and $\lambda_{F_k}$ so that for $\lambda>\lambda_c$ there is chaos in the sense that the level fluctuations start coming close to GOE fluctuations and for $\lambda>\lambda_{F_k}$ (note that $\lambda_c<\lambda_{F_k}$) one has the Gaussian form not only for the smoothed state densities but also for the strength functions [12]. Therefore, $\lambda>\lambda_{F_k}$ region is called the Gaussian domain. It should be noted that $\rho^H(E)$ will be Gaussian even below $\lambda<\lambda_{F_k}$, but with fluctuations approaching Poisson for $\lambda=0$ (for $\lambda=0$ the Gaussian form arises due to the action of the central limit theorem); see Figs. 2 and 3 ahead for examples.

Occupation numbers are given by the expectation values $\langle n_i\rangle^E$ of the number operators $n_i$. Then the single-particle entropy $S^{sp}(E)$ is defined by

$$S^{sp}(E)=-\sum_i \{\langle n_i\rangle^E \ln(\langle n_i\rangle^E)+(1-\langle n_i\rangle^E)\ln(1-\langle n_i\rangle^E)\}. \tag{1}$$

In order to derive an expression for $S^{sp}$ first a form for $\langle n_i\rangle^E$

 

is needed. Considering the linear response of $\rho^H(E)$ under the deformation $H \to H_\zeta = H + \zeta n_i$ it is easily seen that [13]

$$\langle n_i \rangle^E = -[\rho^H(E)]^{-1} \lim_{\zeta \to 0} \int_{-\infty}^{E} \frac{\partial \rho^{H_\zeta}(x)}{\partial \zeta} dx. \tag{2}$$

Note that under $H \to H_\zeta$, the single-particle energy $\epsilon_i \to \epsilon_i + \zeta$; without loss of generality, the single-particle energies $\epsilon_i$ are assumed to be zero centered. With $H$ represented by EGOE$(1+2)$, $H_\zeta$ for $\zeta$ small is also represented by EGOE $(1+2)$, and therefore the shape of $\rho^H(E)$ will be unchanged (from the Gaussian form) under the $\zeta$ deformation. Using this and applying Eq. (2) one gets

$$\langle n_i \rangle^E \overset{EGOE(1+2)}{\longrightarrow} \langle n_i \rangle^m + \langle n_i [H - \epsilon_H(m)] \rangle^m [E - \epsilon_H(m)]/\sigma_H^2(m). \tag{3}$$

In Eq. (3), $\epsilon_H(m) = \langle H \rangle^m$ and $\sigma_H(m) = \{\langle H^2 \rangle^m - [\epsilon_H(m)]^2\}^{1/2}$ are the centroid and width that define $\rho^H(E)$. The linear form (with respect to $E$) as given by Eq. (3) is seen in many EGOE$(1+2)$ and nuclear shell model calculations [6]. Just as with the state density, though the $\langle n_i \rangle^E$ smoothed form is well represented by Eq. (3), the fluctuations will be large for $\lambda < \lambda_c$; see Refs. [6,12], for examples. For the EGOE$(1+2)$ Hamiltonian $H = h(1) + \lambda V(2)$ one can consider $h(1)$ and $V(2)$ to be orthogonal in a well defined sense (see Ref. [12]) and then

$$\langle n_i [H - \epsilon_H(m)] \rangle^m = [m(N-m)/N(N-1)]\epsilon_i, \tag{4}$$

and also $\sigma_H^2(m) = \sigma_h^2(m) + \sigma_V^2(m)$; $\langle n_i \rangle^m = m/N$. Assuming that we have a uniform single-particle spectrum with spacing $\Delta = 1$, $\sigma_h^2(m) = [m(N-m)(N+1)/12]$ and $\sigma_H^2(m) = [m(N-m)(N+1)/12] + [m(m-1)(N-m)(N-m-1)N(N-1)/4(N-2)(N-3)]\lambda^2$; note that $\lambda$ is expressed in units of $\Delta$. Using, with $\rho(\epsilon)$ denoting single-particle density, $\int - -\rho(\epsilon) d\epsilon = [\Delta]^{-1} \int - - d\epsilon$, the sum in Eq. (1) is converted via Eq. (4) into an integral. Evaluating the integral and then expanding it in powers of $\hat{E} = [E - \epsilon_H(m)]/\sigma_H(m)$ gives a remarkably simple expression, when truncated to $\hat{E}^2$ term, for $\exp(S^{sp})$ divided by its maximum value,

$$\exp[S^{sp}(E) - S^{sp}_{max}] = \exp\left(-\frac{1}{2}\zeta^2 \hat{E}^2\right),$$

$$\zeta^2 = \sigma_h^2(m)/\sigma_H^2(m). \tag{5}$$

Note that the correlation coefficient $\zeta$ in Eq. (5) is the same as the one that enters in the EGOE$(1+2)$ formula for $S^{info}$ as given in Ref. [12], and we will return to it later. Using the expressions for $\sigma_h^2$ and $\sigma_H^2$, it is easily seen that in the dilute limit $\zeta^2 = [1 + 3m\lambda^2]^{-1}$. Figure 1 gives a comparison of Eq. (5) with numerical EGOE$(1+2)$ calculations for a system of $m = 6$ spin-less fermions in $N = 12$ single-particle states for $\lambda$ varying from 0.01 to 5. In this example, $\lambda_c \sim 0.05$ and $\lambda_{F_k} \sim 0.2$ [6,12]. For $\lambda \sim 0$, $\zeta \sim 1$ and therefore $\exp(S^{sp})$ is of Gaussian form as given by Eq. (5). As pointed out before,

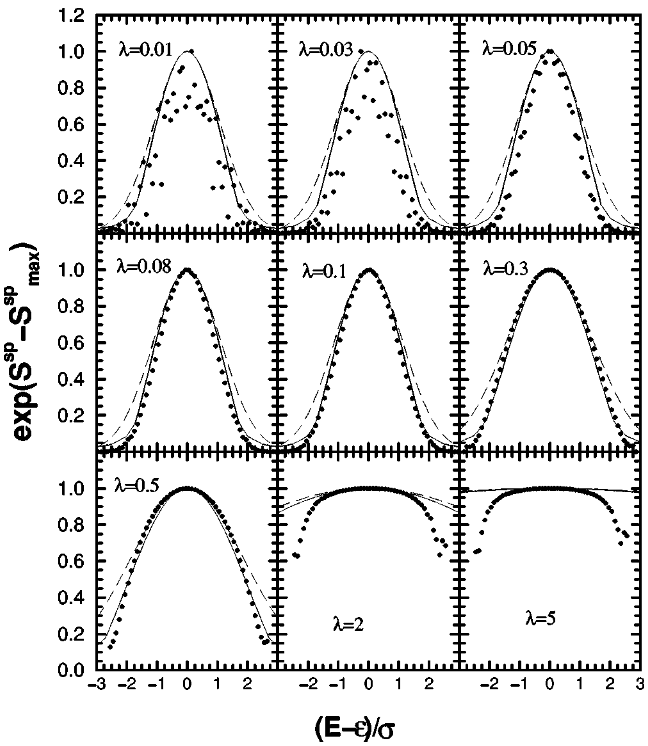


FIG. 1. Single-particle entropy $S^{sp}$ vs energy for a 25 member EGOE$(1+2)$ for various values of the interaction strength $\lambda$ in $\{H\} = h(1) + \lambda\{V(2)\}$ for a system of six fermions in 12 single-particle states; the matrix dimension is 924. The single-particle energies used in the calculations are $\epsilon_i = (i + 1/i), i = 1,2,\ldots,12$, just as in Ref. [6]. In the figures $\exp(S^{sp} - S^{sp}_{max})$ is plotted against $\hat{E} = (E - \epsilon)/\sigma$, where $\epsilon$ is the spectrum centroid and $\sigma$ is the width. The EGOE$(1+2)$ results are obtained by averaging over a bin size of 0.1 and the average values are shown in the figures as filled circles at the center of the bin. The dashed curves correspond to Eq. (5) and the continuous curves are obtained by combining to Eq. (6) with Eq. (1) as explained in the text.

here the fluctuations are expected to be large (for $\lambda \lesssim \lambda_c$) as seen in the figure. For $\lambda > \lambda_c$ (i.e., for $\lambda = 0.08$ and beyond) the fluctuations are small and Eq. (5) gives a good description of the numerical results. For $\lambda \gg \lambda_{F_k}$ (in Fig. 1 for $\lambda = 2,5$ cases) it is seen that $\zeta \to 0$ and then $\exp(S^{sp})$ approaches a constant. This can be seen also from Eq. (3) as in this case the occupancies are given just by the first term. It should be noted that the numerical results do deviate from Eq. (5) predictions for $|\hat{E}| \gtrsim 1.5$. Therefore the $\hat{E}^4$ correction to Eq. (5) is calculated but it is found give negligible contribution. Thus the corrections will not come by adding higher powers of $\hat{E}$ in Eq. (5) but by reexamining Eq. (3). Recognizing [14] that to a good approximation one can write $\rho^H(E)$ as a convolution, $\rho^H(E) = \rho^h \otimes \rho^V[E]$ ($\otimes$ denotes convolution) and then applying Eq. (2) gives [15]

$$\langle n_i \rangle^E = \langle n_i \rangle^m \rho^H_{n_i}(E)/\rho^H(E) = \left(\frac{m}{N}\right) \frac{\exp\left[-\frac{1}{2}\left(\frac{E - \epsilon_{n_i}(m)}{\sigma_H(m)}\right)^2\right]}{\exp\left[-\frac{1}{2}\left(\frac{E - \epsilon_H(m)}{\sigma_H(m)}\right)^2\right]}, \tag{6}$$

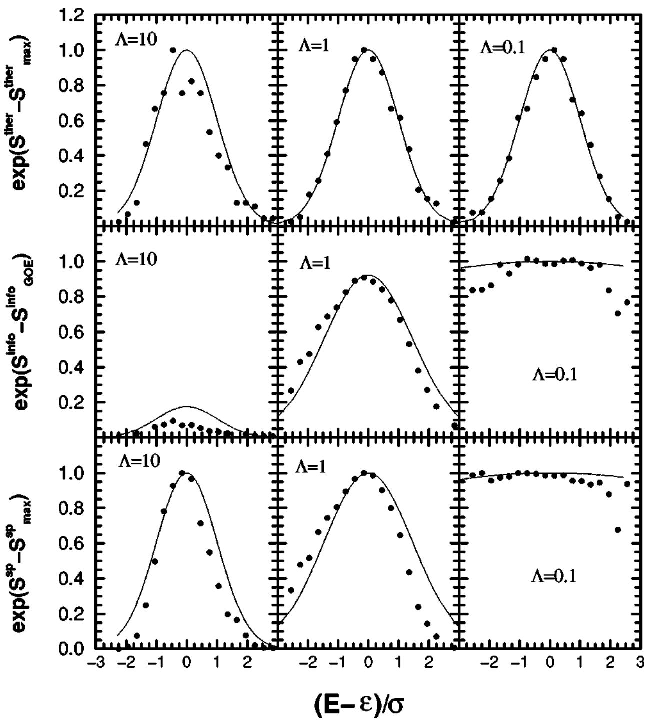


FIG. 2. Thermodynamic entropy $\exp(S^{ther}-S^{ther}_{max})$, information entropy $\exp(S^{info}-S^{info}_{GOE})$ and single-particle entropy $\exp(S^{sp}-S^{sp}_{max})$ vs $(E-\epsilon)/\sigma$ for the angular momentum $J=0$ and isospin $T=0$ levels in the nuclear shell model $(2s1d)^{m=8}$ space (matrix dimension is 325). The Hamiltonian $H=h(1)+V(2)$ is defined by Kuo's [20] two-body matrix elements $[V(2)]$ [20] and $^{17}$O single-particle energies $[h(1)\Leftrightarrow\epsilon_{d_{5/2}}=-4.15$ MeV, $\epsilon_{d_{3/2}}=0.93$ MeV, $\epsilon_{s_{1/2}}=-3.28$ MeV$]$. In the calculations, as described in the text, the diagonal matrix elements of the Hamiltonian in the $(2s1d)^{m=8,J=0,T=0}$ space are multiplied by $\Lambda$ and results for the three entropies are shown in the figure for $\Lambda=10$, 1, and 0.1. All the shell model calculations are carried out using the Rochester–Oak Ridge shell model code [21]. The shell model results are averaged over a bin size of 0.3 and the average values are shown in the figure as filled circles at the center of the bin. The continuous curves are the EGOE$(1+2)$ predictions as given by Eq. (5).

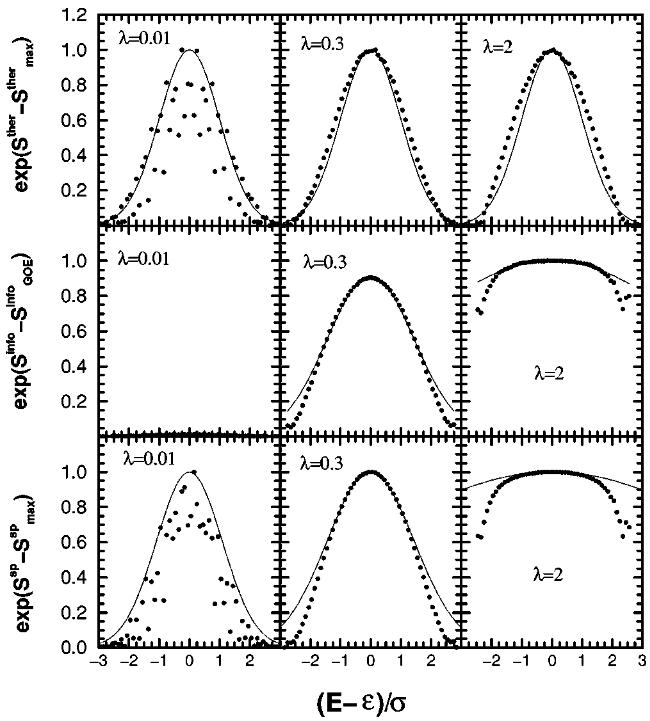


FIG. 3. Same as Fig. 2 but for three values of λ in the EGOE $(1+2)$ example in Fig. 1. The filled circles are EGOE$(1+2)$ results as in Fig. 1 and the continuous curves are the theoretical EGOE$(1+2)$ predictions as given by Eq. (5). Calculations are also carried out for a ten member 3432 dimensional EGOE$(1+2)$ with seven fermions in 14 single-particle states and the results are found to be close to the six fermion example shown in the figure.

where $\epsilon_{n_i}(m)-\epsilon_H(m)=\langle n_i[H-\epsilon_H(m)]\rangle^m/\langle n_i\rangle^m=[(N-m)/(N-1)]\epsilon_i$. Substituting Eq. (6) in Eq. (1), the sum in Eq. (1) can be converted into an integral as before. However, we could not simplify it any further. Therefore, the sum is evaluated numerically and then $\exp[S^{sp}(E)-S^{sp}_{max}]$ is calculated. These results are compared with numerical EGOE$(1+2)$ calculations in Fig. 1. It is clearly seen that Eqs. (6) and (1) give a very accurate description of the numerical results. It is worth pointing out that the convolution form for $\rho^H(E)$ used in deriving Eq. (6) is also employed recently in the study of the thermodynamics of chaotic systems [2,16]. Finally, as Eq. (5) gives a reasonable description of $S^{sp}$, in the following discussion Eq. (5) is employed.

Returning to Zelevinsky *et al.* [1], study of different definitions of entropies, nuclear shell model results with eight nucleons (see Fig. 2) are compared with numerical EGOE $(1+2)$ calculations (see Fig. 3) and also the theoretical forms . As pointed out before, with nonsingular one-body Hamiltonians $h(1)$ (see for example, Ref. [17]), the EGOE $(1+2)$ state density will be a Gaussian even for small values of λ. Then the exponential of $S^{ther}=\ln\rho^H(E)$ will be essentially a Gaussian for all λ values

$$\exp[S^{ther}(E)-S^{ther}_{max}]=\exp\left(-\frac{1}{2}\hat{E}^2\right). \tag{7}$$

The form for $S^{info}$ in terms of the correlation coefficient $\zeta$, valid in the Gaussian domain (and which can be extended to regions below $\lambda<\lambda_{F_k}$ as here $S^{info}$ will be very small compared to the GOE value), is given by [12]

$$\exp[S^{info}(E)-S^{info}_{GOE}]=\sqrt{1-\zeta^2}\exp\left(\frac{1}{2}\zeta^2\right)\exp\left(-\frac{\zeta^2\hat{E}^2}{2}\right). \tag{8}$$

All the EGOE$(1+2)$ results in Fig. 3 are well described by Eqs.(5), (7), and (8). More striking is that the EGOE$(1+2)$ results are in one to one correspondence with the nuclear shell model results in Fig. 2 (also see Fig. 3 in Ref. [1]). The example in Fig. 2 is for eight nucleons and in Ref. [1] a larger system with 12 nucleons was studied. However, the results are essentially same. In the shell model calculations (exactly as in Ref. [1]), the diagonal matrix elements in the many-particle Hamiltonian matrix are multiplied by a parameter $\Lambda$ and then $S$'s are studied as a function of $\Lambda$.

Then $\Lambda \rightarrow 0$ corresponds to $\lambda \rightarrow \infty$ in EGOE$(1+2)$ and similarly $\Lambda \gg 1$ corresponds to $\lambda \rightarrow 0$. Finally $\Lambda = 1$ corresponds to the actual nucleon-nucleon interaction used in the shell model and it is well known [18,6] that for this value one is in the Gaussian ($\lambda > \lambda_{F_k}$) domain. As seen from Fig. 3 and Eqs. (7), (8), and (5), $\zeta \sim 1$ for $\lambda \sim 0$ and then $S^{info} \sim 0$ but $S^{ther}$ and $S^{sp}$ are Gaussian in form. The same result is seen in the shell model results in Fig. 2 (for $\Lambda$ large). For $\lambda = 0.3$ (this is similar to $\Lambda = 1$ in the shell model) $\zeta \sim 0.7$, and then all the three entropies look similar. In other words in the chaotic Gaussian domain (but not for $\lambda$ very much greater than $\lambda_{F_k}$) one has thermalization in the sense that all different definitions of entropy coincide. Finally for $\lambda = 2$ (similar to very small value of $\Lambda$ in the shell model), $\zeta \sim 0$ and therefore $S^{info}$ and $S^{sp}$ approach their maximum values while $S^{ther}$ still retains the Gaussian form.

In conclusion $\exp[S^{info}(E) - S^{info}_{GOE}]$ changes from 0 to 1 as $\lambda$ goes from 0 to $\infty$. Similarly $\exp[S^{sp}(E) - S^{sp}_{max}]$ changes from Gaussian to 1 while $\exp[S^{ther}(E) - S^{ther}_{max}]$ is always a Gaussian. Thus all the three entropies will be approximately same for some intermediate values of $\lambda$. The best value appear to come from the condition that $\exp[S^{info}(E) - S^{info}_{GOE}] = 0.9$ at $\hat{E} = 0$ and this gives $\zeta^2 = 1/2$. The $\Lambda = 1$ in Fig. 2 and $\lambda = 0.3$ in Fig. 3 come very close to this situation. The critical $\lambda_c$ determined by $\zeta^2 = 1/2$ appear to be closely related to the duality issue in EGOE$(1+2)$ discussed recently by Jacquod and Varga [19]. Finally, the results in Ref. [1] are completely explained by Eqs. (5), (7), and (8) and it is established that they have their basis in EGOE$(1+2)$.

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