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Power spectrum analysis of the average–fluctuation density separation in interacting particle systems

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ABSTRACT

The power spectrum analysis using the Lomb–Scargle false alarm probability statistic shows a clear separation between the average and fluctuating parts of the state density in embedded two-body random matrix ensembles with a mean-field for both fermion and boson systems as well as in the nuclear shell model.

1. Introduction

The separation of averages and fluctuations in energy levels, transition strengths, etc., provides a physical basis for statistical spectroscopy of finite quantum systems with interactions such as nuclei, atoms and molecules [1]. These two distinct parts can then be studied separately [2]: the average properties using the spectral distribution methods of French [2–6] and fluctuations that follow the Gaussian Orthogonal Ensemble (GOE) of random matrices introduced by Wigner [7] (also the unitary ensemble GUE and symplectic ensemble GSE in some situations). Normally one uses the nearest neighbor spacing distribution (NNSD) and the Dyson–Mehta Δ_3 statistic [8] for establishing GOE fluctuations. Analysis using the nuclear data ensemble [9,10] gave first conclusive demonstration of GOE fluctuations in nuclei and now there exist other examples from a wide variety of quantum systems [11,12].

The GOE corresponds to ensembles of asymptotically large real-symmetric matrices which apart from rotational and time reversal invariance have no other specific properties of the Hamiltonian. In a many-particle system, GOE describes a situation in which all particles interact simultaneously. It is clear then that Hamiltonian (H) matrices, for an m particle system occupying N single particle states, are dominated by m-body interactions. However, the particle–particle interactions for systems such as nuclei, atoms, quantum dots, small metallic grains, etc., are, in general, two-body in character. This, together with numerical examples from nuclear shell model [13–16] and more recently for atoms [17] led to the introduction of two-body random ensembles (TBRE). For spinless fermion systems, with the two-particle H taken as GOE and then constructing the many-particle H matrix, with the m-particle basis states being direct products of single particle (sp) states, gives the Embedded Gaussian Orthogonal Ensemble of two-body interactions [EGOE(2)] in m-particle spaces. Similarly, for interacting boson systems, the embedded Gaussian orthogonal ensemble of two-body interactions can be defined and to distinguish these from those of fermion systems, they are denoted by BEGOE(2) [18]. One of the most significant features of Embedded ensembles for interacting particle systems is the separation of information re-

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garding energy levels (also for other observables) into averages and fluctuations. For fermion systems in the dilute limit ($m \to \infty$, $N \to \infty$, $m/N \to 0$) with EGOE(2) [1,19] and boson systems in the dense limit ($m \to \infty$, $N \to \infty$, $m/N \to \infty$) with BEGOE(2) [20], the nature of this separation is understood analytically using the binary correlation approximation. There are also numerical calculations [20,21] and shell model examples [1] that provide qualitative, though not quantitative, support to the EGOE(2) and BEGOE(2) analytical results.

By drawing an analogy between the energy spectrum and time series, the study of spectral fluctuations using a power spectrum analysis was introduced many years back by one of the authors (RJL) [22]. Recently, this has been emphasized by the Madrid group (Gómez and collaborators) [23–26] in terms of $1/f$-noise signature of quantum chaos. In the present work we estimate the power spectra of deviations between the smooth distribution functions and the exact one, using a normalized periodogram given by Lomb [27] and Scargle [28]. This technique, initially used for analyzing astronomical data, is quite powerful for finding and testing the significance of weak periodic signals in unevenly spaced data [28,29]. The Fortran subroutine [30] used for the evaluation of the Lomb–Scargle statistic F returns the maximum periodogram value and the value of F which estimates the significance of that maximum against the hypothesis of random noise. The frequency at which the maximum occurs is denoted by f_p and $\Lambda = (1-F)\times 100$ is a measure, in percentage, of the significance of the signal at f_p. Thus the power spectra of the deviations between the exact and smooth distribution functions can provide a 'quantitative measure' (Λ parameter) for the separation that exists between the smooth and fluctuating parts (in the past the r.m.s. deviation has been used; see Figs. 1–4 ahead).

Realistic Hamiltonians include, besides the two-body interactions $V(2)$, a mean field producing one-body part $h(1)$. Therefore, it is more realistic to consider [31] embedded ensembles of (1+2)-body Hamiltonians EGOE(1+2) and BEGOE(1+2) with $H = h(1) + \lambda\{V(2)\}$, where λ is the strength of the two-body interaction in units of average spacing of the sp levels defining $h(1)$. Note that $\{V(2)\}$ represents EGOE(2) or BEGOE(2). We have also considered fermions with spin 1/2 degree of freedom, i.e. EGOE(1+2)-s [32]; here the interaction will have two parts as the two particle spin $s = 0, 1$ and hence $H = h(1) + \lambda_0\{V^{s=0}(2)\} + \lambda_1\{V^{s=1}(2)\}$. The purpose of the present Letter is to apply the periodogram analysis to study the average–fluctuation separation in energy levels for EGOE(1+2), EGOE(1+2)-s, BEGOE(1+2) and a realistic nuclear shell model example for ^{24}Mg. Now we will give a preview.

Analytical results for level motion in dilute fermion and dense boson systems, obtained using the binary correlation approximation, are briefly discussed in Section 2. The periodogram method is discussed in Section 3 and results of the periodogram analysis of average–fluctuation separation for the four examples considered are presented in Section 4. Concluding remarks are given in Section 5.

2. Average–fluctuation separation in EGOE(2) and BEGOE(2)

Given a normalized state density $\rho(E)$, it is possible to expand it in terms of its asymptotic (or smoothed) form $\bar{\rho}(E)$ and the orthonormal polynomials $P_\mu(E)$ defined by the asymptotic density. In general, for $\bar{\rho}(E)$ a Gaussian, i.e. $\bar{\rho}(E) = \rho_{\mathcal{G}}(E) = (\sqrt{2\pi}\sigma)^{-1}\exp(-(E-E_c)^2/2\sigma^2)$ and using the Gram–Charlier (GC) expansion we have,

$$\rho(E) = \rho_{\mathcal{G}}(E)\left\{1 + \sum_{\zeta\geqslant 3}(\zeta!)^{-1} S_\zeta He_\zeta(\hat{E})\right\}. \tag{1}$$

In Eq. (1), $\hat{E} = (E-E_c)/\sigma$ is the standardized energy variable. The centroid $E_c = \langle H\rangle^m$ and the variance $\sigma^2 = \langle H^2\rangle^m - E_c^2$ of the Gaussian $\rho_{\mathcal{G}}$ are the same as that of ρ. He_ζ are Hermite polynomials and S_ζ are, in principle, related to higher moments of the state density $\rho(E)$. We will apply Eq. (1) to EGOE(2) and BEGOE(2) by noting that for fermions in the dilute limit and bosons in the dense limit $\bar{\rho}(E) = \rho_{\mathcal{G}}(E)$. Thus, at this stage distinction between Boson and Fermion systems is not important. Since S_ζ's change from member to member of the EGOE(2) or BEGOE(2) ensemble, one can treat them as independent zero-centered random variables,

$$\overline{S_\zeta} = 0, \qquad \overline{S_\zeta S_{\zeta'}} = 0 \quad \text{for } \zeta \neq \zeta'. \tag{2}$$

This is consistent with the result $\bar{\rho}(E) = \rho_{\mathcal{G}}(E)$ where the 'bar' denotes an ensemble average. Each ζ term in Eq. (1) represents an excitation 'mode' and the wavelength of the modes is proportional to ζ^{-1}. The distribution function $F(E)$, the integrated version of $\rho(E)$, is given by $F(E) = d\int_{-\infty}^{E}\rho(E')\,dE'$ where d is the dimensionality. Deviation of a given level with energy E from its smoothed (with respect to the ensemble) counterpart $\bar{E}$ gives the level motion. In terms of $F(E)$ and the local mean spacing $\overline{D(E)}$, we have $\delta E = E - \bar{E} = [F(E) - \overline{F(E)}]\overline{D(E)}$. Then the variance of the level motion is given by the ensemble average of $\frac{(\delta E)^2}{\overline{D(E)}^2}$. Using Eq. (1) and adding centroid and variance fluctuations [then the summation in Eq. (1) extends to $\zeta \geqslant 1$], we have easily

$$\begin{aligned}\frac{\overline{(\delta E)^2}}{\overline{D(E)}^2} &= \overline{\left[F(E) - \overline{F(E)}\right]^2} \\ &= d^2\sigma^2\left[\rho_{\mathcal{G}}(E)\right]^2\left\{\sum_{\zeta\geqslant 1}(\zeta!)^{-2}\overline{S_\zeta^2}\left[He_{\zeta-1}(\hat{E})\right]^2\right\}.\end{aligned} \tag{3}$$

Therefore we need $\overline{S_\zeta^2}$ for EGOE(2) and BEGOE(2) and they are related to the co-variances $\Sigma_{p,q} = \overline{\langle H^p\rangle\langle H^q\rangle} - \overline{\langle H^p\rangle}\,\overline{\langle H^q\rangle}$. Now applying the so-called binary correlation approximation, first used by Wigner for GOE, it can be shown that [1,19,20], for m fermion or bosons in N sp states,

$$\overline{S_\zeta^2} \xrightarrow[\text{dilute limit}]{\text{EGOE(2)}} 2\zeta\binom{m}{2}^{2-\zeta}\binom{N}{2}^{-2}, \qquad \overline{S_\zeta^2} \xrightarrow[\text{dense limit}]{\text{BEGOE(2)}} 2\zeta\binom{N}{2}^{-\zeta}. \tag{4}$$

Then the final result for level motion in fermion systems in the dilute limit is [1,19],

$$\begin{aligned}\frac{\overline{(\delta E)^2}}{\overline{D(E)}^2} &\overset{\text{EGOE(2)}}{=} \binom{N}{m}^2\binom{m}{2}^2\left[\rho_{\mathcal{G}}(E)\right]^2 \\ &\quad\times\left\{\sum_{\zeta\geqslant 1}(\zeta!)^{-2}2\zeta\binom{m}{2}^{2-\zeta}\binom{N}{2}^{-2}\left[He_{\zeta-1}(\hat{E})\right]^2\right\} \\ &\xrightarrow{\hat{E}=0} \frac{1}{\pi}\binom{N}{m}^2\binom{m}{2}\binom{N}{2}^{-2} \\ &\quad\times\left\{1 + \frac{1}{12}\binom{m}{2}^{-2} + \frac{1}{320}\binom{m}{2}^{-4} + \cdots\right\}.\end{aligned} \tag{5}$$

Similarly for boson systems in the dense limit the result is [20],

$$\begin{aligned}\frac{\overline{(\delta E)^2}}{\overline{D(E)}^2} &\overset{\text{BEGOE(2)}}{=} \binom{N+m-1}{m}^2\binom{m}{2}^2\binom{N}{2}^{-2}\left[\rho_{\mathcal{G}}(E)\right]^2 \\ &\quad\times\left\{\sum_{\zeta\geqslant 1}(\zeta!)^{-2}2\zeta\binom{N}{2}^{-\zeta}\left[He_{\zeta-1}(\hat{E})\right]^2\right\} \\ &\xrightarrow{\hat{E}=0} \frac{1}{\pi}\frac{\binom{N+m-1}{m}^2}{\binom{N}{2}} \\ &\quad\times\left\{1 + \frac{1}{12}\binom{N}{2}^{-2} + \frac{1}{320}\binom{N}{2}^{-4} + \cdots\right\}.\end{aligned} \tag{6}$$