Uncertainties in the analysis of neutron resonance data

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Recent analyses of the distribution of reduced neutron widths in the Nuclear Data Ensemble (NDE) and in the Pt isotopes find strong disagreement with predictions of random-matrix theory. These analyses combine the maximum-likelihood method with a cutoff on the reduced neutron widths. We show that the method introduces a systematic error (the “cutoff error”). That error (seemingly taken into account for the Pt data) increases with increasing cutoff and decreasing number of data points. We reanalyse the NDE taking the cutoff error into account. While differing in detail, our results confirm the earlier conclusion that the NDE disagrees significantly from RMT predictions.

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I. PURPOSE

Early work on the distribution of widths and spacings of neutron resonances in a set of nuclei (the “Nuclear Data Ensemble”) (NDE) indicated agreement with predictions of Random Matrix Theory (RMT). Firm and unbiased conclusions can only be drawn, however, if s-wave and p-wave neutron resonances are cleanly separated. That was not possible or not done at the time. The problem was emphasized in Ref. [4], and in Refs. [1, 2] it was addressed with a help of a cutoff on the reduced neutron widths that depends on neutron resonance energy, variation of a technique originally applied in Ref. [3] to a much smaller data set. The ensuing re-analysis of the NDE [4] and the analysis of new data on the Pt isotopes [5] using different versions of the cutoff method have both cast serious doubt on the validity of random-matrix theory (RMT) in nuclei. (Ref. [7] even carries the title “Neutron Resonance Data exclude RMT.”) Indeed, for the Pt isotopes, the analysis rejects agreement with RMT with a statistical significance of at least 99.997% probability [5]. Some of these results have found wide attention [3] eroding, as they seemingly do, one of the cornerstones of the statistical theory of nuclear reactions [12, 13].

While fully in agreement with the authors of Refs. [4, 5] concerning the need for a clean separation of s-wave and p-wave resonances, we show in this paper that the cutoff procedure actually used in Ref. [4] for the analysis of the NDE introduces a systematic error (this additional error appears to have been included in Ref. [3]). Typically, that error is as large as the error deduced from the width of the maximum of the likelihood function. Valid conclusions on agreement with RMT predictions can be drawn only if that error is properly taken into account in the data analysis.

In Section II, we describe the maximum-likelihood method as used in the analysis of neutron resonance data with a cutoff. Section III illustrates how the combination of applying a cutoff procedure to the data and finite-size-of-data effects can produce maximum-likelihood results that are very different from the underlying data. In Section IV, we describe simulations that quantify the magnitude of these effects and demonstrate that the effects are indeed significant for this particular analysis. Section V provides specific numerical results for the NDE, and we summarize our results in Section VI.

II. MAXIMUM-LIKELIHOOD ANALYSIS

For resonances close to threshold (located at energy $E = 0$), s-wave (p-wave) neutron widths have an intrinsic energy dependence $E^{1/2}$ ($E^{3/2}$, respectively), with $E$ taken at the neutron resonance energy. The transition to reduced widths removes the $E^{1/2}$ dependence of s-wave neutron widths. The remaining linear energy dependence of p-wave resonance widths is used to suppress the latter with the help of a cutoff first proposed in Ref. [4]. Cutoffs that depend both linearly [4] and non-linearly [5] on resonance energy have been employed. All measured neutron widths smaller than the cutoff were removed from the data set. The distribution of the remaining widths was then analyzed using a maximum likelihood (ML) method. The method tests for agreement with the Porter-Thomas distribution (PTD) predicted by RMT. The PTD is a $\chi^2$-distribution with a single degree of freedom ($\nu = 1$). For comparison, distribution functions with other values of $\nu$ were admitted. The test determined which of these gave best agreement with the data. This led to the above-mentioned rejection of RMT.

The normalized $\chi^2$-distribution for $\nu$ degrees of free-
with a cutoff with value $x_{\text{min}}(i)$ at resonance energy $E_i$, and with reduced widths $x_i > x_{\text{min}}(i)$. The likelihood function $L$ is the product of the corresponding probabilities,

$$L(\nu, \langle x \rangle) = \prod_{i=1}^{N_{\text{incl}}} \frac{1}{C_i} g(x_i, \nu, \langle x \rangle) .$$

(3)

The maximum of $\ln L$ as a function of $\nu$ and $\langle x \rangle$ determines the most likely values of these parameters. The width of $\ln L$ in the vicinity of the maximum determines the statistical significance with which a value of $\nu$ that differs from the value at the maximum, is rejected. That is the basis for the figures cited above of 99.17 per cent for the NDE and of 99.997 per cent for the Pt isotopes. (In actual fact the method used in Ref. [3] is slightly different. Instead of the product of normalization factors $C_i$, a single joint normalization factor $C$ to the power $N_{\text{incl}}$ was used. That factor was defined as a suitable average of the $C_i$. For the ML analysis with an energy-independent cutoff studied in the present paper the two methods are identical. Moreover, the additional error due to the cutoff and explained below seemingly was taken into account in Ref. [3].)

### III. TEST OF THE CUTOFF METHOD

The reliability of the maximum-likelihood analysis with a cutoff is adversely affected by (i) the cutoff itself (i.e., even for an infinite data set) and (ii) by finite-size-of-data effects. We display these features by using a combination of analytical reasoning and numerical results. The maximum-likelihood method determines the extremum of $\ln L(\nu, \langle x \rangle)$ as a function of $\nu$ and $\langle x \rangle$. At the extremum, we have

$$\frac{\partial}{\partial \nu} \ln L(\nu, \langle x \rangle) = 0 , \quad \frac{\partial}{\partial \langle x \rangle} \ln L(\nu, \langle x \rangle) = 0 .$$

(4)

We use an energy-independent cutoff $x_{\text{min}}$. Combining that with Eqs. (1) and (2) we find that Eqs. (4) take the form

$$\ln \left( \frac{\nu}{2} \right) - \ln \langle x \rangle - 2 \frac{\partial \ln \Gamma \left( \frac{\nu}{2}, \frac{x_{\text{min}}}{2} \right)}{\partial \nu}$$

$$+ \langle \ln x_i \rangle + 1 - \langle x_i \rangle = 0 ,$$

(5)

$$\langle x \rangle = \langle x_i \rangle + \frac{x_{\text{min}}}{\Gamma(x, y)} \frac{\partial \Gamma(x, y)}{\partial y} \bigg|_{x=(\nu/2),y=\nu/(2)} .$$

(6)

Here $T = x_{\text{min}}/\langle x \rangle$ and

$$\langle \ln x_i \rangle \equiv \frac{1}{N_{\text{incl}}} \sum_{i=1}^{N_{\text{incl}}} \ln x_i , \quad \langle x_i \rangle \equiv \frac{1}{N_{\text{incl}}} \sum_{i=1}^{N_{\text{incl}}} x_i .$$

(7)

The quantities in Eqs. (7) depend on the actual data set and on the value chosen for $x_{\text{min}}$ (which determines the number $N_{\text{incl}}$ of resonances retained in the analysis). The values for $\langle x_i \rangle$ and $\langle \ln x_i \rangle$ given by Eqs. (7) determine $\nu$ and $\langle x \rangle$ as solutions of Eqs. (5) and (6).

We investigate the method by considering Eqs. (5) and (6) separately. For fixed input values of $x_{\text{min}}$, $\langle x_i \rangle$, and $\langle \ln x_i \rangle$, each of these two equations connects $\nu$ with $\langle x \rangle$ and, thus, defines a curve in the two-dimensional $\nu - \langle x \rangle$ plane. The point of intersection of these two curves determines the most likely values of $\nu$ and $\langle x \rangle$. We show how these curves (and their point of intersection) change with both a change of the cutoff parameter $x_{\text{min}}$ and a change of the number $N$ of resonance widths used in the analysis. Our input values are $\nu = 1$ and $\langle x \rangle = 1$. If correct, the maximum-likelihood analysis must reproduce these values.

We begin with the case $N = \infty$ (which implies $N_{\text{incl}} = \infty$). In that case there is no finite-size-of-data error. Given the Gaussian distribution with unit width of the reduced width amplitudes $y_i$, both $\langle x_i \rangle$ and $\langle \ln x_i \rangle$ with $x_i = y_i^2$ can be calculated analytically for every value of $x_{\text{min}}$. For $x_{\text{min}} = 0$ we obtain the two curves shown in Fig. [1]. The horizontal dashed line corresponds to Eq. (5), and the solid curve that intersects the dashed line nearly vertically corresponds to Eq. (6). As expected, the two curves have a single well-defined point of intersection at $\nu = 1$ and $\langle x \rangle = 1$. Both curves change as $x_{\text{min}}$ is increased. The curve representing Eq. (6) is deformed and rotated in a counter-clockwise direction while the curve representing Eq. (5) is likewise deformed but rotated in a clockwise direction. For $x_{\text{min}} = 0.02$ and for $x_{\text{min}} = 0.2$, the results are shown in Fig. [2]. The two curves still intersect at $\nu = 1$ and $\langle x \rangle = 1$ but become ever more parallel as $x_{\text{min}}$ increases. The effect of this is that any changes in the values of $\langle x_i \rangle$ or of $\langle \ln x_i \rangle$ that occur for finite values of $N$ cause significant shifts in the values of $\nu$ and $\langle x \rangle$ that maximize the likelihood function $L$. The fluctuations in $\langle x_i \rangle$ or $\langle \ln x_i \rangle$ for spectra of finite size $N$ are expected to be of order $1/\sqrt{N}$. For $N = 100$, a
reasonable spectrum size for nuclear data, that amounts to 10%. In Figs. 3 and 4 we illustrate the effect such fluctuations might have by changing in Eq. (5) (somewhat unrealistically) \( \langle x_i \rangle \) and \( \langle \ln x_i \rangle \) separately and independently. For \( N = \infty \) and \( x_{\text{min}} = 0.2 \), Fig. 3 shows how the curve representing Eq. (5) is changed when \( \langle x_i \rangle \) is varied while \( \langle \ln x_i \rangle \) is held fixed. Fig. 4 shows the same for fixed \( \langle x_i \rangle \) and a variation of \( \langle \ln x_i \rangle \). We note that an increase in \( \langle x_i \rangle \) causes the curves to shift in one direction while an increase in \( \langle \ln x_i \rangle \) causes them to shift in the other direction. We see that as a result of the finite-size-of data-errors in \( \langle x_i \rangle \) and \( \langle \ln x_i \rangle \), the curves change significantly, and so do (as it turns out) their points of intersection. The dependence of the curve representing Eq. (6) on changes of \( \langle x_i \rangle \) is similar to that shown in Fig. 3.

IV. SIMULATIONS

We have shown that applying a cutoff as described in Refs. [6] and [4] has the potential to shift significantly the ML values of \( \nu \) and \( \langle x \rangle \). We now show that significant shifts of \( \nu \) do actually occur in finite data sets. We have simulated finite values of \( N \) with the help of a random-number generator. We have drawn \( N \) real numbers \( y_i, i = 1, \ldots, N \) from a Gaussian probability distribution with unit width. The squares determine \( N \) widths \( x_i = y_i^2 \). By construction, in the limit \( N \to \infty \) these obey the PTD with \( \langle x \rangle = 1 \). Each of these widths is associated with one of \( N \) resonances. We have repeated that procedure 2500 times, thereby generating for each value
of \( N \) an ensemble of widths. For every member of the ensemble, we use the same cutoff \( x_{\text{min}} \) and determine \( N_{\text{incl}}, \langle x_i \rangle \) and \( \langle \ln x_i \rangle \). These values are used to construct the curves representing Eqs. (5) and (6). As a general rule we find that for finite \( N \) and with increasing \( x_{\text{min}} \), the curve representing Eq. (5) (Eq. (6)) is rotated in the clockwise direction (in the counter-clockwise direction), as in the case for \( N = \infty \). In addition, the shapes of the two curves are tilted in a way that depends on the specific \( N \) values of the widths \( x_i \). Fig. 5 shows two cases for \( N = 100 \), a value relevant to the sets of neutron widths. In both cases, the rotation of the two curves with increasing \( x_{\text{min}} \) is clearly seen. In one case, the point of intersection of the two curves representing Eqs. (5) and (6) occurs for \( \nu \) significantly less than unity; for the other case, the point of intersection produces a value of \( \nu \) noticeably larger than unity.

Fig. 6 shows a scatter plot of the values of \( \langle x_i \rangle \) and \( \langle \ln x_i \rangle \) over the ensemble of 2500 random drawings of \( N = 100 \) widths when a cutoff \( x_{\text{min}} = 0.2 \) is employed. We note that the fluctuations used in Figs. 3 and 4 are realistic. Cases where values \( \nu < 0.1 \) or \( \nu > 2.3 \) are obtained as solutions of Eqs. (5) and (6) are indicated separately in the figure. For every value of \( \langle x_i \rangle \) the highest (lowest) values of \( \nu \) occur for the highest (lowest) values of \( \langle \ln x_i \rangle \). The values \( \nu < 0.1 \) and \( \nu > 2.3 \) are chosen so as to obtain approximately similar numbers of extreme cases.

As a summary of these results, Fig. 4 shows the distribution of \( \nu \) values that are obtained as solutions of Eqs. (5) and (6) for the 2500 random drawings of \( N = 100 \) widths with cutoff values of \( x_{\text{min}} = 0.1 \) and \( x_{\text{min}} = 0.2 \). The corresponding means and standard deviations of these distributions are 1.06 and 0.42 for \( x_{\text{min}} = 0.1 \) and 1.10 and 0.59 for \( x_{\text{min}} = 0.2 \). This illustrates both a small bias toward increasing values of \( \nu \) obtained with this method (a fact which was mentioned briefly by Camarda) as well as a significant increase in the standard deviations as the cutoff parameter \( x_{\text{min}} \) is increased.

V. APPLICATIONS

We now apply this method to the NDE. In each case, we estimate \( \sigma_C \), the uncertainty associated with the combination of the finite-size-of-data effect and the application of a cutoff, by utilizing the simulation process described in Section IV: 2500 sets of widths, each set of size \( N \), are sampled from a Porter-Thomas distribution. A cutoff varying linearly with energy is then applied, as described in Ref. 4; the cutoff is parameterized by a quantity \( T_{\text{max}} \), where \( x_{\text{min}} = T_{\text{max}} E_{\text{n}}/E_{\text{max}} \) (\( E_{\text{n}} \) is the
neutron energy of the resonance in question, and $E_{\text{max}}$ is the maximum energy in that set of widths). The values of $N$ and $T_{\text{max}}$ for each member of the NDE are taken from Ref. [4]. We assume equally spaced resonances in our simulations. It is known that neutron resonance energy levels show significant short- and long-range correlations [1–3]. Because of the ensuing stiffness of the spectrum, this assumption of equal spacings should have minimal impact on our results. We take $\sigma_c$ to be the half-width of the central 68% of the distribution of the parameter $\nu$. The overall uncertainty is then obtained by combining $\sigma_c$ in quadrature with the uncertainty $\sigma_{\text{ML}}$ given by the previous maximum-likelihood analysis.

Table I summarizes the results. The first five columns are taken from Ref. [4]. The next column shows $\sigma_c$. The last column shows the total uncertainty when $\sigma_c$ is included.

In general, $\sigma_c$ in each case has approximately the same magnitude as the value of $\sigma_{\text{ML}}$ for that nuclide. The resulting weighted average of $\nu$ for the NDE when the cutoff error is included is $1.25 \pm 0.13$, as compared to the value $1.217 \pm 0.092$ listed in Ref. [4]. Even though the overall uncertainty is larger when $\sigma_c$ is included in the analysis, the weighted average of $\nu$ has also increased so that the level of significance changes very little from the figure given in Ref. [4]. Most of the increase occurs because the overall uncertainty for the largest data set, $^{232}\text{Th}$, is increased by a relatively smaller amount than the other data sets, and the value of $\nu$ for these data is rather high. To put this in perspective, the weighted average of $\nu$ when $^{232}\text{Th}$ is not included is $1.20 \pm 0.13$, a value which does not show nearly as significant a difference from the RMT expectation of $\nu = 1$.

VI. CONCLUSIONS

It has been known for a long time that various eigenvalue statistics (such as $\Delta_3$ [13]) are extremely sensitive to missing or spurious levels. The effects of spurious or missing levels on the reduced-width distribution have not been nearly as well studied. Koehler [4] has analyzed the reduced neutron widths in the nuclear data ensemble using a cutoff method to remove the smallest reduced widths, many of which probably belong to $p$-wave resonances. Unfortunately, the procedure also carries the risk of removing small $s$-wave resonances that should be
TABLE I. Results for the data sets included in the Nuclear Data Ensemble. The first three columns summarize the data. The next two show the cutoff parameter \( T_{\text{max}} \) used by Koehler [4] in his analysis, the resulting maximum-likelihood estimate for \( \nu \), and the uncertainty \( \sigma_{\text{ML}} \). The last two columns show the values of \( \sigma_c \) and the resulting overall uncertainties resulting from the application of a cutoff that is linear in energy, as described in the text.

| Nuclide | \( N \) | \( E_{\text{max}} \) (keV) | \( T_{\text{max}} \) | \( \nu \) | \( \sigma_c \) | \( \nu \) |
|---------|---------|-----------------|------------|-----------------|---------|--------|
| \( ^{64}\text{Zn} \) | 103 | 367.55 | 0.05 | 1.54 ±0.29 | 0.22 | 1.54 ±0.30 |
| \( ^{66}\text{Zn} \) | 65 | 297.63 | 0.05 | 0.74 ±0.27 | 0.30 | 0.74 ±0.30 |
| \( ^{68}\text{Zn} \) | 45 | 247.20 | 0.05 | 0.95 ±0.32 | 0.36 | 0.95 ±0.51 |
| \( ^{114}\text{Cd} \) | 17 | 3.3336 | 0.45 | 2.0 ±1.2 | 1.3 | 2.0 ±1.8 |
| \( ^{152}\text{Sm} \) | 70 | 3.665 | 0.1 | 1.55 ±0.40 | 0.33 | 1.55 ±0.50 |
| \( ^{154}\text{Sm} \) | 27 | 3.0468 | 0.1 | 1.32 ±0.65 | 0.57 | 1.32 ±0.86 |
| \( ^{156}\text{Gd} \) | 54 | 1.9908 | 0.2 | 2.94 ±0.51 | 0.46 | 2.94 ±0.69 |
| \( ^{158}\text{Gd} \) | 47 | 3.9827 | 0.2 | 2.94 ±0.74 | 0.49 | 2.94 ±0.73 |
| \( ^{160}\text{Gd} \) | 21 | 3.9316 | 0.2 | 0.83 ±0.75 | 0.80 | 0.83 ±1.10 |
| \( ^{161}\text{Dy} \) | 18 | 2.0431 | 0.2 | 1.41 ±1.0 | 0.90 | 1.41 ±1.3 |
| \( ^{162}\text{Dy} \) | 46 | 2.9572 | 0.2 | 0.99 ±0.47 | 0.48 | 0.99 ±0.67 |
| \( ^{164}\text{Dy} \) | 20 | 2.9687 | 0.2 | 2.3 ±1.2 | 0.81 | 2.3 ±1.4 |
| \( ^{166}\text{Er} \) | 109 | 4.1693 | 0.3 | 1.85 ±0.49 | 0.35 | 1.85 ±0.60 |
| \( ^{168}\text{Er} \) | 48 | 4.6711 | 0.3 | 2.16 ±1.2 | 0.56 | 2.16 ±1.4 |
| \( ^{170}\text{Er} \) | 31 | 4.7151 | 0.3 | 2.16 ±1.6 | 0.71 | 2.16 ±1.8 |
| \( ^{172}\text{Yb} \) | 55 | 3.9000 | 0.06 | 0.70 ±0.30 | 0.34 | 0.70 ±0.45 |
| \( ^{174}\text{Yb} \) | 19 | 3.2877 | 0.06 | 1.29 ±0.68 | 0.62 | 1.29 ±0.92 |
| \( ^{176}\text{Yb} \) | 23 | 3.9723 | 0.06 | 1.09 ±0.65 | 0.53 | 1.09 ±0.76 |
| \( ^{182}\text{W} \) | 40 | 2.6071 | 0.15 | 1.50 ±0.62 | 0.51 | 1.50 ±0.80 |
| \( ^{184}\text{W} \) | 30 | 2.6208 | 0.15 | 0.99 ±0.54 | 0.61 | 0.99 ±0.81 |
| \( ^{186}\text{W} \) | 14 | 1.1871 | 0.15 | 2.33 ±0.93 | 1.0 | 2.33 ±1.4 |
| \( ^{232}\text{Th} \) | 178 | 2.988 | 0.26 | 1.78 ±0.36 | 0.25 | 1.78 ±0.42 |
| \( ^{238}\text{U} \) | 146 | 3.0151 | 0.47 | 1.02 ±0.39 | 0.33 | 1.02 ±0.51 |

We have studied in detail how applying a constant cutoff affects the maximum-likelihood analysis of sets of theoretical and of computer-generated neutron widths generated from a PTD. Expressing the condition for the maximum of the likelihood function \( \ln L \) in terms of two equations, we have investigated numerically the dependence of these two equations on the cutoff \( x_{\text{min}} \) and on the number \( N \) of resonance widths. We have found it convenient to represent the two equations graphically, their point of intersection giving the values of \( \nu \) and \( \langle x \rangle \) that correspond to the maximum of \( \ln L \). We have focused on a realistic cutoff value \( x_{\text{min}} = 0.2 \) amounting to 20 per cent of the mean value of all widths. For \( N = \infty \), i.e., in the absence of finite-size-of-data-errors, the cutoff rotates the two curves in such a way that they run almost parallel. Therefore, any changes in the values of \( \langle x_i \rangle \) or of \( \langle \ln x_i \rangle \) that occur for finite values of \( N \) can cause significant shifts in the values of \( \nu \) and \( \langle x \rangle \) that maximize the likelihood function \( L \). The rotation persists for finite values of \( N \) but in addition each of the two curves is deformed, causing the wide scatter of solutions \( \nu \) shown in Fig. 7 for realistic cutoff values 0.1 and 0.2. The full width at half maximum of both distributions shown in Fig. 7 is about unity. We conclude that in realistic cases systematic errors (due to the cutoff) and finite-size-of-data errors (due to the finite number \( N \) of resonance widths experimentally available) combine in such a way that the resulting error on \( \nu \) is of order unity. We refer to the combination of both errors as the cutoff error.

The implications of the cutoff error for the NDE are displayed in Table I. Compared to the analysis of Ref. [4], the overall error is significantly increased for every nucleus. The weighted average over all nuclei gives \( \nu = 1.25 \pm 0.13 \). As expected, the total error is larger than that obtained in Ref. [4]. However, the mean value of \( \nu \) is also increased in such a way that the significance of the deviation of \( \nu \) from the RMT value remains nearly the same. We conclude that inclusion of the cutoff error does not remove the strong discrepancy (first displayed in Ref. [4]) between the distribution of neutron widths as predicted by RMT and the NDE. It must be borne in mind, however, that the strong discrepancy is essentially caused by the deviation from the PTD found for \( ^{232}\text{Th} \).

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