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REVIEW OF THE DIFFERENT METHODS TO DERIVE AVERAGE SPACING FROM RESOLVED RESONANCE PARAMETERS SETS

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RESUME:

「このことは、「このことを見る」ということに、「このことは、「このこと」ということに、「このこと」ということに、「このことに、「このこと」ということに、「このこと」ということに、「このこと」ということ

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The average spacing of resonances is an important parameter for statistical model calculations, especially concerning non fissile nuclei.

The different methods to derive this average value from resonance parameters sets have been reviewed and analyzed in order to tentatively detect their respective weaknesses and propose recommendations. Possible improvements are suggested.

I - INTRODUCTION -

For statistical model calculations the required parameters are neutron strengh functions, average radiative widths and the average spacing <D> of "S" resonances. These parameters are generally obtained from the analysis of the resonance parameters sets. The fact that the experimental resolution and sensitivity are limited in quality will result in an incomplete (missing levels) or distorded (error on partial width determination) information on the resonance parameters.

Generally, this fact has no practical consequence on strength functions *or* **Gamma width determination. On the contrary, in most cases average spacing cannot be directly deduced from resonance sequency and it is difficult to correct exactly for missing resonances.**

As a fact, a look in the littérature shows that, concerning this parameter, discrepancies by a factor 2 are common and even in some cases they can reach a factor 10.

However the importance of average spacing is basic since the average capture cross-section for non fissile nuclei : σ_c =2π² χ ² g_j 1/<Ū> <Γn><Γγ>/ \langle rn>+<Γγ> strongly depends on <D> **either on tne whole statistical energy range (large values of <D>), or *n the high energy part (small valuesof <0>). In these cases ry<<Tn and the above expression reduces to :** $\sigma_c = 2\pi^2 \pi^2 g_f$ $\langle \Gamma \gamma \rangle / \langle \mathcal{D} \rangle$ **.**

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On the other hand and more generally, the average spacing is a normalization constant for compound nucleus level density which governes the behaviour with the energy of the partial widths (except for fission width).

The need for an average spacing determination of good quality is justified by the progresses made recently in the theoretical knowledge of level densities.

II -THEORETICAL LAWS FOR RESONANCE PARAMETER DISTRIBUTIONS - 6ENESIS

11-1/ Leyel,_sp.açings :

Considering a compound nucleus at a finite excitation energy, the following assumptions were first made : 1) the distribution of resonance energies Er is not different from The distribution of the eigenvalues E_{λ} of the Hamiltonian H of the **compound nucleus ; 2) the distribution of a limited size sample is not different from**

the complete set.

In absence of very precise informations on the nuclear forces, the only thing which can be done is to assume a statisti**cal distribution for eigenvalue spac'ngs that directly result from a guess about the statistical nature of H matrix elements. In the frame of this hypothesis, WIGNER [1] first showed tîiat the probability f(D) to find a spacing between D and D+dD is proportional to the spacing itself. f(D) * D , with consequently for spacing distribution law a form :**

 $p(0) = D \exp \left\{-\int_0^D f(D) dD\right\} = De^{-D^2/2}$

o More precisely he guessed that the exact law should be

$$
p\left(\frac{D}{D}\right) = \frac{\pi}{2} \frac{D}{D} exp - \frac{\pi}{4} \left(\frac{D}{D}\right)^2
$$
 (1)

This law shows that nul spacings are excluded ("Level repulsion" property) and large spacings are poorly probable.

All the theoritical work developped afterwards considered different statistical distributions for H matrix elements.

By numerical computations of matrices of relatively high order (» 40) whose elements were independently distributed according to Gaussian Law with 0 mean, many authors did calculate spacings, collected in histograms well represented by the law (1).

The extension of such calculations to matrices of *very* **high order 1s really hard , but MEHTA [31 determined the upper and lower bounds for the theoritical integral distribution law :**

$$
F_{1ow} = 1 - exp \left\{-\left(\frac{\pi}{4} - \frac{D}{cD^2}\right)^2\right\}
$$
 (2)

$$
F_{upper} = 1-\exp\left\{-\left(\frac{\pi}{4} \frac{D}{}\right)^2\right\} \left\{1-\frac{1}{3}\left(\frac{\pi}{4} \frac{D}{}\right)^2\right\} \quad (3)
$$

These bounds are verified by WIGNER's surmise.

Proceeding from MEHTA's work, GAUDIN obtained the distribution function of spacings as an infinite product rapidly **converging, differing from WIGNER's surmise only by less than 5* up to D/<D> < 2.5 (See Fig. 1). For D/<D> < 2, HEHTA proposes :**

$$
F_{\mathbf{N}}(D/) = 1 - \left[1 + 0.078(\frac{\pi}{2} \frac{D}{D})^{2}\right] - 1.003 \times exp\left[-\frac{1}{4}(\frac{\pi}{2} \frac{D}{D})^{2}\right] \quad (4)
$$

which is a better approximation of the exact integral distribution given by GAUDIN [14] than what can be extrapolated from (1).

DYSON [4] proposed a new ensemble E in which a compound nucleus system is represented by a N x N unitary matrix S, instead of an Haniltonian H, the relationship between S and H being unspecified. The energy levels are related to the eigenvalues of the matrix S which are N complex numbers exp. iej distributed on the unit circle. According to Dyson the basic hypothesis is that "the behaviour of n consecutive levels of an actual system, where n is small compared to the total number of levels, is statistically equivalent to the behaviour in the ensemble E of n consecutive angles 6 on the unit circle, where n is small compared to N". Dyson imagined different systems. In particular, if the S matrices are symétrie unitary matrices, the ensemble E is the Ei orthogonal ensemble such as the system is unvariant under time inversion or space rotation, which are obvious physical requirements. For large values of spacings, Dyson gave the relationship :

$$
p\left(\frac{D}{D)} = A\frac{D^{17/8}}{D} \exp \left\{ -\left(\frac{\pi}{4} \frac{D}{D}\right)^2 - \frac{\pi}{4} \frac{D}{D}\right\}
$$
 (5)

From It, we see that Wigner's law underestimates the frequency of large spacings. That has no practical consequences since the probability of large values of D is *very* **small.**

Now, it is worth mentionning the correlations.

The correlations (short range, long range) which have been foreseen by theory and put in evidence by experiment cannot be extracted from Wigner's formula.

PORTER [5] using matrices of order 3 from the Gaussian Ensemble and KAHN [6] with matrices of high order from orthogonal ensemble obtained very close results for the first order spacing **distribution.**

Using matrices of order 10 from Gaussian Orthogonal Ensemble, PORTER [7] calculated nth order spacing distribution (n « 1,...9). His results were confirmed by GARRISON [8] on experimental distributions.

As concluding remark, Wigner's conjecture can be considered as an excellent approximation of what we think to be the "truth" as far as the spacing distributions of a single class level population are concerned and for D/<D> less than 2.5.

In the case of superposition of two uncorrelated clas**ses of level the spacing distribution given by LYNN [2] 1s :**

2

$$
p(x) = \frac{1}{\overline{x}_1 + \overline{x}_2} \left[\frac{\pi x \overline{x}_1}{2 \overline{x}_2^2} \exp\left(-\frac{\pi x^2}{4 x_2^2}\right) \left\{1 - \text{erf}\left(\frac{x \sqrt{\pi}}{2 \overline{x}_1}\right) \right\} + 2 \exp\left\{-\frac{\pi x^2}{4} \left(\frac{1}{2} + \frac{1}{x_2^2}\right) \right\} + \frac{\pi x \overline{x}_2}{2 \overline{x}_1^2} \exp\left(-\frac{\pi x^2}{4 \overline{x}_1^2}\right) \left\{1 - \text{erf}\left(\frac{x \sqrt{\pi}}{2 \overline{x}_2}\right) \right\} \right] \qquad (6)
$$

 $\frac{D}{5}$. where $x =$

II-2/ Neutron widths distribution :
The neutron widths of same spin and parity fluctuate strongly from resonance to resonance. The general expression of neutron width being $\Gamma_n = 2P_L\gamma_n^2$, these fluctuations are due to
reduced neutron width γ_n^2 since the penetration factor varies smuothly with energy.

In the frame of R matrix theory :
\n
$$
\gamma_{\lambda(c)} = \left(\frac{\hbar^2}{2Ma_c}\right)^{1/2} \int_{r_c = a_c} r_c^* \chi_{\lambda} ds_c
$$

where x_{λ} is the eigenfunction in the internal region and φ_{n}^{*} the joint surface function. According to PORTER-THOMAS [11] the integral can be approximated by sum over many cells in the configuration space. If the linear dimensions of cells are correctly cho-
sen (π/K) , the number of cells is large $(KR/\pi)^{3A}$ and the contributions from cells of positive and negative signs are equally probable. The application of the central limit theorem results in Gaussian form with 0 mean for $Y_{\lambda}(c)$ distribution.

The frequency function for the reduced widths follows from this fact :

$$
p(\gamma_n^2) d\gamma_n^2 = \frac{1}{\sqrt{2\gamma_n^2 + (\gamma_n^2)^2}} exp(-\frac{\gamma_n^2}{\gamma_n^2}) d\gamma_n^2
$$
 (7)

" It has to be noted that Porter-Thomas frequency function is a particular case of the "chi squared" frequency function with v degrees of freedom:

$$
p_{v}(x)dx = \Gamma(v/2)^{-1}(v/2 < x>)^{v/2}(v-2)/2 e^{-vx/2 < x> dx}
$$
 (8)

III - EXAMINATION OF POSSIBLE ERRORS ON RESONANCE PARAMETERS COMING FROM EXPERIMENTAL TECHNICS AND ANALYSIS METHODS -

The resonances are revealed when transmission or reaction cross-sections are measured with low energy incident neutrons. In this chapter, we investigate the possible causes of errors on the knowledge on resonance parameters due to the imperfections of the experimental technics and the analysis methods of the raw data.

III-1/ Experimental effects :

. Effects due to sample thickness :

The area of a weak resonance is : $A_T = \pi/2$ n σ_0 Γ for **total cross-section, and Ar •» w/2 o0 rr for reaction crosssection (o0 * 4irX*g rⁿ /r, r resonance total width).**

So, a compromise is to be found in transmission experi**ment between the sample thickness and sensitivity threshold taking into account the statistical fluctuation and the fact that the potential transmission introduces an important background compared to small resonances. Reaction cross-sections measurements are certainly more efficient to reveal weak resonances.**

Connected with sample thickness are the neutron multiple scattering and self screening effects. They affect only reaction crosssections data and are calculated by NONTE-CARLO and analytical Methods respectively. They déforme the shape of the cross-secti >n with poor consequences on level energy determination, but with substantial modification of partial widths.

. Doppier and energy resolution effects :

These effects have consequences on both level spacings and resonance widths. The Doppier effect is assumed to be Gaussian In shape with a width defined as

$$
\Delta = 2 \sqrt{k \frac{E}{A} T_{eff}}
$$

^T eff *s tn ^e effective temperature of the sample as defined by LAMB [10]. It is an experimental parameter of importance. By reducing T^e ff by a factor 4 (T going from 300°K to 77"K) resulting in a reduction of A by a factor 2, it was possible to detect three new resonances in 235U [9].

^E 3/2 The energy resolution is expressed as *all)* **« k » <ei At 1n time of flight experiment. 36.15L**

The Doppier effect is preponderant at low energy and up to some KeV.

These effects have consequences on both level spacings and resonance widths due to the fact that the doublets may not be separated.

. Neutron background determination :

An error on neutron background determination reacts directly on partial width values. But, according to many authors [12], [13], this error can be revealed by the shape analysis method.

111-2/ Effects.of analysis.methods : There are two methods to analyze raw data : Area Analy**sis method, and Shape Analysis Method :**

•«MMMH J

. Area analysis method :

The total resonance area is expressed in terms of the partial widths of the resonance and sample thickness e. For different values of this latter parameter a system of curves F(rn»rY,e) is obtained whose convergence zone determines Fn and *Ty* **with more or less accurate results.**

The advantage of this method is that the resonance area is not sensitive to Ooppler ani Resolution effects.

The disadvantages are that this method can hardly be applied to non-isolated resonances and to detect errors on background determination.

. Shape analysis method :

Jf obtained by a sample of small thickness, the raw data are written in the following way :

 $\sigma_{\mathbf{eff}}(E) = \sigma(E) \times D(E) \times R(E)$ for reaction cross-section **data. For transmission data we have Tr = (e-n crfE)xD(E)) x R (£)**

D(E) and R(E) are Doppler broadening and Resolution functions respectively. o(E) which is the "True" cross-section is calculated by a formalism which can be very sophisticated (multichannel, multilevel), but which has to be adequately chosen in function of the type of crocs-section. On the other hand, Doopler and Resolution widths must be small compared to natural resonance widths. This method uses the whole of experimental informations. It is fast and can detect errors in normalization or background determination.

It is basically the more efficient method if used with least squares procedure.

IV - REVIEW OF THE DIFFERENT METHODS USED TO DERIVE AVERAGE SPACIN6S -

There are three classes of methods :

- **. the method of MONTE-CARLO simulation ;**
- **. the methods wh<ch use the statistics concerning the position of the levels ;**
- **. the methods based on the fit of the reduced neutron width distribution by a PORTER-THOMAS Law.**

IV-1/ Method_of.MgNT|:CARLO.simylat1gn.{,Mn :

A set of resonance parameters is generated using WIG⁺ **NER's and PORTER-THOMAS laws with estimated values for <D> and <gTn>. It 1s used to simulate a total cross-section in the energy interval of interest taking Into account the experimental effects (Resolution, Doppler). This simulated cross-section is analyzed 1n the same way as the experimental cross-section. The percentage of missing resonances found in the simulated cross-section 1s supposed to be the same for the experimental one. This method 1s valid 1f the percentage of loss of resonances 1s not sensitive to the starting value of <D>. This method was used, for example, by DERRIEN [15], for 241 Am.**

IV-2/ Methods using statistics concerning the position of the levels

There is a method, often used even nowadays, which consists of the plot of the cumulative number $N(E)$ of levels as a function of energy ("Staircase" method). This method is based on the assumption, very questionable, that in the energy interval ΔE where the behaviour of N(E) is linear with the energy there are no missing resonances, and <D> is given by <D> = $\Delta E / N(E) \Delta E$

One method, directly derived from the previous one, is based on the Δ_3 statistics given by Dyson and MEHTA [16]. The best fit of N(E) is given by least squares procedure and a parameter Δ is defined as :

The Δ_3 parameter for the theoretical distribution is $1/\pi^2$ (Log. N-0.0687) with a variance independent of N $1.17/\pi^2$ = 0.11 for a multiplicity equal to 1). If Δ is $\sigma(\Delta_3)$ = such as : $\Delta_3 - \sigma(\Delta_3) < \Delta < \Delta_3 + \sigma(\Delta_3)$, the experimental set of re-
sonances is supposed complete and <D> is given by <D> $\pm \Delta E/f_{\Delta E}(AE+B) dE$.

This method has theoretical basis of high quality, but does not seem to be adequate for mean spacing determination because : - not very accurate : for a sample of 100 resonances,

the accuracy allowed for Δ is $\sigma(\Delta_2)/\Delta_3 = 0.24$; - it is not true that the omission of a few levels or the presence of spurious resonance will cause a large discrepancy between the theoretical value and the experimental value of Δ_3 . (see 148Nd and 151Sm treated as examples).

IV-3/ Methods based on PORTER-THOMAS law : In addition to <D> these methods give access to <grn> and then to neutron strength function.

The missing level estimator (M3) [17] uses properties of PORTER-THOMAS law resulting from partial integrations. According to KEYWORTH and al, the method consists in "calculating the quantity nEgrn/(25Fn)² starting with the largest value of grn in the interval and adding additional levels, one at a time, going from larger to smaller in the ordered array of observed values of gin. When this quantity equals 1.206, the total number of levels in the interval is n/0.617". This method which is quick and does not require any judgement is sensitive to the quality of the determination of the largest widths.

Least squares fitting procedure (M4):
In this method initiated at SACLAY [9], the fit concerns the part of the integral distribution above a given threshold of gIn^o, which is relatively small compared to the mean value. The assumption is made that only the small values of grn^o are missed with no consequence for the shape of the distribution above this threshold. In the case of the presence of "p" wave resonances the method is also applied if it is still possible to choose a threshold which eliminates the quasi totality of the "p" wave resonances. Several authors use the method by varying the threshold and keeping the value which gives the best fit to the remaining distribution.

Maximum likelihood method : 'ESTIMA" method *(HS)* **:**

For a distribution of reducedneutron width of a single class, the likelihood function is defined as the product of the frequences of each datum x_1 having a frequency function $Pv(x)$:

 $L(\nu,\bar{x}) = \prod_{i} P_{\nu}(x_i)$

The values of parameters which maximise the function L or its logarithm are the most likely values.

In ESTIMA code [19], [20], [21], the parameter v is kept equal to 1 with the justification that a departure from unity can be caused by instrumental bias or by surimposition of two populations. Consequently, the conditlonsof application of this code are the following :

- **in the enargy interval AE of interest, the unresolved doublets are judged very improbable on the basis of the experimental conditions ;**
- **the analyzed set of resonances contains only "sure" "s" wave resonance defined as such either by the author of the experiment, or by using a criterion based on the comparison with the possible largest mûjhitude for the "p" wave neutron widths for the considered nucleus. (In a recent code [22] the probability for a resonance to be "p" wave is explicitly included in the likelihood function).**

A maximum of informations (detection of systematic errors) is obtained if the method is applied to truncated distributions. At each position of the threshold corresponds a theoretical distribution fitting the data, characterized by a value for <grn> and resulting in an estimated total number Nt of resonances In the energy interval under analysis. So, a set of most likely values is obtained for <g**rn> and N_t.These values fluctuate with the threshold positions. Those which correspond to a "stabilization" are judged as "most physical" (see figure 4) .**

The average spacing is obtained by $\langle D \rangle = \Delta E / N_f^{SL}$.

The oscillations in the stabilization region give the error on the estimation of N|t. The "sampling" error 1s given by Dyson and Mehta as :

 $\frac{\Delta D}{D} = \frac{0.45}{N} \sqrt{\text{Log}(2\pi N) + 0.343}$,

where N 1s the number of the "observed" resonances. A check of the final results is obtained by loocking at the distributions of gTn around <gTn> as function of energy (partial integration, see fig. 7 and 10).

V - INTERCOMPARISON OF THE VARIOUS METH00S -

It is interesting \star ² "now for the reviewed methods the degree of sensitivity to the experimental effects. These ones have² **the following consequences on-the spacing and the reduced neutron width distributions.**

Spacing distribution :

the loss of resonances results In a deformation of the distribution In Its whole and there 1s no possibility to correct 1t. On the other hand, due to Its principle Itself the Ai statistics 1s unable to correct for a constant percentage of missing resonances.

Reduced neutron width distribution :

The loss of resonances (weak resonances) has no consequence on the shape of the distribution above a given threshold. The contamination by "p" wave resonances is easily detectable :

- **either the "p" wave resonances have small <gTn>. In that case only & small part of the distribution is perturbed which has to be analyzed above a given threshold ;**
- **or the "p" wave resonances have average width comparable in magnitude to those of "s"wave resonances (sample of resonances extending up to high energy or nuclei of 3p region with A * 90). In that case, two solutions : take into account the probability of existence of "p" wave resonances or work on sample populated only with sure "s" wave resonances.**

The detection of contamination by doublets requires in many cases a further analysis which can be a critical study of experimental conditions (Doppler effect, energy resolution) or a study of the variation of the largest widths as a function of energy (see figure lObis). It has to be noted that even-even nuclei have a small probability to exhibit doublets ("repulsion effect").

The presence of very large (or small) neutron widths has as no influence on the results given by the maximum likelihood methods or xz procedure provided that the threshold is position ned at low energy. The results obtained by Missing Level Estimator can be affected by such defaults.

In Annex one finds a partial illustration of the considerations mentionned above.

148Nd and 151Sm treated as sample cases show how discrepant can be the results on <D> obtained by the different methods from the same set of resonances :

Method Nucleus	M1	M2	M3	M4	M5
151 Sm	1.62	1.73	1.58	1.11	1.05
148 Nd	91.	113.	158.	171.	191.

- CONCLUSION -

The parameters obtained for 15lSm and 148Nd show clearly that there 1s a large discrepancy in the indications given by the methods based on spacing distribution (Ml, M2) and those given by the methods based on neutron width distribution (M3, M4, M5). So, 1t 1s obvious that the choice of the method to derive average spacing can be at the origin of large errors. But 1t 1s also obvious, and that 1s probably the essential point, that the choice of the resonance sampling plays a major role. In this choice the following considerations should be taken Into account :

1/ The analysis of set of resonance parameters should be performed jointly with a critical analysis of the experlmen-

tal conditions (sample thickness, resolution, background) and Of the method used to obtain the resonance paraneters (shape or area analysis, formalism , ...) ;

y **The priority should be given to the quality of the sampling rather than to the number of resonances.**

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ANNEX

151Sm

SOME COMMENTS ON THE CONDITIONS OF THE EXPERIMENT OF KIROUAC **AND** EILAND (Physical Review C, 11, 3, 895, 1975)

- ANNEX -

The experiment was performed by time of fligth method with a Linac and a 31.6 m fligth path. The nominal resolution was 4.4 ns/m at 20 ev and seems to be good enough to separate most important resonances up to about 100 ev. The sample thicknesses were 0.2858 x 10-3 and 0.0728 x 10-3 at/b giving a potential transmission of about 1, which is not adequate for the detection of weak resonances. We can Infer from this fact that there is probably an important loss of weak resonances - even at low energy where the resolution is good - which are hided by the statistical fluctuations in the experimental transmission curves. On figure 10 bis, we see that there are no resonances below a threshold $S_A(E) = 8.10^{-4} E^{\frac{1}{2}}$ (ev) in the energy range 0 ev to 100 ev. **Above this energy, a mathematical expression of the sensitivity threshold is rather difficult to be justified on the basis of technical arguments. The only comments which can be made are of qualitative nature :**

- the missed resonances have increasing value of gin

- the observed resonances have an increasing average value (existence of doublets, neutron background determination ?)

- the number of non separated doublets is Increasing (between 100 ev and 150 ev the number of resonances having gTn such as 0.2<gTn> \gTn< <grn> is reduced by a factor 2, the sensitivity threshold being unchanged).

It seems from this examination of KIROUAC and EILAND experiment that the resonance sampling to be treated should stop at 100 ev neutron energy, with the very simple question : how many resonances are missed below the threshold SA(E) » 8.10-4 $E^{1/2}$ (ev) 2 **(ev).?** ***

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Fig.1

 $Fig. 2$

 $\boldsymbol{\mathcal{B}}$

Fig.3

AFTER REFERENCE [19]

 $\mathcal{L}^{(1)}_{\mathcal{L}^{(1)}_{\mathcal{L}^{(1)}}}$

 $\frac{1}{4}$

 \vec{z}_i

 \overline{A}

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 $1 -$

 2_o

┑

 D^{obs} ev

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