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Data-adaptive unfolding of nonergodic spectra: Two-Body Random Ensemble

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Abstract. The statistics of spectral fluctuations is sensitive to the unfolding procedure that separates global from local properties. Previously, we presented a parameter-free and data-adaptive unfolding method that we demonstrated to be highly effective for standard random-matrix ensembles from Random Matrix Theory (RMT). More general ensembles often break the ergodicity property, which leads to ambiguities between individual-spectrum averaged and ensemble-averaged fluctuation measures. Here, we apply our data-adaptive unfolding to a nonergodic Two-Body Random Ensemble (TBRE). In the present approach, both fluctuation measures can be calculated simultaneously within the same unfolding step, and possible arbitrariness introduced by traditional unfolding procedures are avoided.

1. Introduction

Standard matrix ensembles from Random Matrix Theory (RMT) [1], such as the Poisson ensemble and the Gaussian Orthogonal Ensemble (GOE), have been enormously successful in the modelling of the fluctuations of excitation spectra of quantum systems, that are regular and chaotic, respectively [2]. Recently, RMT has been applied as well in multivariate statistics to model the fluctuations of eigenspectra of correlation matrices of complex systems [3]. However, this RMT modelling is not completely realistic because many-body systems are effectively governed by one- and two-body forces, while canonical RMT implicitly assumes many-body forces between the constituents [4]. A stochastic modelling of the one- and two-body interaction yields a much smaller number of independent random variables, e.g., when a two-body random ensemble (TBRE) [5, 6], or a k -body embedded Gaussian ensembles (EGE) [7] is used. These more general ensembles introduce new statistical features that are absent in standard RMT, such as Gaussian instead of semicircular level densities [5] and nonergodicity [4, 5, 8, 9].

One of the difficulties in the statistical study of spectral fluctuations is the *unfolding* procedure which serves to separate the global level density density $\bar{\rho}(E)$ from the local fluctuations



$\tilde{\rho}(E) = \rho(E) - \bar{\rho}(E)$. The unfolding procedure is not trivial, and statistical results can be sensitive to the unfolding applied [10, 11]. In principle, the mean level density $\bar{\rho}$ can be determined as the average over all spectra of the ensemble, or – alternatively – as a running average over each spectrum individually. If the ensemble under study is *ergodic*, then the resulting *ensemble averaged* and *individual-spectrum averaged* fluctuation statistics are equivalent. The breaking of ergodicity creates an ambiguity in the characterization of the spectral fluctuations as the two measures lead to different results. In this case, the ensemble average is not representative for the individual realizations of the spectrum and an individual-spectrum unfolding is more appropriate [4, 5, 8]. When a correct unfolding is applied to a nonergodic ensemble that is chaotic, then spectral fluctuations of the GOE-type should result [9].

Previously, in Refs. [12, 13, 14], we proposed an unfolding method that is data-adaptive and model-free, and that expresses a spectrum in an exact way as the superposition of global and fluctuation normal modes. In this way, possible artifacts introduced by standard unfolding techniques are avoided. We presented two versions of the method. A first version is based on Singular Spectrum Analysis (SSA), which is a univariate time-series technique, and which can be applied to individual spectra to calculate individual-spectrum averaged statistics [12]. The SSA-based method includes one free parameter, but we demonstrated that the statistical results are parameter independent. The second version is based on a multivariate time-series technique, Singular Value Decomposition (SVD) [13], which is applied to an ensemble of spectra. The SVD-based method is preferable as it does not include any parameters. Also, within this approach, both spectrum-averaged and ensemble-averaged fluctuation statistics can be calculated [14]. In Ref. [12], an SSA-based data-adaptive unfolding was successfully applied to the individual spectra of a nonergodic TBRE ensemble. The purpose of the present contribution is to study an SVD-based data-adaptive unfolding of a TBRE ensemble.

2. SVD-based data-adaptive unfolding

Following the discussion of Ref. [13, 14], we consider an ensemble of $m = 1 \dots M$ excitation spectra $E^{(m)}(n)$, where each spectrum consists of $n = 1 \dots N$ levels. Each spectrum can be accommodated in a row of the $M \times N$ dimensional matrix \mathbf{X} , which is interpreted as a multivariate time series,

$$\mathbf{X} = \begin{pmatrix} E^{(1)}(1) & E^{(1)}(2) & \dots & E^{(1)}(N) \\ E^{(2)}(1) & E^{(2)}(2) & \dots & E^{(2)}(N) \\ \vdots & \vdots & \ddots & \vdots \\ E^{(M)}(1) & E^{(M)}(2) & \dots & E^{(M)}(N) \end{pmatrix}. \quad (1)$$

Singular Value Decomposition (SVD) decomposes \mathbf{X} in a *unique* and *exact* way as,

$$\mathbf{X} = \mathbf{U}\mathbf{\Sigma}\mathbf{V}^T = \sum_{k=1}^r \sigma_k \mathbf{X}_k = \sum_{k=1}^r \sigma_k \vec{u}_k \vec{v}_k^T, \quad (2)$$

where $\mathbf{\Sigma}$ is an $M \times N$ -dimensional matrix with only diagonal elements which are ordered *singular values* or weights $\sigma_1 \geq \sigma_2 \geq \dots \geq \sigma_r$, with $r \leq \text{Min}[M, N] = \text{rank}(\mathbf{X})$. The vectors \vec{v}_k are orthonormal, and correspond to the k th columns of the $N \times N$ -dimensional matrix \mathbf{V} . They are *normal modes*, and they constitute a basis for the row space of \mathbf{X} . The vectors \vec{u}_k are orthonormal as well, corresponding to the k th columns of the $M \times M$ -dimensional matrix \mathbf{U} , and can be interpreted as the associated *projection coefficients*. The elementary matrices $\mathbf{X}_k = \vec{u}_k \vec{v}_k^T \equiv \vec{u}_k \otimes \vec{v}_k$ are calculated from the outer product of \vec{u}_k and \vec{v}_k . In this way, any

matrix row of \mathbf{X} containing a particular excitation spectrum $E^{(m)}(n)$ can be written as,

$$E^{(m)}(n) = \sum_{k=1}^r \sigma_k U_{mk} \vec{v}_k^T(n). \quad (3)$$

The square of a singular value or weight gives a *partial variance*, $\lambda_k = \sigma_k^2$, which is the fraction of the total variance $\lambda_{\text{tot}} = \sum_{k=1}^r \lambda_k$ of the multivariate time series \mathbf{X} carried by the normal mode \vec{v}_k .

A first result of Ref. [13] is that the main feature of a typical energy sequence $E(n)$ is a dominant monotonous trend $\bar{E}(n)$, whereas the superposed fluctuations $\tilde{E}(n) = E(n) - \bar{E}(n)$ are usually orders of magnitude smaller. Consequently, the global properties of a spectrum are represented by non-oscillating normal modes \vec{v}_k associated to the first few $k = 1, \dots, n_T$ dominant partial variances λ_k in the so-called *scree diagram* of ordered partial variances, which can be distinguished easily from the much smaller higher-order partial variances λ_k with $k = n_T + 1, \dots, r$ corresponding to oscillating normal modes \vec{v}_k associated to the fluctuations.

Another result from Ref. [13] is that when the data-adaptive unfolding of Eq. (2) is applied to the standard Poisson or GOE matrix ensembles, the part of the scree diagram associated to the fluctuation normal modes obeys the power law,

$$\lambda_k \propto 1/k^\gamma, \quad (4)$$

indicating that the long-range correlations of the fluctuations are scale invariant (fractal). The exponent γ characterizes the *rigidity* of the fluctuations, with $\gamma = 2$ in the case of soft spectra (Poisson), and $\gamma = 1$ in the case of rigid spectra (GOE). On the other hand, any particular spectrum from the ensemble can be unfolded separately using Eq. (3), after which its individual fluctuations can be studied with, e.g., Fourier spectral analysis. In the case of the standard random-matrix ensembles, the Fourier power spectrum of the fluctuations of the individual eigenspectra also obeys a power law,

$$P(f) \propto 1/f^\beta, \quad (5)$$

with $\beta = \gamma = 2$ (Poisson) and $\beta = \gamma = 1$ (GOE), such that the scale invariance property does not seem to depend on the particular basis used for the decomposition. In Ref. [14], it was argued that Eq. (4) can be interpreted as an ensemble-averaged fluctuation measure, because it quantifies the scaling properties of the normal modes in common to all the spectra of the ensemble, whereas Eq. (5) was interpreted as an individual-spectrum averaged fluctuation measure. Note that within the present SVD-based approach, both measures can be calculated within one and the same unfolding procedure. In contrast, in the traditional approach, each measure is obtained after a separate unfolding procedure which makes a consistent comparison between both measures difficult (see, e.g., [4]).

3. Two-Body Random Ensemble (TBRE)

In the present contribution, we consider an ensemble of theoretical excitation spectra for the ^{48}Ca atomic nucleus. The spectra are calculated with a nuclear shell-model code, based on ANTOINE [20], and using random interactions (TBRE [5, 21]). The nucleus ^{48}Ca is an obvious choice to study within the nuclear-shell model framework, because an inert ^{40}Ca core can be assumed, and calculations can be carried out in the full neutron fp shell. The level fluctuations of ^{48}Ca have been thoroughly studied in literature and have been found to correspond with GOE

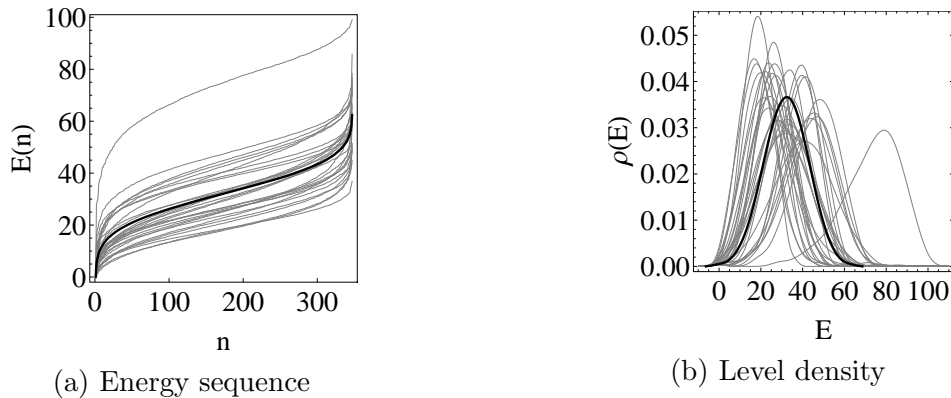


Figure 1. TBRE ensemble of $M = 30$ spectra, each with $N = 347$ levels. (a) Energy sequences $E^{(m)}(n)$ with $n = 1, \dots, N$ and $m = 1, \dots, M$. (b) Level densities $\rho(E)$. It can be appreciated that the ensemble mean (thick black curve) is not representative for the individual realizations of the spectrum (gray curves).

predictions [15, 16, 17, 18, 19], which permits to verify the validity of the present SVD unfolding method. Fluctuation studies must be applied to levels with the same quantum numbers; we arbitrarily choose the $J^\pi = 0^+$ subspectrum. The ensemble consists of $m = 1, \dots, M$ energy sequences $\{E^{(m)}(n), n = 1, \dots, N\}$ with $N = 347$ and $M = 30$, see Fig. 1. Shown are the energy sequences $E(n)$ (panel a) and also the level densities $\rho(E)$ (panel b). Note that the level densities have a gaussian shape instead of obeying the semicircle distribution typical for GOE ensembles. It can be seen that the ensemble average is not representative for the individual realizations of the excitation spectrum, which is an indication of the nonergodicity property of this ensemble [4, 5]. To take into account only the bulk (central part) of the spectrum when performing the SVD-based unfolding procedure, 10% of the lower and upper levels will be discarded. In Ref. [12], when the SSA-based data-adaptive unfolding was applied to the individual spectra of this TBRE ensemble, a scree diagram and Fourier power spectrum were obtained that obey the power laws of Eq. (4) and Eq. (5) with exponents $\gamma \approx \beta \approx 1$, indicating the expected GOE-type fluctuations, in confirmation with results from other authors [5, 21].

4. Results

Applying the SVD-based data-adaptive unfolding of Eq. (2) to the TBRE ensemble of Fig. 1, a scree diagram of ordered partial variances λ_k is obtained, where λ_k with $k = 1, \dots, 3$ are orders of magnitude larger than the higher-order λ_k , see Fig. 2(a). Inspection of the associated normal modes \vec{v}_k , confirms that \vec{v}_k with $k = 1, \dots, 3$ do not oscillate, whereas the higher-order normal modes \vec{v}_k do oscillate, see Fig. 2(b). The former suggests that the global spectral properties of the TBRE ensemble are described by the first $n_T = 3$ normal modes. The higher-order partial variances λ_k with $k = n_T + 1, \dots, r$ follow the power law of Eq. (4) with $\gamma \approx 1.83$, which is much closer to the Poisson limit than to the GOE limit, and which is in contradiction with the result $\gamma \approx 1$ from Ref. [12]. This result seems to confirm that, in the case of nonergodic ensembles, the ensemble-averaged fluctuation measure of the power law of Eq. (4) of the scree diagram is not reliable. The close-to Poissonian statistics appears to indicate that the normal modes \vec{v}_k are rather uncorrelated. To check this idea, we consider the participation ratio $\text{PR}(k)$,

$$\text{PR}(k) = 1 / \sum_{m=1}^M U_{km}^2, \quad (6)$$

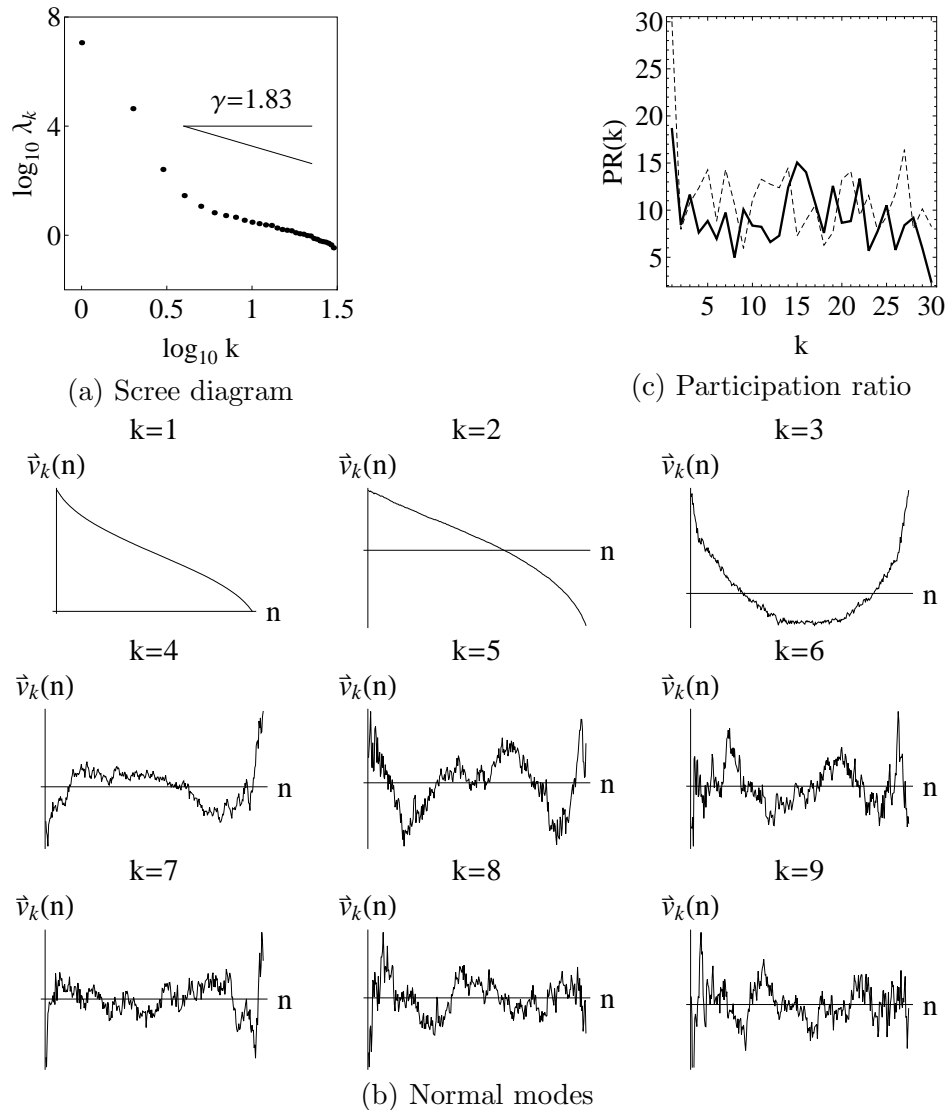


Figure 2. SVD decomposition of the ensemble of TBRE spectra of Fig. 1. (a) Scree diagram of ordered partial variances λ_k , where the λ_k with $k = 1, \dots, n_T$ describes the global spectral properties, the λ_k with $k = n_T + 1, \dots, r$ obey the power law of Eq. (4) with $\gamma = 1.83$ and describes the local spectral properties. (b) First 9 normal modes \vec{v}_k . (c) Participation ratio $PR(k)$ of the normal modes \vec{v}_k of the TBRE ensemble (thick curve) compared to an equivalent GOE ensemble (dashed curve).

which gives the number of spectra of the TBRE ensemble to which the normal mode \vec{v}_k significantly contributes [22]. In Fig. 2(c), the participation ratio $PR(k)$ of the TBRE ensemble is compared with the participation ratio of a GOE ensemble with the same dimensions M and N . Overall, it can be appreciated that the normal modes \vec{v}_k contribute to a larger number of spectra in the ergodic GOE case than in the nonergodic TBRE case. It can be appreciated, however, that the most important difference resides in the first dominant normal mode \vec{v}_1 , which contributes to all $M = 30$ spectra in the GOE case, and to only two thirds of the spectra in the TBRE case. As each specific normal mode does contribute to some spectra and does not contribute to some other spectra, the set of normal modes partially decorrelates, and their

scaling properties deviates towards Poisson statistics.

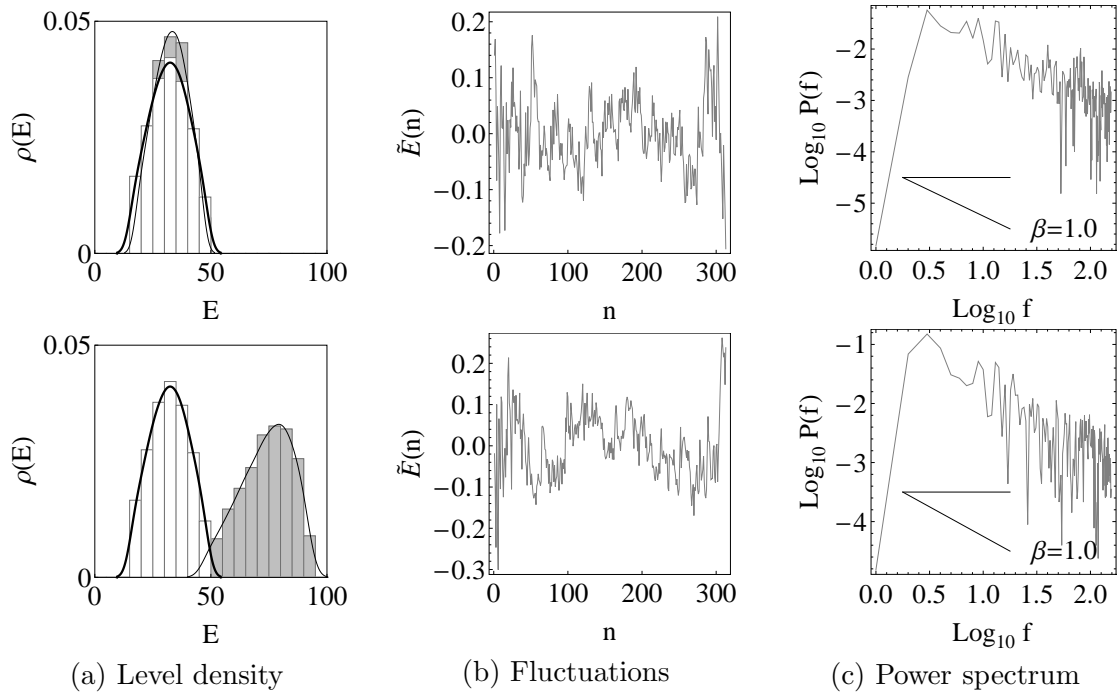


Figure 3. Data-adaptive unfolding of the TBRE ensemble of Fig. 1. Results of the unfolding are shown for two different spectra; one spectrum lies close to the ensemble average (upper row) and the other spectrum lies far from the ensemble average (lower row). (a) Empirical level density of the individual spectrum (gray histogram) compared to the ensemble average (white histogram); compared to the data-adaptive global level density $\rho(\bar{E})$ for the realization (thin curve) and for the ensemble average (thick curve). (b) Fluctuations of the realization. (c) The Fourier power spectrum of the fluctuations of the realization behaves as the power law of Eq. (5) with $\beta = 1$.

Using the expression of Eq. (3), each separate spectrum can be expressed exactly as a weighted sum of normal modes, such that also an individual-spectrum averaged fluctuation measures can be calculated. The global part of an individual spectrum is given by [13],

$$\bar{E}^{(m)}(n) = \sum_{k=1}^{n_T} \sigma_k U_{mk} \vec{v}_k(n), \quad (7)$$

and the local fluctuating part can be expressed as [13],

$$\tilde{E}^{(m)}(n) = \sum_{k=n_T+1}^r \sigma_k U_{mk} \vec{v}_k(n). \quad (8)$$

In Fig. 3, two specific spectra from the ensemble are represented. The first spectrum is selected from a region close to the ensemble average, and the second spectrum is chosen far from the ensemble average. Shown are (a) the histogram of the levels of the spectrum compared to the SVD-based data-adaptive global level density $\rho(\bar{E})$, (b) the local fluctuations $\tilde{E}(n)$, and (c) the corresponding Fourier power spectrum $P(f)$. It can be appreciated that the Fourier power spectrum of the fluctuations of the individual spectra obeys the power law of Eq. (5) with exponent $\beta \approx 1$, in correspondence with the results with SSA-based data-adaptive unfolding [12], and in correspondence with results from other authors using traditional unfolding [5, 21].

5. Conclusion

In the present contribution, we applied a SVD-based data-adaptive unfolding technique that we first presented for standard ergodic random-matrix ensembles from RMT to a nonergodic TBRE ensemble. Ensemble averaged and individual-spectrum averaged statistics can be calculated in a parameter-free and consistent way within the same unfolding procedure. In a forthcoming publication, we will apply the SVD-based unfolding to a random-matrix model with tunable nonergodicity to study its effect on the statistical properties [23].

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