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ANALYSIS OF THE ^{238}U RESONANCE PARAMETERS USING RANDOM-MATRIX THEORY

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ABSTRACT

Random-matrix theories (RMTs) provide valuable statistical tools to analyze neutron-resonance data. The predictive power of the random-matrix theories, which do not contain any adjustable parameters, is striking, and the application is rather simple and fast. A new evaluation of ^{238}U resonance parameters has recently been performed at the Oak Ridge National Laboratory; the objective of this paper is to illustrate the use of RMT in the field of resonance-parameter evaluation with the newly evaluated ^{239}U energy levels and widths. Several statistics were computed using the s-wave resonances up to 20 keV and compared to the Gaussian Orthogonal Ensemble predictions. It is shown that a good agreement is observed between RMT and the experimental data up to 2.5 keV. The F-Dyson statistic was especially investigated because of its claimed ability to detect locally missed and spurious levels in the sample (p-resonances contamination or unresolved multiplets). As expected, the entire set of evaluated ^{238}U s-wave resonances up to 20 keV disagrees significantly with the theory. There are two reasons for this: First, it is difficult to distinguish s- and p-wave resonances in the analysis. Second, especially above 10 keV, it is impossible to determine reliable resonance energies from the available experimental data. It is concluded that the use of RMT can help nuclear data evaluators to improve their evaluations in the resonance range.

KEYWORDS: ^{238}U, resonance parameters, statistical analysis, GOE, random-matrix theory

1. INTRODUCTION

In the early 1950s, the study of many-particle energy spectra such as those measured by neutron-induced reactions showed that energy levels could not be considered as a random sequence but featured striking properties such as level-repulsion effect or spectrum rigidity. With the pioneering work of Wigner, it was recognized that statistical properties of the energy spectrum of a compound nucleus could be mathematically investigated with the help of random-matrix theories (RMTs) [1]. The energy levels, seen as eigenvalues of a nuclear Hamiltonian, can be obtained by diagonalizing large matrices whose properties preserve the usual space-time symmetries. Because individual elements of the matrix are unknown, Wigner first studied a special ensemble of real symmetric matrices, the Gaussian Orthogonal Ensemble (GOE), whose elements are independent and randomly distributed.

Subsequently, several random-matrix ensembles were introduced to study the nonconservation of space-time invariants. The Gaussian Unitary Ensemble (GUE) of complex matrices preserves rotational invariance but violates time-reversal, while the Gaussian Symplectic Ensemble (GSE) of quaternion matrices obeys time-reversal invariance but not rotational invariance. The three ensembles GOE, GUE, and GSE have been extensively studied by analytical methods and Monte Carlo computer simulations. Dyson proposed an alternative to Gaussian ensembles and defined three "circular" ensembles COE, CUE, and CSE to simplify mathematical treatments while still predicting the same fluctuation properties as Gaussian ensembles (see Reference [1] for details). In the early seventies, the Two-Body Random Hamiltonian Ensembles (TBRE) were investigated independently by French and Wong, and Bohigas and Flores, as discussed in [2]. This ensemble arose from the development of nuclear shell model calculations, where the nuclear spectra are described by an effective two-body interaction. Using numerical techniques, an important result was demonstrated by Wong et al. [3]: predictions of the usual observables from GOE and TBRE are very similar, making it difficult to decide experimentally which ensemble was the most appropriate.

Experimental checks of RMT began in the sixties when the Columbia group first gave convincing evidence for RMT using spectroscopic neutron data [4]. On a larger scale, Haq et al. [5], using a larger set of selected neutron and proton resonance spectra, showed impressive agreement between RMT and experiments. It is worth mentioning that RMTs have provided a way to address the breaking of symmetry and invariance by testing experimental data against GOE, GUE (time-reversal invariance) and other ensembles (characterizing the breaking of isospin or parity conservation).

2. FLUCTUATION PROPERTIES OF SPECTRA

The fluctuation properties of energy-level spectra are well understood with the two-level correlation function $R_2(r)$ that defines the probability density of observing two levels in the intervals $[x_1,x_1+dx_1]$ and $[x_2,x_2+dx_2]$ separated by $|x_1-x_2| = r$ (assuming all levels are equivalent). Here r is the energy interval measured in units of the average spacing D. This function should be equal to unity for a random sequence; however within the framework of RMT, the deviation from unity is defined by the so-called two-level cluster function $R_2(r) = 1-Y_2(r)$ that has been extensively worked out by Dyson and Mehta [1]. For GOE, Y_2 is given by:

$$\boldsymbol{Y}_{2,\boldsymbol{GOE}}(\boldsymbol{r}) = \left(\frac{\sin \pi \boldsymbol{r}}{\pi \boldsymbol{r}}\right)^2 + \left(\frac{\boldsymbol{d}}{\boldsymbol{dr}}\frac{\boldsymbol{d}\sin \pi \boldsymbol{r}}{\pi \boldsymbol{r}}\right)\int_{r}^{\infty}\frac{\sin \pi \boldsymbol{r}'}{\pi \boldsymbol{r}'}\boldsymbol{dr}'. \tag{1}$$

Similar equations can be found for GUE and GSE. Experimentally, it is not easy to test the two-level cluster function for large r. Instead, one has to consider different integrated forms of Y_2.

3. NUMERICAL SIMULATION OF RANDOM MATRICES SPECTRA

The fluctuation properties predicted by random matrix theories have been thoroughly studied by analytical methods. In the present work, we are instead using computer-generated sets of GOE matrices of high-dimension (≈2000) to compare experimental data with theoretical results. After the matrices are diagonalized, the resulting spectrum (which followed the unphysical Wigner semi-circle distribution) was unfolded to obtain the constant level density.

4. ^{238}U RESONANCE-PARAMETER SET

The spin of the ^{238}U nucleus is $I = 0$ so that s-wave neutrons form the ^{239}U compound nucleus with unambiguous spin $J = 1/2$. In contrast, p-wave resonances can form $J = 1/2$ or $J = 3/2$, making it difficult to obtain a pure sample (with only resonances with specific J^{π}). We considered the sample of s-wave resonances recently evaluated at ORNL [6]. This evaluation is based on a comprehensive experimental database from thermal energy to 20 keV. Several transmission and capture measurements presented in Table I, mostly performed at the Oak Ridge Electron Linear Accelerator (ORELA), were fitted with the Reich-Moore approximation of the R-matrix theory using the SAMMY code [12]. Careful attention was paid to the study of experimental conditions (normalization, background, resolution function, temperature). Complementary techniques have permitted the separation between s-waves and p-waves:

- The theory of conditional probability gives the probability of a resonance with a given $g\Gamma_n$ to be $l = 0$ or $l = 1$ [13]. This method suggests the orbital angular momentum, by discriminating resonances according to the magnitude of their neutron reduced widths.
- Corvi et al. [14] have determined the orbital angular momentum of ^{238}U resonances by analyzing the γ-ray spectrum following resonant capture. They noticed that the γ transitions involved in the decay of the compound nucleus are not the same in the case of s-wave or p-wave resonances. The γ multiplicity is enhanced for p-waves, providing a way to identify the orbital momentum. Below 1.6 keV, the present ^{238}U evaluation adopted the l-assignment of Corvi et al.
- The simultaneous fitting of transmission and capture measurements and the analysis of the goodness of fit permitted the assignment of l for resonances with large reduced neutron widths.

Table I. Overview of the experimental database used in the analysis of ^{238}U resonances

Energy range	Reference	Measurement type
6 eV - 100 keV	de Saussure et al. (1973) [7]	Capture
0.5 eV - 4 keV	Olsen et al. (1977) [8]	Transmission
300 eV - 100 keV	Olsen et al. (1979) [9]	Transmission
250 eV - 130 keV	Macklin et al. (1988) [10]	Capture
1 keV - 100 keV	Harvey et al. (1988) [11]	Transmission

Above 10 keV, poor experimental resolution makes resonance analysis difficult so that even resonance energies could not be reliably determined. A "pseudo-resonance" approach was used; a set of resonances is proposed that fits the transmission and capture data but does not represent actual resonances. It is expected that the statistical tests will fail in this energy range.

5. STATISTICAL TESTS OF SPECTRUM FLUCTUATIONS

5.1. The variance of the number of levels $\Sigma^2(r)$

The most obvious test is to study the number of levels in an energy interval of a fixed length r (which is given in units of D). The fluctuations of the number of levels are measured by the so-called number variance $\Sigma^2(r)$ and somehow probe the two-level cluster function Y_2.

$$\Sigma^2(r) = r - 2\int_0^r (r' - r) Y_2(r') dr'. \quad (2)$$

This integral has been analytically evaluated by many authors, and the results for GOE can be safely approximated for large r as $\Sigma^2(r) = \frac{2}{\pi^2}[ln(2\pi r) + \gamma + 1 - \pi^2/8)]$. Here $\gamma \approx 0.5772$ is the Euler constant. In the case of ^{238}U resonances, the calculation of the number variance is not very accurate for $r > 10$. As shown in Fig. 1, the agreement between the data and GOE is fairly good even if we consider all the s-wave resonances up to 10 keV.

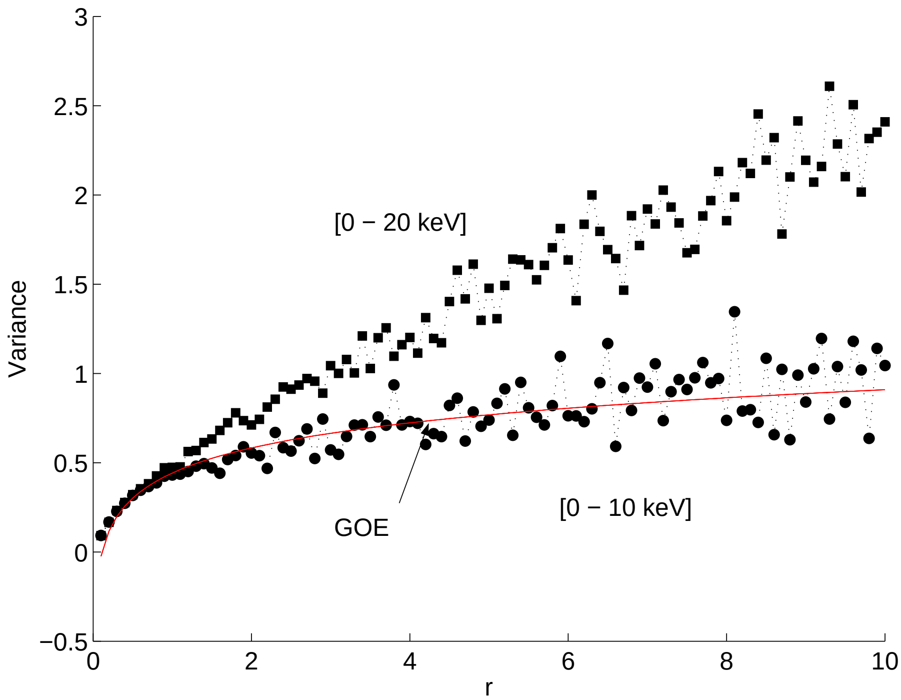

Figure 1. Experimental number variances compared with GOE prediction.

5.2. Δ_3 Mehta-Dyson statistics and the $\rho(D_i, D_{i+1})$ test

The statistic Δ_3 developed by Dyson and Mehta is a popular measure of long-range correlations. It is defined as the mean square of the deviation of the cumulative number of levels from a fitted straight line.

$$\Delta_3(r) = min_{A,B}\frac{1}{r}\int_0^r [N(r') - Ar' - B]^2 dr' \tag{3}$$

where r represents the energy interval measured in units of D. Again, Δ_3 is directly related to the two-level cluster function:

$$\Delta_3(r) = \frac{r}{15} - \frac{1}{15r^4}\int_0^r (r'-r)^3(2r^2 - 9rr' - 3r'^2)Y_2(r')dr'. \tag{4}$$

For large r, Dyson and Mehta, within the framework of COE, calculated the average value of $\Delta_3(r) = \frac{1}{\pi^2}[ln(2\pi r) - \gamma - 5/4 - \pi^2/8]$ and predicted a constant variance $Var\ \Delta_3 = (0.11)^2$. Above 2.5 keV, we note in Fig. 2 that the experimental Δ_3 becomes higher than the theoretical value, suggesting the presence of p-resonance contamination or spurious levels (doublets, multiplets).

The short-range correlations are measured by the linear correlation coefficient between nearest-neighbor level spacings. Mehta, using analytical methods, predicts a negative correlation value of $\rho(D_i, D_{i+1}) = -0.27$ for GOE. From the physics point of view, this negative correlation illustrates the rigidity of GOE spectrum; i.e., if a small spacing is observed, the neighbor spacing will tend to be higher. The calculations presented in Table II in various energy ranges show strikingly good agreement with experiment up to 10 keV.

Table II. Experimental linear correlation coefficient ρ and Mehta-Dyson statistic Δ_3 compared with the theoretical predictions

Energy range	ρ (theory -0.27)	Δ_3 exp.	Δ_3 theo.
0 - 500 eV	-0.28	0.216	0.315 ± 0.11
0 - 1 keV	-0.23	0.223	0.381 ± 0.11
0 - 3 keV	-0.32	0.513	0.494 ± 0.11
0 - 5 keV	-0.29	0.674	0.545 ± 0.11
0 - 10 keV	-0.25	1.494	0.616 ± 0.11

5.3. The spacing variance σ_k test

Statistical analysis of the resonance parameters is often based on the distribution of the nearest-neighbor spacings and the comparison with the Wigner surmise. Exact GOE calculations lead to a distribution nearly indistinguishable from the Wigner formula. However, RMTs also provide

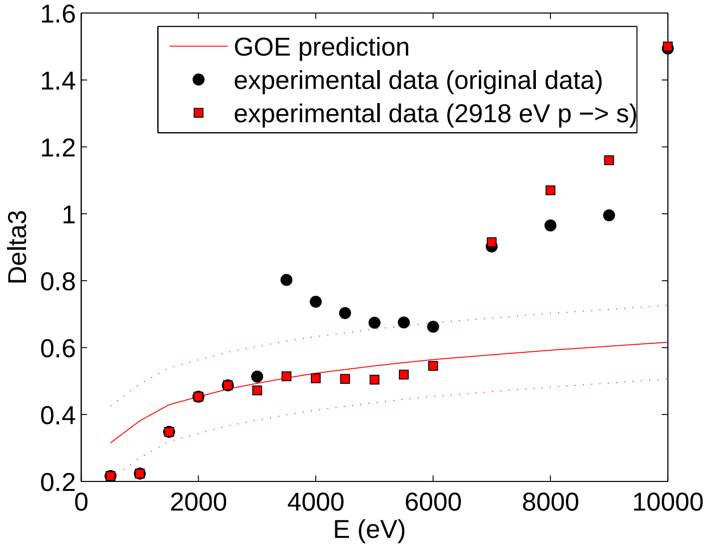

Figure 2. Experimental Δ_3 compared with GOE prediction. Note a significant improvement when the spin assignment of only one resonance (2919 eV) is changed (see text for details).

theoretical forms of the spacing distribution (and the associated spacing variance σ_k) of higher order k [i.e, the distribution of spacings between two resonances having k resonances between them]. The k-order spacing distribution in the case of ^{238}U is displayed in Fig. 3.

Figure 4 compares the variance of the k-order spacing distribution with the GOE simulation. Good agreement is noticed for s-wave resonances below 4 keV. As expected, the complete set of resonances up to 20 keV clearly disagrees with GOE mainly because of the pseudo-resonance representation.

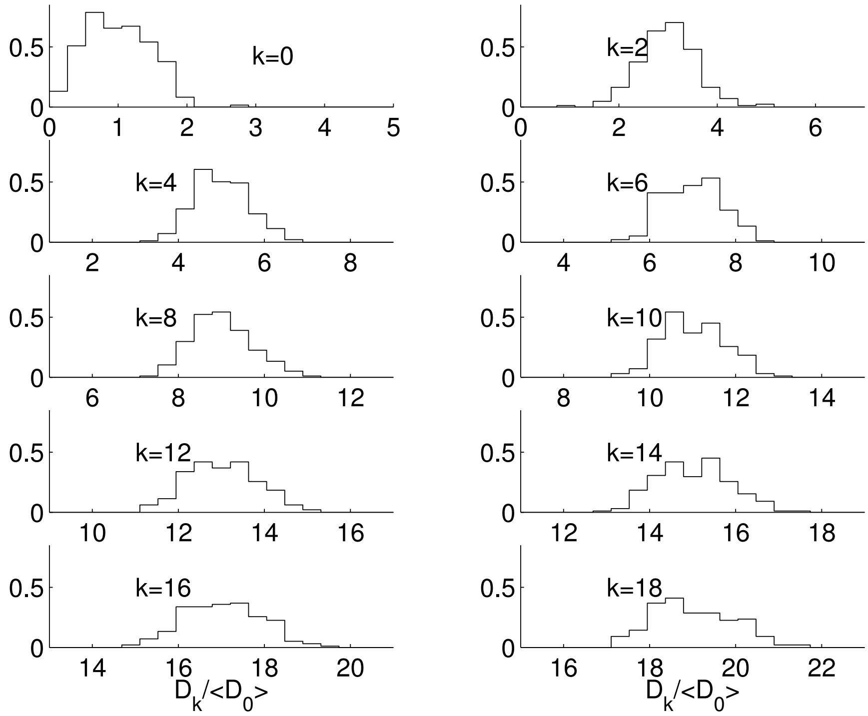

Figure 3. Distribution of the k-order spacings for ^{238}U s-wave resonances below 10 keV.

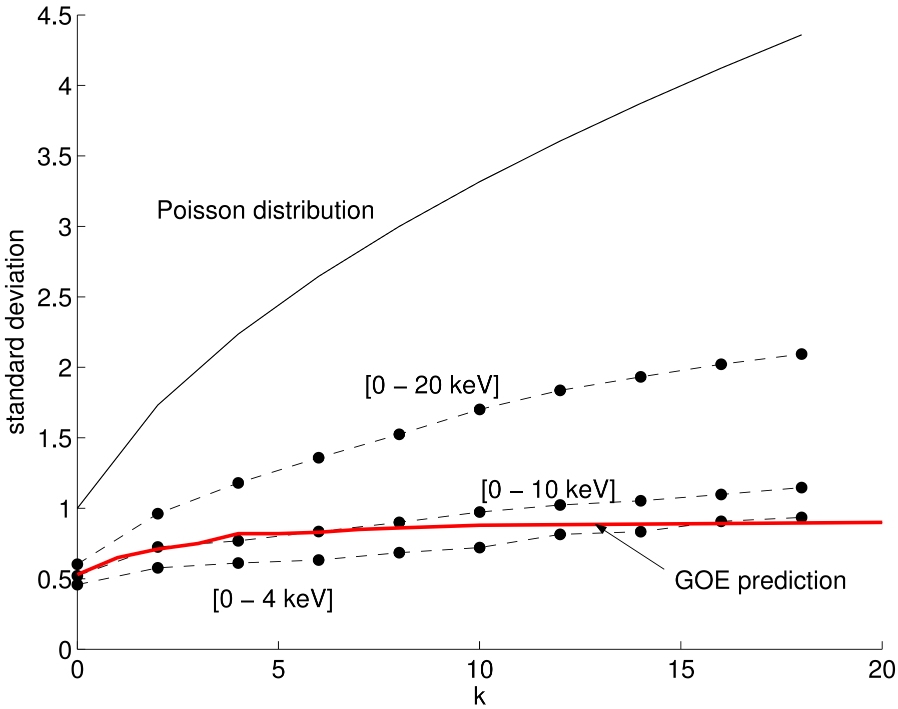

Figure 4. Comparison between experimental and theoretical variances of the k-order spacings.

5.4. The F-Dyson statistic

As discussed in [4], the F statistic was introduced by Dyson, to provide a method to detect missed and spurious levels. For each resonance i, one needs to compute:

$$F_i = \sum_{j \neq i} f(y_{ij}) \quad y_{ij} = \frac{x_i - x_j}{L} \tag{5}$$

$$f(y) = \begin{cases} \frac{1}{2} \ln \frac{1+\sqrt{1-y^2}}{1-\sqrt{1-y^2}} & |y| < 1 \\ 0 & |y| \geq 1 \end{cases} \tag{6}$$

The sum extends to all levels x_j within $x_i - L < x_j < x_i + L$. Dyson claimed that the expectation value of F should be $L/D\pi - ln(L/D\pi) - 0.656$ for each level and that the variance of F is $\sigma^2(F) = ln(L/D\pi)$. If one level is missing, the local values of F should drop, while a spurious level will cause a rise in F. Various choices of L/D were tested; Fig. 5 displays the values of F for each resonance below 5 keV with $L/D = 10$.

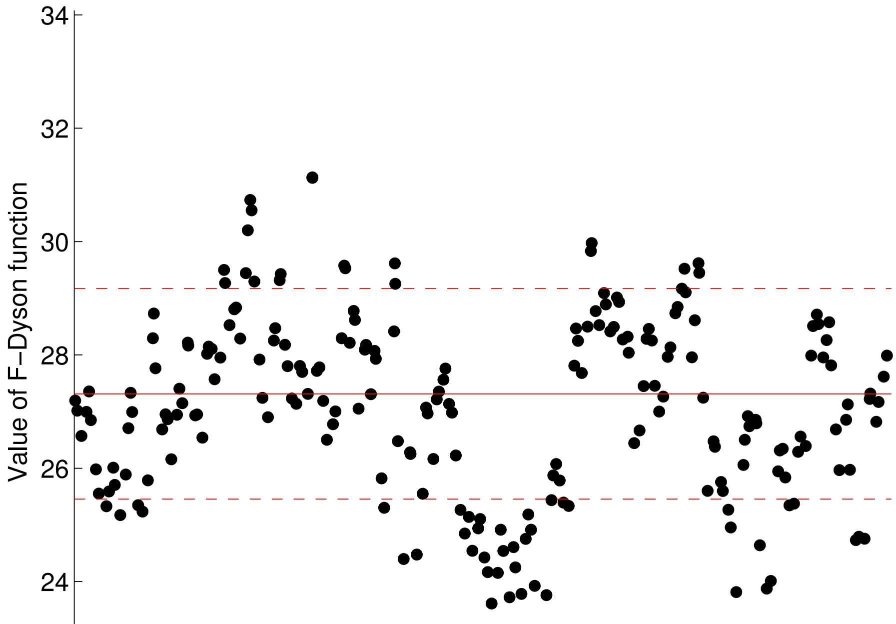

Figure 5. Values of the F-Dyson function for s-wave ^{238}U resonances below 5 keV.

Around 1420 eV, a group of levels with F-values outside the $2\sigma(F)$ band is observed, so that one can suspect the presence of spurious levels. As shown in Fig. 6 and 7, a close examination of the data between 1390 eV and 1450 eV shows 5 s-wave resonances (1394 eV, 1405 eV, 1420 eV, 1427 eV and 1444 eV) and 5 p-wave resonances (1400 eV, 1410 eV, 1414 eV, 1417 eV and 1427 eV). After changing the assignment of only one of the resonances from *s* to *p*, the F-statistic was recomputed; all the discrepant F-values in this energy range were eliminated. However, given the magnitude of the reduced neutron widths, the Bayes formula gives less than 6% probability that one of these levels is p-wave, so that it was not possible in this case to draw conclusions regarding the presence or contamination of the s-sequence by p levels within this energy range.

A significant drop in F is observed around (2800 to 3100 eV) which suggests missed levels. This observation confirmed the results obtained with the Δ_3 statistics. Figures 8 and 9 show the capture and transmission measurements performed in this energy region. Spin assignments for two resonances were investigated. For instance, the 2919-eV resonance had been considered as a p-wave in the original resonance set in agreement with the magnitude of its reduced neutron width that give a probability of 85% to be p. However, if we change the spin assignment of this resonance, the F-Dyson statistic and especially the Δ_3 statistic are greatly improved as shown in Figs. 2 and 10. To further investigate this point, the SAMMY fits were performed for this resonance using either *p* or *s* assignment. The χ^2 of the fit for the thick sample transmission measured by Olsen is slightly improved ($\chi^2 = 1.17 \rightarrow 1.03$) when this resonance is *s*, making plausible this assumption. Other resonances such as the 2989-eV resonance were investigated, but no firm conclusion could be drawn from the Bayes formula, the goodness of SAMMY fit, and the random-matrix statistics.

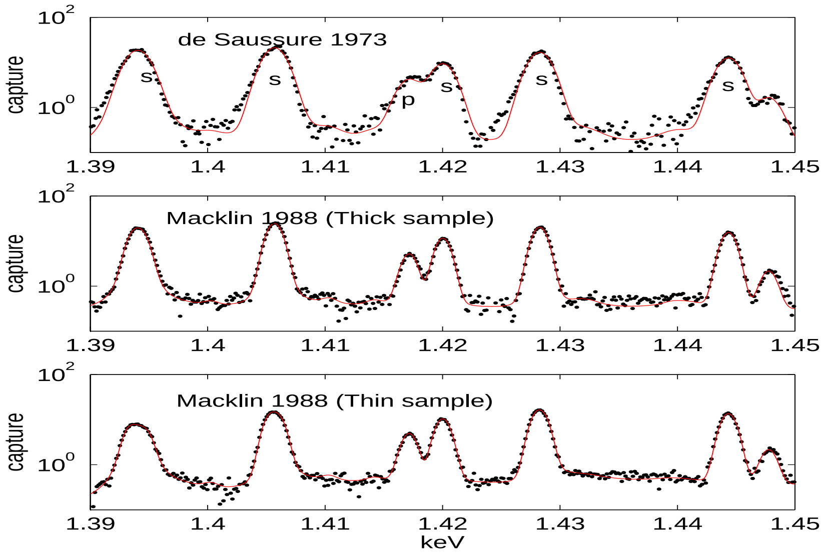

Figure 6. SAMMY fit of the capture experimental data.

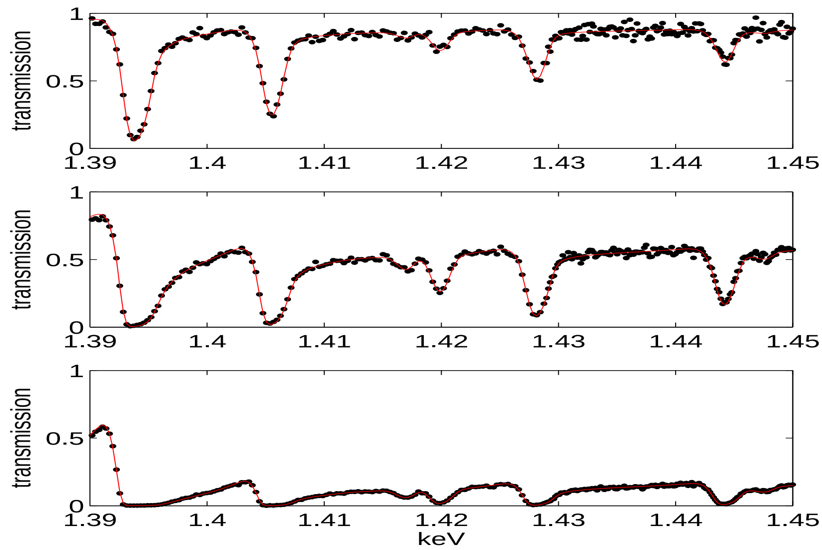

Figure 7. SAMMY fit of the transmission data from Olsen et al. (only the thickest samples are displayed).

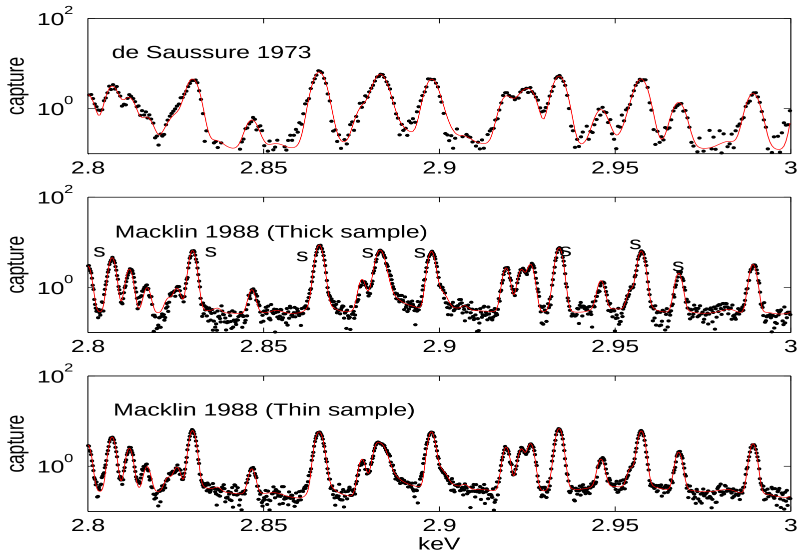

Figure 8. SAMMY fit of the capture experimental data.

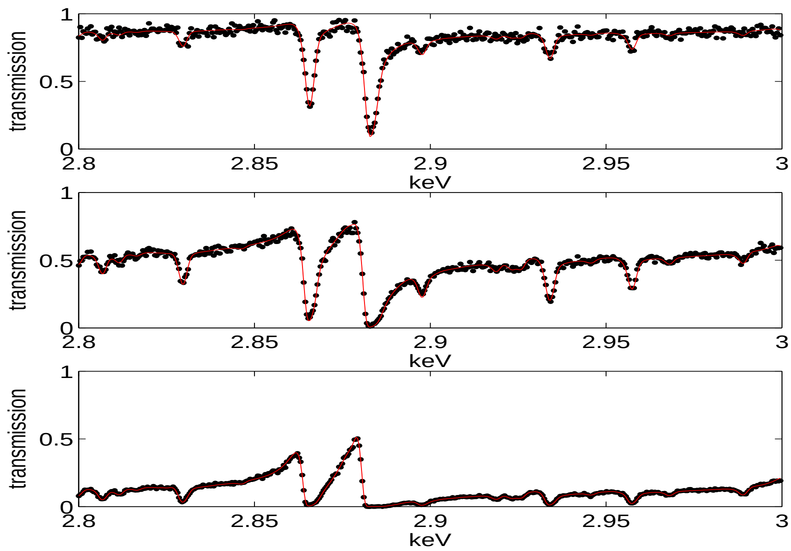

Figure 9. SAMMY fit of the transmission data from Olsen et al. (only the thickest samples are displayed).

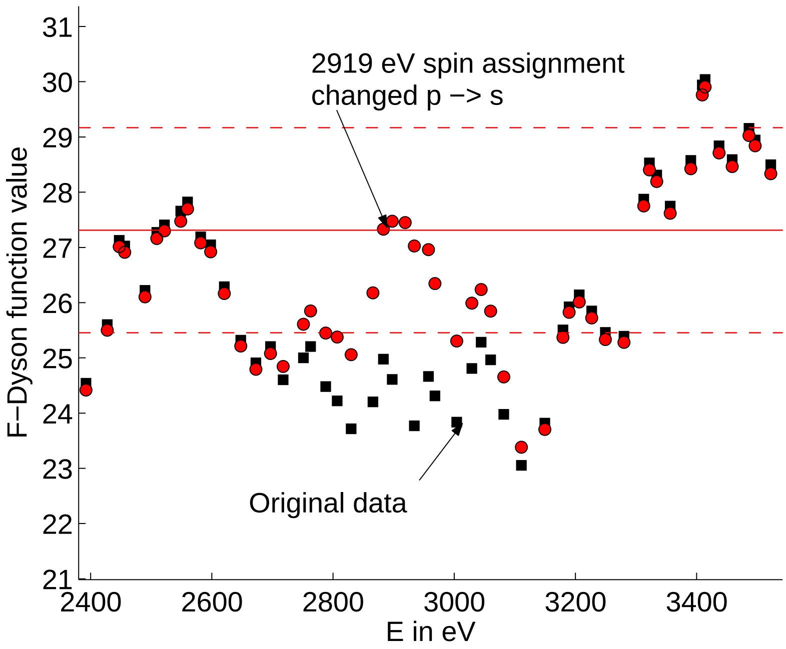

Figure 10. Values of the F-Dyson function for s-wave ^{238}U resonances when the spin assignment of only one resonance (2919 eV) is changed from $l = 1$ (p-wave) to $l = 0$ (s-wave).

The F-Dyson statistic seems to be a useful tool to locally test experimental nuclear spectra and detect missed or spurious levels. Sometimes, however, it might be not clear if the rise or drop in F can be reliably associated with missed levels or if it is a statistical effect. Investigation with numerically generated GOE matrices confirmed the $\sigma^2(F)$ value even though the individual spectra often presented local deviations from the F-Dyson prediction.

6. CONCLUSIONS

In the resonance analysis process, evaluators sometimes cannot assign the correct angular momentum or spin of resonances because of the lack of experimental data. RMT should provide a means of testing the various assumptions that are made. Random Matrix Theory should also help to determine whether a sample of resonances is pure or not, which is of importance in the determination of average parameters such as the average spacing or the neutron strength function. This paper illustrates some of the statistical tests that can be used. In the case of the evaluation of ^{238}U resonance parameters recently completed, remarkable agreement between GOE (analytical or numerical prediction) and the evaluated energy levels is observed below $\approx$ 2.5 keV. It is also demonstrated that the change in the spin assignment of one or two resonances of the ^{238}U set can improve the agreement with GOE up to 5 keV. As shown in Table III, the set of p-wave resonance parameters ($J = 1/2$ or $J = 3/2$) disagree strongly with all of these statistical tests, illustrating the difficulty of determining the correct spin assignments from available experimental data.

Table III. Synthesis of the statistics for ^{238}U s- and p- waves resonances compared with GOE results

Statistic	GOE theory	Exp. data ^{238}U $l = 0$ $J^{\pi} = 1/2^{+}$	Exp. data ^{238}U $l = 1$ $J^{\pi} = 1/2^{-}$	Exp. data ^{238}U $l = 0$ $J^{\pi} = 3/2^{-}$
		[0 - 2.5 keV]	[0 - 2.5 keV]	[0 - 2.5 keV]
Δ_3	0.476 ± 0.11	0.487	0.388	8.65
ρ	-0.27	-0.32	0.09	-0.02
$\sigma(F)$	1.86	1.38	3.41	5.66
$\Sigma(1)$	0.44	0.45	0.56	0.70
$\Sigma(3)$	0.66	0.49	1.79	1.89
$\Sigma(6)$	0.80	0.55	4.85	3.71
σ_0	0.53	0.50	0.78	0.77
σ_6	0.82	0.65	2.34	1.91
σ_{10}	0.89	0.68	2.85	2.38

In the present paper, the various tests are all related to the two-level cluster function; however, one can probe higher-order cluster functions (three-level or four-level) that would require the analysis of higher moments of distribution (skewness and excess of the spacing distribution for instance). An extension of this work concerns the statistical properties of reduced neutron widths that, within the framework of RMT, are obtained from the eigenvectors of the random matrices.

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