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We analyze the fluctuation properties of nuclear energy levels and widths with new spectrally averaged measures. A remarkably close agreement between the predictions of random-matrix theories and experiment is found.

[Fluctuation properties of energy levels, width fluctuations, level repulsion, random matrices, neutron resonances]

1. Introduction

This paper deals with the current status of the random matrix theories with regard mainly to the nuclear energy level fluctuations i.e. departures from spectral uniformity, and also to widths fluctuations. Specifically the question is how well the ensemble results agree with experiment. And if the agreement is good, then : what is the source of this agreement and what limits can one impose on the mechanisms which affect the fluctuations. We are mainly concerned here with the first question for which we rely for the most part on our recent work[1]. We refer only briefly to the latter two questions for which also the answers are emerging.

The nuclear data relevant for fluctuation studies consists of slow-neutron resonances of medium and heavy nuclei and also of proton resonances of some light nuclei. Most of the neutron data come from systematic measurements of total neutron cross-sections performed at Columbia during the sixties and early seventies. There are also measurements in which the spin of the levels are measured directly. These include mainly (n,γ) measurements performed at Geel, Livermore and Oak Ridge. Besides the neutron measurements, detailed nuclear resonance parameters have been extracted from high resolution inelastic proton scattering experiments performed at Duke.

The principal random matrix model, valid for space rotation and time reversal invariant systems, is Wigner's Gaussian Orthogonal Ensemble (GOE), consisting of asymptotically large real symmetric matrices, in which the distinct matrix elements are distributed independently with essentially the same zero-centered Gaussian law. For energy levels the main predictions are due to Dyson and Mehta[2]. The close-lying levels behave as if they are repelling each other and the distant ones display a long range order, the resultant spectral rigidity being then akin to a crystalline structure. For widths the model predicts a χ^2-distribution known after the names of Porter and Thomas[3]. The early theoretical work in the subject is reviewed in Refs [4-6]. For later developments as well as upto-date references see Ref.[7].

The GOE predictions are very sensitive to spurious and missing levels, especially for energy level fluctuations, imposing stringent conditions on the quality of data. Ideally the observed level sequence should be pure (all levels should have the same spin and parity) and complete (no missing level). Because of this, while the main GOE predictions have been known for almost two decades, good quality data required to test the model have come relatively recently. Earlier analyses of individual level sequences indicate "overall good agreement" between theory and experiment ; see Ch.VI of Ref.[7] for a review.

The present analysis makes much sharper comparisons between theory and experiment than the previous ones. The main reason for this improvement is not due to the additional data of the last few years, but rather to making better use of the theory when compared with experiment. Indeed, there are two disconcerting features in the previous analyses : the predictions of the theory have not been tested in a systematic way nor much attention has been paid to sample size effects. We resolve these difficulties here. We ask : what features of the theory are observed in the data and with what accuracy. We attempt to test directly the (fundamental) k-level correlation functions which are essentially the joint probability functions and of which the two level properties are the most significant. We go on to other fluctuation measures (which in fact derive from the correlation functions) so as to improve the statistical significance of the testing procedure. Moreover, since the theory is parameter-free, we combine all the data into a nuclear data ensemble (NDE) of approximately 1700 levels, this improving the statistics even more dramatically. Our main conclusion is that the agreement between theory and experiment is remarkably good.

Some comparison between theory and experiment is also made for widths, although in this case conclusions are less significant because the theoretical distribution itself has been used to a large extent to make spin and parity assignment of the levels.

In the next section we review the GOE predictions for the energy levels and in section 3 we present the results of comparison with the NDE. Section 4 deals with width fluctuations. The concluding section discusses the implications of the agreement.

2. GOE Predictions for the Energy Levels

Dyson's[2] k-level cluster functions* $Y_k(k\geq 1;Y_1\equiv 1)$ provide a natural hierarchy for energy level fluctuation studies. Essentially these are the k-level correlation functions, viz the joint-probability densities of observing k levels at given positions, from which the lower order correlation effects have been subtracted out. In particular $(1-Y_2(r))dr$ gives the probability of observing a level in an infinitesimal interval dr

*For a random variable W, we denote its ensemble average by $\bar{W}$ and its ensemble variance $(W-\bar{W})^2$ by Var W. Note, moreover, that we are considering spectra normalized to unit local average spacing.

at a distance r from a given level. These functions are designed in such a way that for the Poisson ensemble, in which the energy levels are chosen randomly in a given interval, the Y_k are all zero for k>1.

For GOE[5,6]

$$Y_2(r) = \left(\frac{\sin\pi r}{\pi r}\right)^2 + \left(\int_r^\infty \frac{\sin\pi r'}{\pi r'}\,dr'\right)\frac{d}{dr}\left(\frac{\sin\pi r}{\pi r}\right), \qquad (1)$$

which is normalized to a total unit integral. It has the value unity at r=0 implying level repulsion and goes to zero as $(\pi r)^{-2}$ for large r(>1) implying spectral rigidity. The latter aspect is more apparent from the number variance[2,7] $\Sigma^2(\bar{n})$, namely the variance of the number statistic n, the number of levels in a given interval of length $\bar{n}$:

$$\Sigma^2(\bar{n}) = \bar{n} - 2\int_0^{\bar{n}} (\bar{n}-r)Y_2(r)dr$$

$$= \frac{2}{\pi^2}\left\{\ell n(2\pi\bar{n})+\gamma+1+\frac{1}{2}[\mathrm{Si}(\pi\bar{n})]^2 - \frac{\pi}{2}\mathrm{Si}(\pi\bar{n}) - \cos(2\pi\bar{n}) - \mathrm{Ci}(2\pi\bar{n}) + \pi^2\bar{n}\left[1-\frac{2}{\pi}\mathrm{Si}(2\pi\bar{n})\right]\right\}$$

$$\xrightarrow{\bar{n}\gg 1} \frac{2}{\pi^2}\left\{\ell n(2\pi\bar{n}) + \gamma + 1 - \frac{\pi^2}{8}\right\}. \qquad (2)$$

Note that its value is ∼ unity for $\bar{n}$=100 and even for $\bar{n} \sim 10^6$ the fluctuation is not more than a couple of levels. This should be compared with $\Sigma^2(\bar{n})=\bar{n}$ for the Poisson ensemble.

Another measure of the spectral rigidity is the Δ_3-statistic of Dyson and Mehta[2]. It measures, for a fixed interval $[x,x+\bar{n}]$, the least square deviation of the staircase N(E), the number of levels with energy less than or equal to E, from the best straight line fitting it :

$$\Delta_3(\bar{n};x) = (1/\bar{n}) \min_{A,B} \int_x^{x+\bar{n}} (N(E)-AE-B)^2 dE \quad . \qquad (3)$$

Its ensemble average is related to Σ^2, and hence to Y_2, by[9]

$$\bar{\Delta}_3(\bar{n}) = (2/\bar{n}^4)\int_0^{\bar{n}} (\bar{n}^3 - 2\bar{n}^2 r + r^3)\,\Sigma^2(r)\,dr \quad , \qquad (4)$$

which may be integrated numerically, or for $\bar{n}$>15 one may use[2] $\bar{\Delta}_3 \simeq \pi^{-2}\,\ell n\,\bar{n} - 0.007$ with good accuracy. Again, in comparison with the Poisson value $\bar{\Delta}_3=\bar{n}/15$, the spectrum is seen to exhibit a long range order. (Note that because of stationarity[10] the ensemble properties are independent of x, the position of the interval).

Usually the most one can hope for is to test the theory for the two level functions and its integrals such as Σ^2 and $\bar{\Delta}_3$. However from a very long sequence of levels or from a collection of many short sequences as is the case for nuclear spectra, it may be possible to observe some higher-than-two level effects as well. Moreover the higher order functions are needed for the calculation of the sample errors of the testing procedure ; thus for example for testing two-point measures one needs to know the k-level functions for k≤4. Although all cluster functions have been evaluated for GOE[11], very few analytic results are available for higher-than-two-point measures. For properties related to Y_k with k>2, we rely mostly on Monte Carlo results that we have obtained from a sample, adequate for our purpose, of 100 GOE matrices of dimensionality 300.

Some examples of higher-than-two-level measures are provided by the distributions and correlation properties of the Δ_3 as well as the number (n) statistics. In this paper some results for Δ_3 are considered (see Fig.2c for Var Δ_3 and Figs.3a,3b for the Δ_3 distribution for $\bar{n}$=10,20). For very large $\bar{n}$,Var Δ_3 approaches[2] the value .011 which should be compared with the Poisson result Var $\Delta_3 = (1+11\bar{n}/30)\bar{n}/210$. Once again it is seen that the fluctuations are small for GOE.

In order to make optimal use of an observed spectrum, we introduce spectral averaged quantities. Consider a sequence containing (p+1) levels. For a statistic $W(\bar{n};x)$ defined in an interval of length $\bar{n}$ at x, the spectral average

$$\langle W(\bar{n})\rangle_p = (p-\bar{n})^{-1}\int_x^{x+(p-\bar{n})} W(\bar{n},y)\,dy \qquad (5)$$

is an estimator of $\bar{W}(\bar{n})$. The variance of $\langle W\rangle_p$, which is the square of the sample error, is also given by the theory :

$$\mathrm{Var}\,\langle W(\bar{n})\rangle_p \equiv \overline{\langle W(\bar{n})\rangle_p^2} - \overline{\langle W(\bar{n})\rangle_p}^2$$

$$= \frac{2\,\mathrm{Var}\,W(\bar{n})}{(p-\bar{n})^2}\int_0^{(p-\bar{n})}(p-\bar{n}-r)C(r;\bar{n})dr$$

$$\simeq \frac{2\,\mathrm{Var}\,W(\bar{n})}{(p/\bar{n})}\int_0^1 C(\lambda\bar{n};\bar{n})d\lambda \quad , \qquad (6)$$

where $C(r;\bar{n})$ is the autocorrelation function of W :

$$C(r;\bar{n}) = (\mathrm{Var}\,W(\bar{n}))^{-1}\left\{\overline{W(\bar{n};x)W(\bar{n};x+r)} - (\bar{W}(\bar{n}))^2\right\}. \qquad (7)$$

The last step of Eq.(6), valid for $p\gg\bar{n}$, follows from the fact that the autocorrelation functions for measures discussed in this paper fall off rapidly, being close to zero for $r\geq\bar{n}$ for $\bar{n}\geq 1$. Notice that as $p\to\infty$, Var $\langle W\rangle_p$ goes to zero, which is nothing but the ergodic property[10] : the spectral average coincides with the ensemble average.

It is seen from (6) that for the sample errors we need Var W as well as the integral $\int C(\lambda\bar{n};\bar{n})d\lambda$ both of which we estimate from our Monte Carlo sample. The details will be published elsewhere. In practice instead of (5) we use a less smooth average in which the integral is replaced by a summation.

3. Comparison with Experiment for Energy Levels

In the conventional analysis one treats the data from each nucleus, containing about 50-100 levels, separately and consequently the statistical significance is poor. As seen from (5) the testing procedure improves as the sample size increases. Moreover since the correlation functions, Eq.(7), fall off rapidly it is not necessary to have one long sequence but a collection of many relatively short sequences could also be used.

Since one expects that the resonance energies of every compound nucleus will share the same fluctuation properties, it seems natural, and in the spirit of random matrix theory, to treat the set (NDE) of nuclear resonance energy data of different nuclei as a sampling of eigenvalues of GOE matrices ; see Ref.[12] for a similar notion for complex atomic spectra. As an example of this procedure, the nearest neighbor spacing distribution is shown in Fig.1. It is clear that a histogram containing ∼ 1700 spacings corresponding to the NDE (Fig.1b) is statistically much more significant, when compared to a theoretical prediction, than a histogram containing only ∼ 100 spacings corresponding to a single nucleus (Fig.1a).

Our NDE consists of 1762 resonance energies corresponding to 36 sequences of 32 different nuclei :

i) Slow-neutron resonance data on ^{64,66,68}Zn (103,65,45 levels[13]), ^{114}Cd (17 levels[14]), ^{152,154}Sm (70, 27 levels[15]), ^{154,156,158,160}Gd (19,47,21,54 levels[16]), ^{162,162,164}Dy (18,46,20 levels[17]), ^{166,168,170}Er (109,48,31 levels[18]), ^{172,174,176}Yb (55,19,23 levels[19]), ^{182,184,186}W(41,30,14 levels[20]), ^{188,192}Os (56,17 levels[21]), ^{232}Th (178 levels[22]) and ^{238}U (146 levels[22]),

ii) (n,γ) reaction data on ^{177}Hf (34'J=3' levels, 23'J=4' levels[23]), ^{179}Hf(25'J=4' levels, 22'J=5' levels[23]) and ^{235}U(58'J=3' levels, 68'J=4' levels[24]),

iii) proton resonance data on ^{44}Ca(52'$1/2^-$' levels, 39'$1/2^+$' levels[25]), ^{48}Ti(66'$1/2^+$' levels[25]) and ^{56}Fe (56'$1/2^+$'levels[25]).

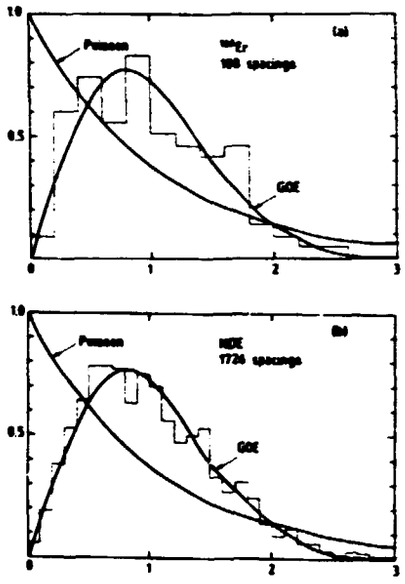

Fig.1. Nearest neighbor spacing histogram for : (a) ^{166}Er, (b) Nuclear Data Ensemble (NDE).

The criterion* for inclusion in the NDE is that the individual sequences be in general agreement with GOE.

We have made an extensive test of the theory by studying the aforementioned functions $Y_2(r)$, $\Sigma^2(\bar{n})$, $\Delta_3(\bar{n})$ as well as others. A complete account will be given elsewhere. Here we restrict ourselves to a few typical examples for the NDE.

Consider first the two-level measures $\Sigma^2(\bar{n})$ and $\bar{\Delta}_3(\bar{n})$. The procedure for calculations is to evaluate for each of the 36 sequences the spectral-averaged measure, say $\langle\Delta_3(\bar{n})\rangle$ for $\bar{\Delta}_3(\bar{n})$, and then take their average, weighted according to the size of each sequence. We have considered the range $0<\bar{n}<100$. The results for $\bar{n}<25$ are shown in Figs.2a, 2b. They are in a remarkably good agreement with GOE. We emphasize that typically the "figure of merit", e.g. $(\mathrm{Var}\langle\Delta_3\rangle)^{1/2}/\bar{\Delta}_3$ for $\bar{\Delta}_3$, is of the order of a few percent in the present analysis, whereas in the conventional analysis it is $\sim$ 20% or more. The values corresponding to the Poisson case as well as the Gaussian Unitarity Ensemble (GUE ; see section 5 below) are also shown for comparison.

To explore higher-than-two level effects we consider the ensemble variance of $\Delta_3(\bar{n})$, which is sensitive to Y_k upto k=4, and the distribution function of Δ_3 for various values of $\bar{n}$ (which involves in principle all order effects). The results are presented in Fig.2c for Var Δ_3 for $\bar{n}\leq 25$ and two examples ($\bar{n}$=10,20) of the distribution function of Δ_3 are shown in Fig.3. The agreement between the GOE predictions and data is again very good.

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*In the previous paper[1] our NDE consisted of 1407 resonance energies corresponding to 30 sequences of 28 different nuclei. In the present NDE we have added 8 new sequences. Moreover, we have not included the modifications suggested by the authors of the Columbia data to account for some missing levels. Instead, we have considered shorter sequences in a few cases and have dropped from the list the ^{111,113,114}Cd-spectra which involved large modifications. Our conclusions, as exemplified by Figs.2,3 are still the same as in Ref.[1].

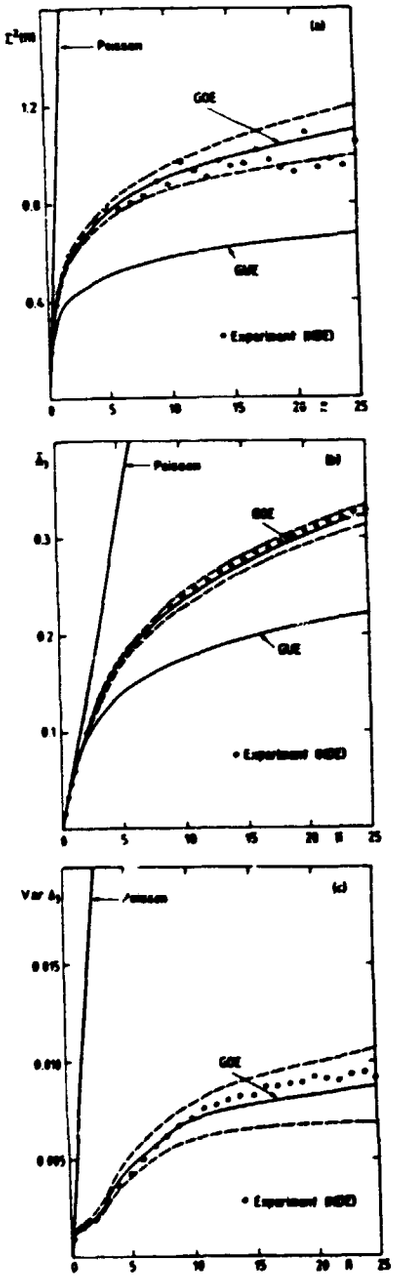

Fig.2. (a) Σ^2, (b) $\bar{\Delta}_3$, (c) Var Δ_3 as functions of $\bar{n}$. Dashed lines correspond, for GOE, to one standard deviation from the average.

4. Width Fluctuations

The main question is whether the transition widths (via which the resonance levels are detected and identified) have a χ^2_1 (Porter-Thomas[3]) distribution :

$$\rho(x) = (2\pi x)^{-1/2}\ \exp(-x/2)\ ;\ x = \Gamma_{ic}/\bar{\Gamma}_{ic}\ , \qquad (8)$$

where the width Γ_{ic} measures the rate of transition from an initial (statistical) state i to a channel state c. Or, equivalently the question is whether the transition amplitudes, whose squares (to within a penetrability factor) are the widths, are Gaussian random variables. This prediction follows directly from the orthogonal invariance of the random matrix ensembles as is the case with GOE ; see Ch.VII of Ref.[7].

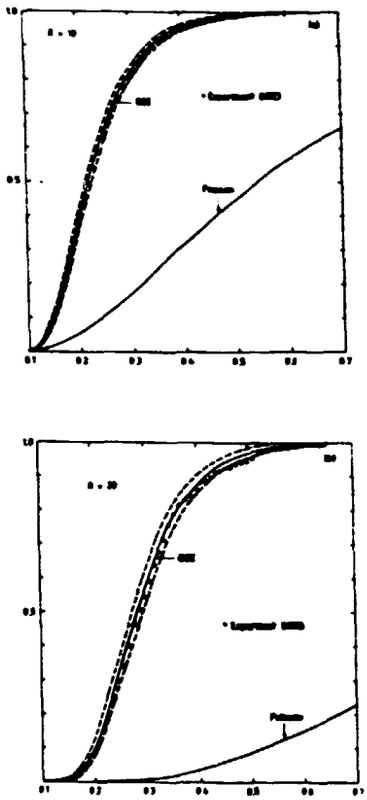

Fig.3. Distribution function of Δ_1 : (a) $\bar{n}$=10, (b) $\bar{n}$=20. Dashed lines correspond, for GOE, to one standard deviation from the average.

The amount of data that can be used to test the theory is much larger than in the case of energy levels. This is because even if some of the resonances are not detected due to very small widths, Eq.(8) can be tested for $x \geq \alpha$, an experimental threshold. In this section we present the results for some of the neutron-widths. A more detailed analysis will be taken up later. For a similar analysis of much older data, see Ref.[27]

We consider an NDE containing 1182 widths corresponding to 21 level sequences* of the previous section : ^{64,66,68}Zn, ^{110}Cd, ^{152,154}Sm, ^{154,156,158,160}Gd, ^{162}Dy, ^{166,168,170}Er, ^{172,174,176}Yb, ^{182,184}W, ^{232}Th and ^{238}U. The transition amplitude distributions are shown in Fig.4 for an individual sequence as well as the NDE. The agreement between theory and data is seen to be very good.

For further tests we calculate ν, the number of degrees of freedom, assuming that the width distribution itself is χ^2_ν with ν not necessarily an integer. A statistically significant departure from ν=1 would then be an indication of a failure of the Porter-Thomas model. A commonly-used procedure is to construct the likelihood function which is the product of the χ^2_ν - densities of the observed (renormalized) widths and then to maximize this function with respect to ν. The sample errors associated with this estimation procedure are obtained by studying the deviations from the maximum. The result would however show departure if some small widths are missing. For a better procedure we may assume a (relative) cut-off α below which the widths are likely to be missed and then do the above analysis for all widths of values $\geq\alpha$ with a truncated

* The widths in each sequence are renormalized to unit average.

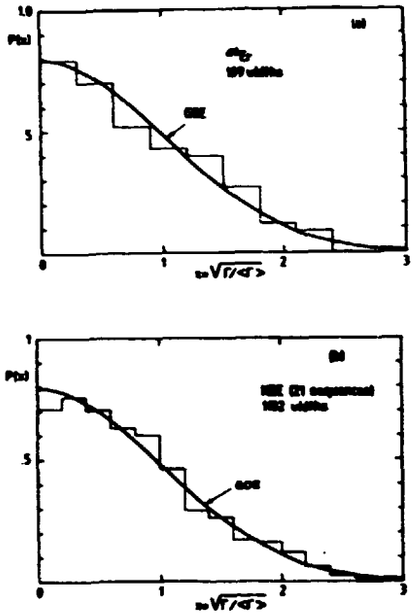

Fig.4. Histogram for the absolute values of transition amplitudes : (a) ^{166}Er, (b) NDE. The theory predicts $P(x)=(2/\pi)^{1/2}\exp(-x^2/2)$.

χ^2_ν-distribution;for details see Refs.[3,27]. We have studied ν as a function of α and a plot is given in Fig.5. The departures from theory for $\alpha \lesssim 10^{-3}$ may be due to the missing small widths. For larger values of α the agreement is again very good.

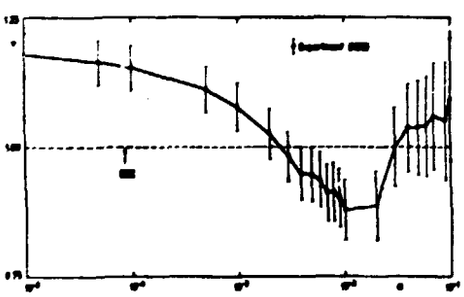

Fig.5. The degree of freedom ν as a function of cut-off α. The error bars correspond to one standard deviation from the estimated ν.

Finally we turn to the question of correlations between the width and energy level fluctuations. The theory predicts the two to be statistically independent. To test this we calculate the correlation coefficient

$$r = \frac{1}{N}\sum_{i=1}^{N}\left(\frac{\Gamma_{ic}-\langle\Gamma\rangle}{\sigma_\Gamma}\right)\left(\frac{E_i-\langle E_i\rangle}{\sigma_E}\right) , \qquad (9)$$

for each sequence. Here N is the number of levels in the sequence and Γ_{ic} the width associated with the level E_i. $\langle\Gamma\rangle$ and σ_Γ are the mean and standard deviation of the Γ_{ic}, and

$$\langle E_i\rangle = Ai+B, \quad \sigma_E^2 = N^{-1}\sum_{i=1}^{N}(E_i-\langle E_i\rangle)^2 , \qquad (10)$$

where A and B are fixed by minimizing* the expression for σ_E^2. For the NDE we take the average of the correlation coefficients for each sequence, weighted according to the size of the sequence. We obtain r(NDE)= 0.017 as compared to the theoretical value 0±0.029 confirming again the predictions.

5. Conclusion

We have established an astonishingly good agreement between a parameter-free theory (GOE) and the data. We emphasize that, apart from rotation and time-reversal invariance resulting in the real symmetric nature of the matrices, GOE takes no account of the specific properties of the nuclear Hamiltonian, e.g. its (1+2)-body nature, its large pairing and quadrupole components, etc. We also recall that the eigenvalues and eigenvector components of realistic (non-random) nuclear shell model matrices show the same fluctuation patterns[7,28]. How can this be understood theoretically ?

To answer this we recall first that there are other classical ensembles in which, like GOE, the orthogonal invariance plays a key role and which also give the same fluctuations[11,29]. But more significantly for the nuclear Hamiltonian, there are Monte Carlo results[28,30] which indicate that ensembles of two-body operators acting in many-particle (shell model) spaces also yield fluctuations characteristic of GOE. More recently[31] it has been demonstrated that adding a GOE matrix H to any real symmetric matrix K,(K+αH), leads very quickly, as α increases, to the same fluctuations. Intermediate fluctuation patterns are to be expected only when the random matrix elements are not much larger than the local average spacing of the given (non-random) matrix K. The good agreement with experiment, coupled with the theoretical understanding which is now emerging, reinforces the belief that GOE fluctuations are to be found in nature under very general conditions.

We mention finally that one can use the close agreement to impose restrictions on mechanisms which would change the fluctuations. In particular if time reversal is not an exact symmetry, the appropriate model would be an ensemble of complex Hermitian matrices in which the real and imaginary parts are sampled independently. The Gaussian Unitary Ensemble (GUE) in which the two parts have the same norm is one such example. It gives very different fluctuation properties than GOE[7]. For example, $Y_2(r)=(\sin\pi r/\pi r)^2$ implying stronger level repulsion than GOE (see Figs. 2a,2b for Σ^2 and $\bar{\Delta}_3$) and widths follow a χ^2_2 distribution. Analytic results for ensembles in which the real and imaginary parts have unequal weights have recently been given[31-33]. It is shown for energy level fluctuations (and is expected to be valid for width fluctuations as well) that even a small magnitude of the imaginary part induces major changes in fluctuation properties, leading very rapidly from GOE to GUE type fluctuations. The results are being used[32] to derive an upper bound on the time reversal non-invariant part of the nuclear Hamiltonian.

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*We remark parenthetically that the expression for A thus obtained is a good estimator of the average spacing ; see section X.B of Ref.[7]. The spectra used in section 3 were normalized by this procedure.