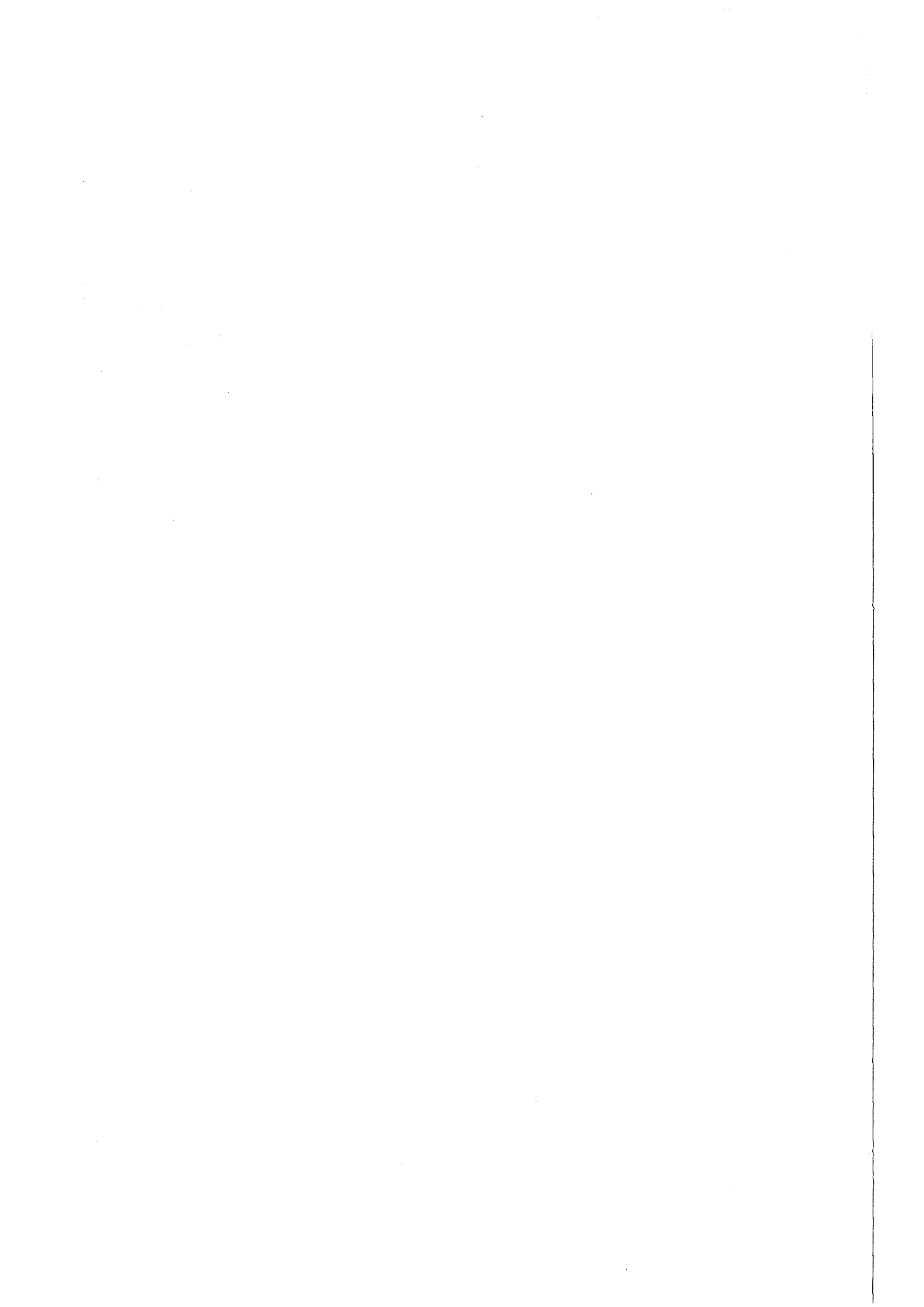


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Abstract

Level densities are most directly obtained by counting the resonances observed in the resolved resonance range. Even in the best measurements, however, weak levels are invariably missed so that one has to estimate their number and add it to the raw count. The main categories of missing-level estimators are discussed in the present review, viz. (i) ladder methods including those based on the theory of Hamiltonian matrix ensembles (Dyson-Mehta statistics), (ii) methods based on comparison with artificial cross section curves (Monte Carlo simulation, Garrison's autocorrelation method), (iii) methods exploiting the observed neutron width distribution by means of Bayesian or more approximate procedures such as maximum-likelihood, least-squares or moment methods, with various recipes for the treatment of detection thresholds and resolution effects. The language of mathematical statistics is employed to clarify the basis of, and the relationship between, the various techniques. Recent progress in the treatment of resolution effects, detection thresholds and p-wave admixture is described.

Statistische Schätzung von Niveaudichten aus aufgelösten Resonanzparametern

Zusammenfassung

Niveaudichten erhält man am unmittelbarsten durch Abzählen der Resonanzen, die im Bereich aufgelöster Niveaus beobachtet werden. Selbst in den besten Messungen werden jedoch unweigerlich schwache Resonanzen übersehen, so daß man ihre Anzahl abschätzen und zu der zunächst erhaltenen Zahl hinzuzählen muß. Die Hauptkategorien von Schätzfunktionen für fehlende Niveaus werden im vorliegenden Bericht diskutiert, und zwar 1) Treppenverfahren einschließlich derjenigen, die auf der Theorie der Hamiltonschen Matrix-Ensembles (Dyson-Mehta-Statistik) basieren, 2) Verfahren, die sich auf Vergleich mit künstlich erzeugten Wirkungsquerschnitten stützen (Monte-Carlo-Simulation, Garrisons Autokorrelationsmethode), 3) Verfahren, welche die beobachtete Verteilung der Neutronenbreiten ausnützen, mit Hilfe Bayesscher oder näherungsweise Prozeduren wie z. B. mit der Methode maximaler Mutmaßlichkeit, mit der Methode der kleinsten Quadrate oder mit Momentenmethoden, unter Verwendung verschiedener Vorschriften zur Behandlung von Beobachtungsschwellen und Auflösungsseffekten. Die Terminologie der mathematischen Statistik wird verwendet, um Grundlagen und die Beziehungen zwischen den verschiedenen Verfahren zu klären. Neuere Fortschritte bei der Behandlung von Auflösungsseffekten, Beobachtungsschwellen und p-Wellen-Beimischung werden beschrieben.

STATISTICAL INFERENCE OF LEVEL DENSITIES
FROM RESOLVED RESONANCE PARAMETERS

1. INTRODUCTION

Accurate information on level densities, apart from providing test material for level density theories [1-4], is indispensable for level-statistical calculations of average partial cross sections. These are roughly proportional to the level density if the relevant mean partial widths are known for instance from analysis of high-resolution neutron (or proton) resonance data. The level densities themselves are also most directly obtained in the resolved resonance region just above the neutron (or proton) separation energy, where it seems simple enough to count the resonances observed in a given energy interval.

This report is based on a paper prepared for the
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Weak levels are always missing, however, because of limited counting statistics and finite instrumental resolution. The preponderance of small values in the Porter-Thomas distribution of entrance-channel widths [5] and hence of weak levels aggravates the problem. As a consequence even the best contemporary high-resolution resonance data, for instance the ^{238}U transmission data shown in Fig. 1, are affected by about 20 % missing s-wave levels, and 30 or 40 % are quite common for less well studied nuclei. Level densities uncorrected for missing levels are therefore useless for most purposes. Nor does it help to take only the low-energy portion of the cumulative level count $N(E)$ with its typical nicely linear behaviour. This linearity is frequently mistaken as an indication that no levels are missed. Of course it indicates merely that the missing fraction does not depend on energy.

The whole problem of level density estimation is truly an evaluator's item - replete with missing data, shaky statistical models suggested by rather abstract spectral theories, rigorous equations which are so intractable that approximations must be invoked, logical and numerical traps etc. Even benchmark calculations have recently made their appearance in this field [7], showing that (and why [8]) impeccably conceived and carefully tested programs can produce less than satisfactory results. Liou [9] has reviewed a number of level density estimation techniques, giving a short functional description of each one. In the present paper (which updates and expands a recent similar review [10]) the emphasis will be on the probability-theoretical aspects. Since the very concept of level density is statistical it seems appropriate to use the tools of mathematical statistics to develop and to compare methods for the estimation of level densities and missing levels. It will then be seen that many of the seemingly quite different techniques which exist are mere variants of the same basic approach.

2. THEORY OF LEVEL STATISTICS

Strictly speaking there is nothing random or statistical about resonance energies or widths. They are determined as eigenvalues and by the eigenfunctions of a Schrödinger equation with suitable boundary conditions. A statistical description is justified only by the complexity of the spectra which reflects the complicated interaction between the many nucleons in the nuclear systems we consider here. The square roots of the reduced neutron (proton, photon, ...) widths, for instance, are essentially surface integrals over rapidly oscillating eigenfunctions in the $3A$ -dimensional configuration space associated with the A nucleons of a given nucleus. Without any further information one can therefore expect them to be normally distributed around zero. This hypothesis leads immediately to the Porter-Thomas distribution [5] for the reduced widths Γ ,

$$p(\Gamma|\langle\Gamma\rangle)d\Gamma = \frac{e^{-x}}{\sqrt{\pi x}} dx, \quad 0 < x \equiv \frac{\Gamma}{2\langle\Gamma\rangle} < \infty. \quad (1)$$

where $\langle\Gamma\rangle$ is the ensemble average (for clarity we omit the usual sub- and superscripts for reduced widths). Recently there were reports that in

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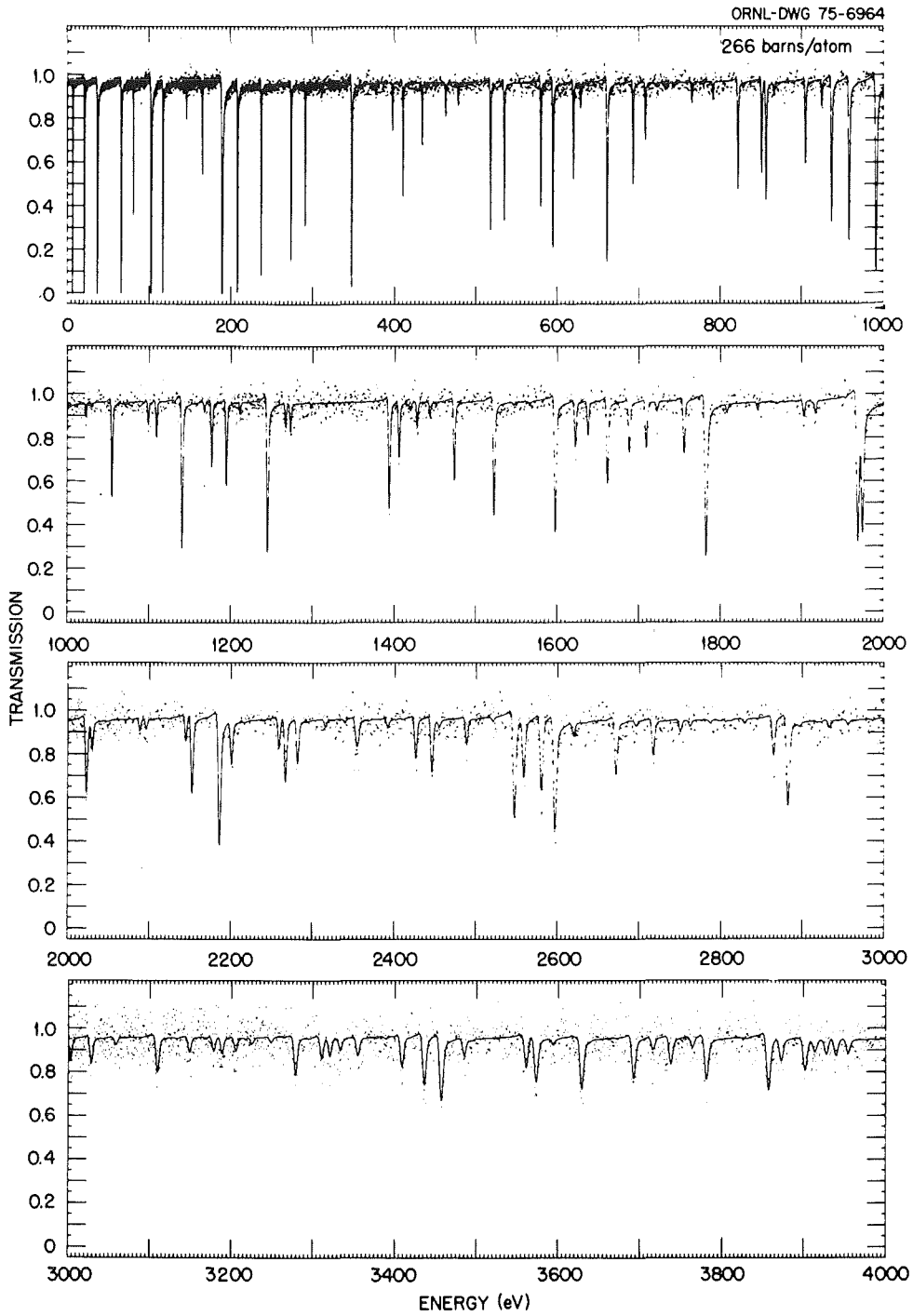


Fig. 1 - Points: high-resolution resonance data (transmission of neutrons through 0.76 mm of ^{238}U measured by time-of-flight), Curve: calculated from ENDF/B-IV total cross sections, Doppler broadened to 300 K (from Olsen et al. 1976, Ref. 8)

large-scale shell model calculations including two-body residual interactions the width distributions deviated from (1) [11, 12]. According to other studies [13, 14] the deviations vanished, however, if the secular variation of the average reduced width was properly taken into account (or if the sampling was restricted to reasonably narrow energy bins). So far all experimental neutron, proton and photon resonance data support local validity of the Porter-Thomas hypothesis.

The level spacing distribution is much more difficult to find. The level energies are the eigenvalues of a Hamiltonian matrix H which can be taken as real and symmetric since the nuclear interaction is invariant under time reversal. Furthermore, the probability density function $p(H)$ must be invariant under rotations in Hilbert space because all representations of H , including the diagonal form, are equally valid. The additional requirement that the matrix elements be independent of each other yields the Gaussian orthogonal ensemble (see [15]). This independence is, however, unfounded physically and leads to an unrealistic semi-circular dependence of level density on energy. Dyson (see [15]) introduced the circular orthogonal ensemble by assuming that some unitary (otherwise unspecified) matrix function S of H has its eigenvalues distributed uniformly around the unit circle. He showed that with this very general assumption one can reproduce any reasonable energy dependence of the level density. Mello et al. [16] studied the more physical statistical shell model where not the elements of H but only those of the residual (two-body) interaction are considered as random variables. Both the orthogonal ensembles and the statistical shell model (or two-body random ensemble) yield a level spacing distribution that is very close to Wigner's famous surmise (see [14, 15])

$$p(D|\langle D \rangle)dD = 2xe^{-x^2} dx, \quad 0 < x \equiv \frac{\sqrt{\pi}}{2} \frac{D}{\langle D \rangle} < \infty, \quad (2)$$

where $\langle D \rangle$ is the ensemble average. In addition to the level repulsion (improbability of small spacings) implied by (2) all random-matrix models predict that nuclear level sequences possess "nearly crystalline" regularity or stiffness in the sense that the cumulative level count $N(E)$ follows closely a straight line with slope $\rho = 1/\langle D \rangle$, excursions by more than one unit being extremely unlikely. This implies that spacings are correlated in such a way that a large spacing is followed by a short one more often than not and vice versa. The mean-square deviation from a best-fit straight line in an interval containing N levels, called the Δ_3 statistic by Dyson and Mehta [17], has the expectation value

$$\langle \Delta_3 \rangle = \frac{1}{\pi^2} \left\{ \ln(2\pi N) + \gamma - \frac{\pi^2}{8} - \frac{5}{4} \right\} \quad (3)$$

($\gamma = 0.5772\dots$ is Euler's constant) and the variance

$$\text{var } \Delta_3 = \frac{1}{\pi^4} \left(\frac{4\pi^2}{45} + \frac{7}{24} \right) \approx 0.012. \quad (4)$$

Absence of levels or presence of spurious levels from other sequences obviously increases Δ_3 . One has therefore tried to use it as a test statistic for the purity of level sequences. According to Dyson the best test statistic for the presence of spurious or missing levels in an almost

pure and complete level sequence is (see [18])

$$F_{\lambda} = \sum_{\mu \neq \lambda} \arccosh \frac{I/2}{|E_{\mu} - E_{\lambda}|} , \quad (5)$$

where μ runs through all levels between $E_{\lambda} - I/2$ and $E_{\lambda} + I/2$ and I is an arbitrary test interval (for instance 20 times $\langle D \rangle$). Expectation value and variance are, with $m \equiv \pi I / (2 \langle D \rangle)$,

$$\langle F_{\lambda} \rangle = m - \ln m - \gamma + 2 , \quad (6)$$

$$\text{var } F_{\lambda} = \ln m , \quad (7)$$

if E_{λ} is a true member of the sequence. If it is the energy of a spurious level in an otherwise pure sequence one gets

$$\langle F_{\lambda} \rangle = m , \quad (8)$$

so that a spurious or missing level should produce, on average, a peak or a dip of magnitude $\ln m$ in an almost constant trend. The catch, however, lies in the words "on average" (see [19]). In practice one finds that the Δ_3 and F_{λ} test criteria for purity and completeness are often satisfied for samples that are known to be neither pure nor complete.

3. ESTIMATION BASED ON LEVEL POSITIONS ALONE

It was already stated that simple ladder estimators such as a straight line fitted to the linear portion of the level number staircase curve $N(E)$ are usually rather worthless, and this is true also if they appear under the more pretentious name of Δ_3 statistic.

The seemingly straightforward approach of fitting the Wigner distribution (2) to the observed distribution of level spacings is ruled out by the bad distortion of the latter if 20 % or more of all levels are missing. Unfortunately none of the tests described so far permits unambiguous identification of spurious or missed levels. Nevertheless, as the Columbia group demonstrated, one can purify almost pure level sequences further by a combination of all available tests [19]. Such an ambitious program involves much judgement and is therefore not easily cast into the form of a computer code. Moreover, as already mentioned the tests based on orthogonal-ensemble theory are not as sensitive as one might expect [20-22]. For instance evaluated ^{238}U resonance parameters, after application of the Δ_3 test, yielded a seemingly pure and complete sequence of s-wave levels [23]. The mean spacing corresponding to the slope of the fitted straight line,

$$\langle D \rangle = 24.78 \pm 0.14 \text{ eV},$$

(see Fig. 2) was obtained from the W statistic recommended by Dyson and Mehta [17] as the optimal estimator for nearly pure level sequences,

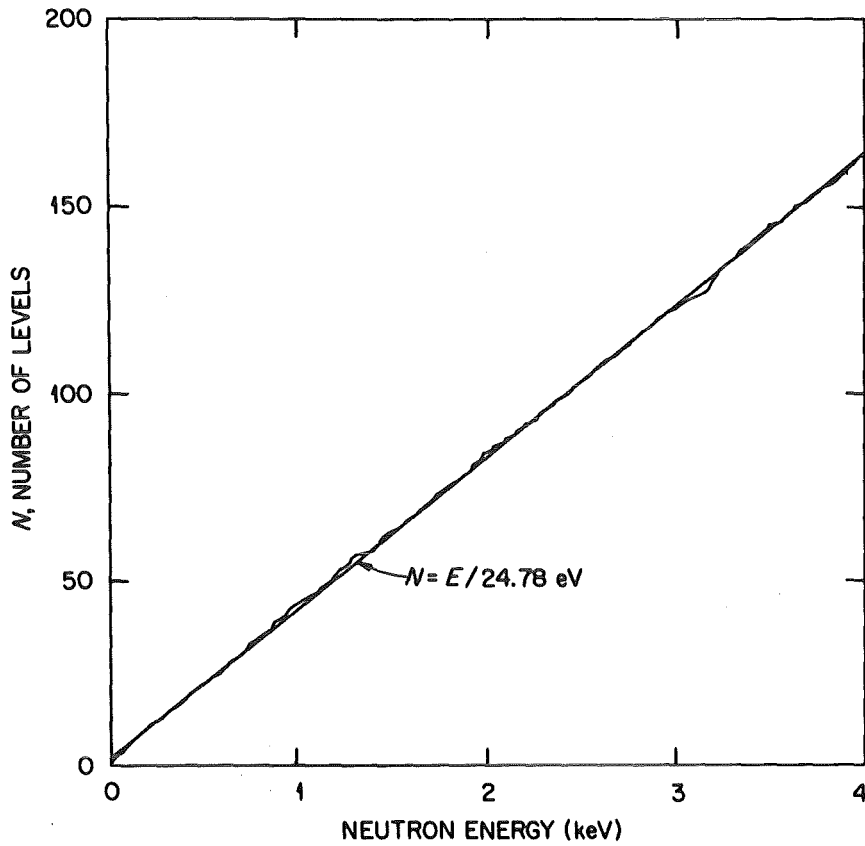


Fig. 2 - Cumulative number of s-wave levels versus neutron energy according to the evaluation of de Saussure et al., Ref. 23. There is no indication from the Δ_3 test that many weak levels are missing as shown clearly by the reduced-width distribution.

$$W = \sum_{\lambda=1}^N \sqrt{1 - \left(\frac{E_{\lambda} - \bar{E}}{I/2}\right)^2}, \quad \langle D \rangle = \frac{\pi I}{4 \langle W \rangle}, \quad (9)$$

where I and \bar{E} are length and midpoint of the energy interval considered. As will be seen below, however, the width distribution shows quite clearly that about 20 % of the levels are missing. Similar discrepancies for the stable iron isotopes [24] can be traced back to the same weakness of the Δ_3 and other related statistics. Now if the ladder tests suggested by orthogonal-ensemble theory are of such doubtful value already in these favorable cases, where levels are well separated and only one spin is possible for s-wave resonances (so that level repulsion is fully effective) they are quite useless for resonance data afflicted by severe level overlap and unknown level spins such as those for ^{233}U , ^{239}Pu and other fissile target nuclei with two superimposed s-wave sequences.

4. ESTIMATION BASED ON LEVEL POSITIONS AND WIDTHS

For the last-mentioned nuclei Monte Carlo techniques have proven useful. One generates artificial cross sections from resonance parameters sampled from the relevant distributions. By varying the mean widths and spacings one tries to make the artificial, Doppler and resolution broadened cross section curves statistically as similar as possible to the measured data. The number of unrecognisable and unresolved levels in the artificial cross section can then be taken as estimate for the number missed in the real data (see e. g. [25, 26]).

The difficult judgement of the statistical similarity between experimental and artificial cross sections was put on a quantitative basis by Garrison [27]. He uses the same energy grid and also the same cross section bin structure for both cross section curves and then generates a bivariate distribution in matrix form by considering all pairs of data points that are separated by the same energy difference ΔE (which is to be chosen as comparable to the mean level spacing). If the two cross sections of such a pair fall into the i -th and the k -th cross section bin the value one is added to the (i,k) matrix element. The two matrices thus created from the experimental and the artificial cross section are then compared by means of either a maximum-likelihood or a chi-square criterion to determine the degree of statistical similarity between both. Varying the level density and the mean widths one can maximise the statistical similarity. This method can cope with data that are quite badly affected by missing levels and unresolved doublets. Garrison's estimate for ^{235}U ,

$$\langle D \rangle = 0.38 \pm 0.04 \text{ eV}$$

[27], deduced from spin-merged data, is consistent with the value

$$\langle D \rangle = 0.44 \pm 0.04 \text{ eV}$$

found later by Moore et al. from spin-separated data measured with polar-

ised beam and sample [20], whereas previous, less quantitative comparisons with Monte Carlo generated cross sections had given much higher values [25]. It is obvious, however, that simpler techniques are required for routine extraction of level densities from the vast body of modern resonance parameter data.

5. ESTIMATION BASED ON WIDTHS

In contrast to the spacing distribution the neutron width distribution is only slightly affected by missing levels. The upper part of the Porter-Thomas distribution, corresponding to the strong levels, can usually be regarded as unperturbed. It is then possible to estimate the mean width from this part, for instance by a straightforward least-squares fit [28]. The expected number of missing levels and the level density can be calculated once the mean width is known. This, in essence, is the basis of the best level density estimation techniques available at present, even if they employ more refined methods. In order to introduce the relevant principles of probability theory we begin with a discussion of the simplest parameter estimation problem involving the Porter-Thomas distribution.

5.1 Unperturbed Porter-Thomas Distribution

Suppose we have a sample of reduced neutron widths $\Gamma_1, \Gamma_2, \dots, \Gamma_N$ from a pure Porter-Thomas distribution. The joint probability that in a random sample of size N , drawn from the distribution (3) with given $\langle \Gamma \rangle$, the sample values lie in the infinitesimal intervals $d\Gamma_1$ at $\Gamma_1, d\Gamma_2$ at $\Gamma_2, \dots, d\Gamma_N$ at Γ_N is

$$L(\Gamma_1, \dots, \Gamma_N | \langle \Gamma \rangle) d\Gamma_1 \dots d\Gamma_N = \prod_{i=1}^N p(\Gamma_i | \langle \Gamma \rangle) d\Gamma_i . \quad (10)$$

The joint probability density function L is called the likelihood function. It specifies the relative probabilities for different samples if the parent distribution and its parameter(s) are given. Our problem, however, is just the reverse. We want the probability density function not for the sample (that is given) but for the parameter $\langle \Gamma \rangle$ of the parent distribution. The recipe for the necessary inversion of conditional probabilities is provided by Bayes' theorem (see e. g. [29]) which thus constitutes the very basis for all scientific inference from experimental (uncertainty-affected) data. It states that the required (a-posteriori) probability is the product of the likelihood function and the a-priori probability for the estimated parameter(s). Writing $p_0(\langle \Gamma \rangle) d\langle \Gamma \rangle$ for our a-priori probability we get

$$p(\langle \Gamma \rangle | \Gamma_1, \dots, \Gamma_N) d\langle \Gamma \rangle \propto L(\Gamma_1, \dots, \Gamma_N | \langle \Gamma \rangle) p_0(\langle \Gamma \rangle) d\langle \Gamma \rangle . \quad (11)$$

This distribution, the Bayesian solution to the estimation problem, is the optimal solution: it contains the complete information about $\langle \Gamma \rangle$ which can

be extracted from the sample, including all error information. Its usefulness depends, however, on knowledge of the prior probability, and this is often unknown in the case of continuous parameters. In our case $\langle \Gamma \rangle$ is a scale factor. Jaynes [30], arguing that the prior probability cannot depend on the scale chosen, showed that for scale parameters the appropriate prior probability is $d\langle \Gamma \rangle / \langle \Gamma \rangle = d \ln \langle \Gamma \rangle$, thus giving a rigorous group-theoretical proof for a conjecture due to Jeffreys [29]. Next the question arises which value of $\langle \Gamma \rangle$ should be quoted as the best estimate, the maximum (mode) of p or the expectation value or something else? The recommended Porter-Thomas distribution should of course be the same whether we estimate $\langle \Gamma \rangle$ or $1/\langle \Gamma \rangle$ (both must be equally possible for a scale parameter). The Jeffreys-Jaynes prior probability suggests that we consider $\ln \langle \Gamma \rangle$ as the basic parameter, hence L as its probability density function. The maximum of L with respect to $\ln \langle \Gamma \rangle$ is then determined by

$$\frac{dL}{d \ln \langle \Gamma \rangle} = \langle \Gamma \rangle \frac{dL}{d \langle \Gamma \rangle} = \frac{1}{\langle \Gamma \rangle} \frac{dL}{d(1/\langle \Gamma \rangle)} = 0, \quad (12)$$

which shows that in each case we have to maximise the likelihood function, and that the recommended value is in fact the same in all three cases.

We could have avoided Bayes' theorem and the Jeffreys-Jaynes prior probability by use of the more familiar maximum-likelihood technique (see e. g. [29]). Writing down L explicitly for the Porter-Thomas distribution one sees that L is a product of one factor containing the sample values and a second factor which depends only on the true mean $\langle \Gamma \rangle$ and the sample average

$$\bar{\Gamma} \equiv \frac{1}{N} \sum_{i=1} \Gamma_i. \quad (13)$$

The factorisation shows that $\bar{\Gamma}$ is a minimal sufficient statistic, i. e. it is a number that can be calculated from the sample, contains all information about $\langle \Gamma \rangle$ that the sample contains and has the smallest scatter around its expectation value among all possible sufficient statistics. Small scatter is one property which a useful estimator must have. The second property is that it should be unbiased which means that its expectation value should be equal to the estimated true value. The sample average $\bar{\Gamma}$ has both properties. Furthermore it maximises the likelihood function, i. e. the value to be recommended is, as might have been expected,

$$\langle \Gamma \rangle = \bar{\Gamma}. \quad (14)$$

The statistic $\bar{\Gamma}$ has a χ^2 -distribution with N degrees of freedom [31],

$$p(\bar{\Gamma} | \langle \Gamma \rangle) d\bar{\Gamma} = \Gamma(N/2)^{-1} e^{-y} y^{N/2-1} dy, \\ 0 < y \equiv \frac{N \bar{\Gamma}}{2 \langle \Gamma \rangle} < \infty \quad (15)$$

(where $\Gamma(N/2)$ is a gamma function, not a width), as follows upon substitution of $\xi_i = \sqrt{\Gamma_i / (2 \langle \Gamma \rangle)}$ and integration in the space of the ξ_i over all angles, for fixed radius. Now (15) is seen to be basically the distribution

of the ratio $\bar{\Gamma}/\langle\Gamma\rangle$. It can be interpreted either as the distribution of $\bar{\Gamma}$ for given $\langle\Gamma\rangle$ or, equally well, as that of $\langle\Gamma\rangle$ for given $\bar{\Gamma}$,

$$p(\bar{\Gamma}|\langle\Gamma\rangle)d\bar{\Gamma} = p(\langle\Gamma\rangle|\bar{\Gamma})d\langle\Gamma\rangle . \quad (16)$$

The importance of this distribution lies in the fact that it contains the uncertainty information about the $\langle\Gamma\rangle$ estimate. One can establish confidence limits for any confidence level P by demanding that y -integration over (15) yield the value P between, and equal values $(1-P)/2$ below and above the limits, and then converting y -limits to $\langle\Gamma\rangle$ -limits. ($P \approx 0.68$ corresponds to the error bars of ± 1 standard deviation usually quoted for Gaussian distributions.)

Exactly the same estimate and the same associated probability distribution would have been obtained immediately with the Bayesian approach, i. e. by insertion of the Porter-Thomas distribution (1) and of the Jeffreys-Jaynes prior in Bayes' theorem, Eq. (11), and determination of the most probable value of $\ln\langle\Gamma\rangle$. In fact, the Bayesian and the maximum-likelihood solution coincide whenever a scale parameter (or a position parameter, with constant prior probability density [30]) is estimated. It should be understood, however, that in more general cases the maximum-likelihood solution only approximates the rigorous Bayesian solution (which is the price one has to pay for not working with the correct prior probability).

5.2. Porter-Thomas Distribution with Given Threshold

Let us now consider a less academic case. We assume that the sample contains only reduced widths that exceed a given detection threshold Γ_c . If the threshold depends on energy we must start from the bivariate distribution (properly normalised to unity)

$$p(\Gamma_i, E_i | \langle\Gamma\rangle, \Gamma_c) d\Gamma_i dE_i = \frac{1}{\text{erfc}\sqrt{x_c}} \frac{e^{-x_i}}{\sqrt{\pi x_i}} dx_i \frac{dE_i}{E_b - E_a} ,$$

$$x_c \equiv \frac{\Gamma_c(E)}{2\langle\Gamma\rangle} < x_i \equiv \frac{\Gamma_i}{2\langle\Gamma\rangle} < \infty , \quad E_a < E_i < E_b , \quad (17)$$

where the bar over the complementary error function denotes the energy average in the interval $(E_a \dots E_b)$. The joint probability to obtain the given sample of level energies and entrance-channel widths is

$$L d\Gamma_1 \dots d\Gamma_N dE_1 \dots dE_N = \left(\frac{2}{\sqrt{\pi} \text{erfc}\sqrt{x_c}} \right)^N e^{-\xi^2} d^N \xi \frac{dE_1 \dots dE_N}{(E_b - E_a)^N} \quad (18)$$

where $\xi^2 = (N/2)(\bar{\Gamma}/\langle\Gamma\rangle)$ is the squared radius and $d^N \xi$ is the volume element in the space of the ξ_i defined before. Factorising L one sees again that the sample average $\bar{\Gamma}$ is a minimal sufficient statistic. As before its distribution can be obtained by integration over all angles in the space of

the ξ_i for fixed level energies E_i . The resulting solid angle factor must then be averaged over level energies. The final distribution can again be interpreted either as that for $\bar{\Gamma}$ or as that for $\langle \Gamma \rangle$. Since the energy-averaged solid-angle factor does not depend on $\langle \Gamma \rangle$ one finds in the latter case

$$p(\langle \Gamma \rangle | \bar{\Gamma}, \Gamma_c) d\langle \Gamma \rangle \propto (\overline{\text{erfc}\sqrt{yz}})^{-N} e^{-y} y^{N/2-1} dy, \\ 0 < y \equiv \frac{N \bar{\Gamma}}{2\langle \Gamma \rangle} < \infty, \quad z \equiv \frac{\Gamma_c(E)}{N\bar{\Gamma}}. \quad (19)$$

Since we estimate a scale factor again, the maximum-likelihood solution coincides with the rigorous Bayesian solution. Maximising L with respect to $\langle \Gamma \rangle$ one obtains

$$\bar{\Gamma} = \langle \Gamma \rangle \left(1 + \frac{2}{\sqrt{\pi}} \frac{e^{-x_c} x_c}{\text{erfc}\sqrt{x_c}} \right). \quad (20)$$

The factor in parantheses corrects for threshold effects. Since it depends on $\langle \Gamma \rangle$ one must solve iteratively, for instance with the Newton-Raphson method. Once $\langle \Gamma \rangle$ is known one knows also $\text{erfc}\sqrt{x_c}$ and thus the estimated true number of levels, $N/\text{erfc}\sqrt{x_c}$.

Although this may not be readily apparent from the available documentation (20) is the basis of the algorithms developed by

- Fuketa and Harvey [32] (with $\Gamma_c/\Gamma = c \cdot E^b$, c and b being given constants characterising experimental conditions),
- Fort et al. [33] (ESTIMA code, $\Gamma_c = \text{const}$, chosen so as to exclude practically all p-wave levels),
- Rohr et al. [34] (MISDO, modified Fuketa-Harvey code with threshold chosen so as to restrict p-wave admixture to a given small fraction).

In none of these algorithms, however, is the $\langle \Gamma \rangle$ -uncertainty calculated from the exact distribution (19).

Another approximate estimation procedure is the moment method. One equates the sample moments with the true (ensemble) moments of the probability distribution whose parameters one tries to estimate. Moore [20] derived a missing-level estimator by equating the first two moments of the distribution of $\sqrt{\Gamma}$ (essentially the width amplitude) with their expectation values, for a sharp width threshold Γ_c .

$$\overline{\sqrt{\Gamma}} \equiv \frac{1}{N} \sum_{i=1}^N \sqrt{\Gamma_i} = \int_{\Gamma_c}^{\infty} \sqrt{\Gamma} p(\Gamma) d\Gamma / \int_{\Gamma_c}^{\infty} p(\Gamma) d\Gamma, \quad (21)$$

$$\overline{\Gamma} \equiv \frac{1}{N} \sum_{i=1}^N \Gamma_i = \int_{\Gamma_c}^{\infty} \Gamma p(\Gamma) d\Gamma / \int_{\Gamma_c}^{\infty} p(\Gamma) d\Gamma. \quad (22)$$

Inserting (1) explicitly one gets

$$\frac{\overline{\Gamma}}{(\overline{\sqrt{\Gamma}})^2} = \sqrt{\frac{\pi}{2}} e^{x_c} \operatorname{erfc}\sqrt{x_c} \left(\sqrt{\frac{\pi}{2}} e^{x_c} \operatorname{erfc}\sqrt{x_c} + \sqrt{2x_c} \right). \quad (23)$$

For given sample averages this is an equation for x_c which can be solved by iteration. If, in addition, the threshold Γ_c is known one obtains $\langle \Gamma \rangle = \Gamma_c / (2x_c)$. Moore, on the other hand, prescribes a value for x_c (e. g. 1/8 for the ^{238}U sample considered in [36]) which determines the right-hand side of (23). He then varies the threshold and thus the number N of levels included, beginning with a high threshold. Lowering the threshold he includes weaker and weaker levels in the sample averages until the left-hand side of (23) equals the fixed number on the right-hand side. The true number of levels is then estimated as $N/\operatorname{erfc}\sqrt{x_c}$. The mean level spacing found with this estimator for ^{238}U was

$$\langle D \rangle = 20.9 \pm 1.5 \text{ eV.}$$

This is to be compared with the 24.78 ± 0.14 eV obtained from essentially the same data base by means of the orthogonal-ensemble statistics Δ_3 and W (see Sect. 3.). The 19% discrepancy corresponds to weak levels that are clearly missing from the width distribution but did not show up in the Δ_3 test because they were fairly uniformly distributed over the energy range covered (0 to 4 keV). This illustrates the insensitivity of the orthogonal-ensemble test statistics mentioned before and the general superiority of estimation procedures based on the width distribution.

An estimator similar to the one devised by Moore could be based on (20). Assuming with Moore that the threshold does not depend on energy one can rewrite (20) as

$$\frac{\overline{\Gamma}}{2\Gamma_c} = \frac{1}{x_c} \left(1 + \frac{2}{\sqrt{\pi}} \frac{e^{-x_c} x_c}{\operatorname{erfc}\sqrt{x_c}} \right). \quad (24)$$

For given right-hand side one can again vary the threshold Γ_c and thereby also the number N of widths included in the statistic $\overline{\Gamma}$ until both sides of (24) are equal. With the final value of N the estimated true number of levels is $N/\operatorname{erfc}\sqrt{x_c}$ as before.

For given threshold, however, it is not more difficult to find $\langle \Gamma \rangle$ and thus $\operatorname{erfc}\sqrt{x_c}$ from (20). Moreover, this rigorous Bayesian approach has the advantage that confidence limits can easily be calculated from the correct distribution (19) whereas for Moore's missing-level estimator and the simpler one based on (24) the correct error estimation recipe is not so obvious.

5.3. Porter-Thomas Distribution with Unknown Threshold

The missing-level estimators discussed in the preceding section require thresholds to be set on the basis of experimental characteristics [32] or of prior knowledge about strength functions [33, 34] or by judging how far the unperturbed part of the width distribution extends [20, 28]. It will be shown now that for a pure Porter-Thomas distribution the threshold can be automatically estimated from the resonance parameters themselves without any other prior knowledge. We adopt the notation

$$u_i \equiv \operatorname{erfc} \sqrt{x_i} \quad , \quad u_c(E) \equiv \operatorname{erfc} \sqrt{x_c(E)} \quad , \quad (25)$$

so that $u_c(E)$ is the fraction of observed levels in the interval dE at E . In this representation the bivariate distribution of level energies and reduced neutron widths (normalised to unity) assumes the simple form

$$p(\Gamma_i, E_i | \langle \Gamma \rangle, \Gamma_c) d\Gamma_i dE_i = \frac{du_i}{u_c} \frac{dE_i}{E_b - E_a} \quad ,$$

$$0 < u_i < u_c(E_i) \quad , \quad E_a < E_i < E_b \quad . \quad (26)$$

This means that in an (E, u) -diagram the sample points (E_i, u_i) are uniformly distributed below the threshold $u = u_c(E)$ as shown schematically in Fig. 3.

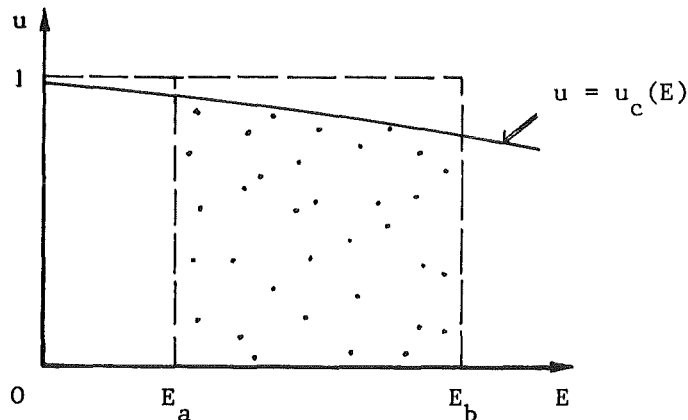


Fig. 3 - Threshold and distribution of sample points in (E, u) representation

Next we factorise, pulling out the energy average denoted by the overbar,

$$u_c(E) \equiv \overline{u_c} f(E) \quad , \quad (27)$$

and assume the energy dependence $f(E)$ to be known. This function can easily be obtained from the resonance data with adequate precision by least-squares fitting of a suitable test function to the cumulative level numbers

$N(E)$. Choosing a polynomial we can write for the fitted function and its derivative

$$\bar{N}(E) - \bar{N}(E_a) = \rho \bar{u}_c \int_{E_a}^E f(E) dE = c_1(E-E_a) + c_2(E-E_a)^2 + \dots \quad (28)$$

$$\frac{d\bar{N}}{dE} = \rho \bar{u}_c f(E) = c_1 + 2c_2(E-E_a) + \dots \quad (29)$$

where the coefficients c_n are known from the fit. The apparent level density $u_c \rho$ is easily expressed by known quantities if we put $E = E_b$ in (28) and utilise $f(E) = 1$. One finds

$$f(E) = \frac{c_1 + 2c_2(E-E_a) + \dots}{c_1 + c_2(E_b-E_a) + \dots} \quad (30)$$

A parabolic fit ($c_3 = c_4 = \dots = 0$), corresponding to a linear energy dependence of u_c , is usually quite adequate. Fig. 4 shows examples for parabolic fits.

Clearly $\langle \Gamma \rangle$ is a scale parameter again but the role of \bar{u}_c is less clear. Not knowing the prior probability we cannot invoke Bayes' theorem. Instead we try to find sufficient statistics by factorisation of L , and then their probability distribution by integration over as many widths and energies as possible. We start with a constant threshold, $f(E) = 1$. The joint probability for the whole sample is

$$L(\Gamma_1, \dots, \Gamma_N | \langle \Gamma \rangle, \Gamma_c) d\Gamma_1 \dots d\Gamma_N = \frac{1}{u_c^N} \frac{e^{-N\bar{\Gamma}/(2\langle \Gamma \rangle)}}{\langle \Gamma \rangle^{N/2}} \prod_{i=1}^N \frac{d\Gamma_i}{\sqrt{2\pi\Gamma_i}} H(\Gamma_i - \Gamma_c) \quad (31)$$

where H is the Heaviside function and Γ_1 the smallest width. This shows that $\bar{\Gamma}$ and Γ_1 are jointly sufficient statistics. Integration over all angles in the $(N-1)$ -dimensional space spanned by ξ_2, \dots, ξ_N results in the distribution

$$p(\bar{\Gamma}, \Gamma_1 | \langle \Gamma \rangle, \Gamma_c) d\bar{\Gamma} d\Gamma_1 \propto \frac{du_1}{u_c} e^{-y} y^{(N-1)/2-1} dy, \quad y \equiv \frac{N\bar{\Gamma} - \Gamma_1}{2\langle \Gamma \rangle} \quad (32)$$

This is the product of the joint probability that Γ_1 lies in $d\Gamma_1$ and all other widths are larger, viz.

$$p(u_1 > u_2 > \dots > u_N | u_c) du_1 = N \left(\frac{u_1}{u_c}\right)^{N-1} \frac{du_1}{u_c}, \quad (33)$$

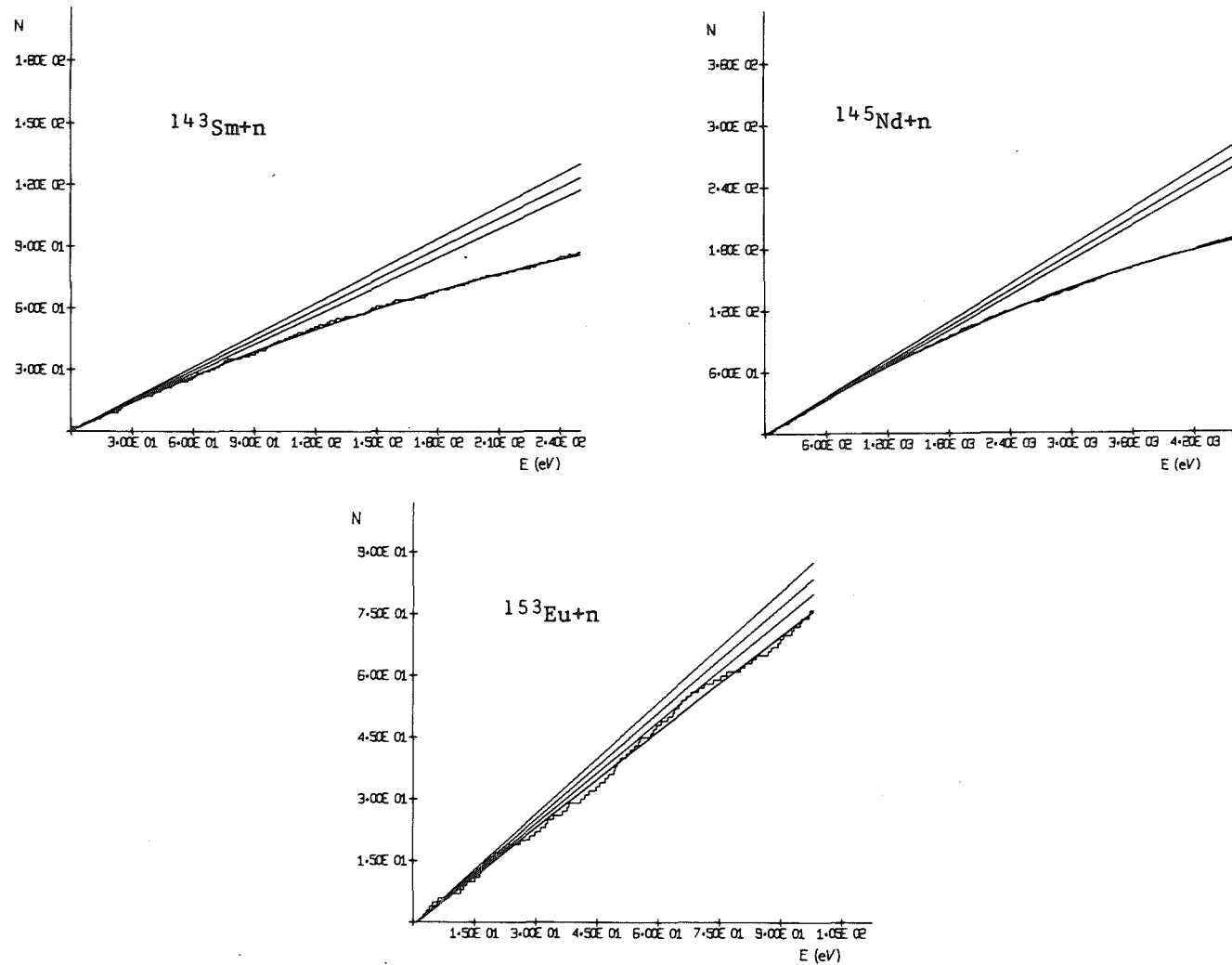


Fig. 4 - Examples for parabolic fits to level number staircase curves $N(E)$.
 Straight lines: STARA estimates and confidence limits for the level density corrected for missing levels (from Ref. 35), maximum-likelihood approach.

and the probability that the sum of these other widths is $N\bar{\Gamma} - \Gamma_1$ given that Γ_1 is the lower threshold, viz.

$$p(\bar{\Gamma} | \langle \Gamma \rangle, \Gamma_1) d\bar{\Gamma} \propto \frac{1}{u_1^{N-1}} e^{-y} y^{(N-1)/2-1} dy \quad (34)$$

Going to $\langle \Gamma \rangle$ and u_c as variables one finds from (32) the joint distribution of the estimated parameters,

$$p(\langle \Gamma \rangle, u_c | \bar{\Gamma}, \Gamma_1) d\langle \Gamma \rangle du_c \propto \frac{u_1}{u_c^N} e^{-y} y^{(N-1)/2-1} dy \frac{du_c}{u_c},$$

$$0 < y \equiv \frac{N\bar{\Gamma} - \Gamma_1}{2\langle \Gamma \rangle} < \infty, \quad 0 < u_c < 1 \quad (35)$$

For given Γ_1 the probability becomes maximal if u_c is minimal, i. e. $u_c = u_1$. This estimate is biased, however, being always low. Calculating the expectation value of u_1/u_c from (33) one finds that

$$u_c = \frac{N+1}{N} u_1 = \frac{N+1}{N} \operatorname{erfc}\sqrt{x_1} \quad (36)$$

is an unbiased estimator of the observable fraction of levels. Differentiation of L with respect to $\langle \Gamma \rangle$ yields

$$\frac{1}{N-1} \sum_{i=1}^N \Gamma_i = \langle \Gamma \rangle \left(1 + \frac{2}{\sqrt{\pi}} \frac{e^{-x_1} \sqrt{x_1}}{\operatorname{erfc}\sqrt{x_1}} \right) \quad (37)$$

Thus $\langle \Gamma \rangle$ can be found from (37) whereupon u_c and the estimated true number of levels N/u_c follow from (36). If the threshold depends on energy (37) remains valid^c but instead of (36) one finds

$$\frac{1}{u_c} = \frac{N+1}{N} \frac{\operatorname{erfc}\sqrt{x_1}}{f(E_1)} \quad (38)$$

In both (37) and (38) the subscript 1 refers now to the sample point which relatively speaking is closest to the threshold, i. e. which has the highest ratio $u_i/f(E_i)$ (but not necessarily the smallest Γ_i).

So far we assumed thresholds to be sharp. In reality, however, thresholds are diffuse. It is then better to base the estimation not on all members of the sample, but to discard the points in the region of the diffuse threshold. It is not difficult to derive the corresponding equations. If the sample members are enumerated in descending order of $u_i/f(E_i)$ and the estimation is based on the members k to N only one finds as generalisation of Eqs. (37) and (38)

$$\frac{1}{N-k} \sum_{i=k+1}^N \Gamma_i = \langle \Gamma \rangle \left(1 + \frac{2}{\sqrt{\pi}} \frac{e^{-x_k \sqrt{x_k}}}{\operatorname{erfc} \sqrt{x_k}} \right), \quad (39)$$

$$\frac{u_c}{c} = \frac{N+1}{N+1-k} \frac{\operatorname{erfc} \sqrt{x_k}}{f(E_k)}. \quad (40)$$

One can begin the estimation with the outermost point ($k=1$) and then move inward point by point to check the stability of the results against threshold variations. It should be pointed out that the rigorous result presented here differs from the maximum-likelihood result given in [8], especially for small samples.

Another way to deal with diffuse thresholds is to replace the Heaviside function in (31) by a function with smooth edges. This precludes a rigorous solution and one has to use the maximum-likelihood approximation, as is done in the STARA code [35]. Fig. 5 shows results for ^{238}U , obtained from the same data base as the mean level spacings quoted before (24.78 ± 0.14 eV [23], 20.9 ± 1.5 eV [36]). The average s-wave level spacing estimated with STARA was [35]

$$\langle D \rangle = 20.4 \pm 0.3 \text{ eV},$$

in good agreement with the value from Moore's missing-level estimator.

5.4 Porter-Thomas Distribution Distorted by Unresolved Multiplets

The level density estimators based on the observed width distribution which we discussed so far gave satisfactory results when tried on Monte Carlo generated resonance parameter sets, with reduced widths sampled from the Porter-Thomas distribution, resonance energies from the Wigner distribution or orthogonal-ensemble theory, and levels with a reduced width below some critical value rejected as missing. It came, therefore, as an unpleasant surprise when in the recent NEADB benchmark exercise [5] all of them systematically underestimated the level density by 4-8 % in cases which must be considered as quite favorable, viz. large, almost pure s-wave samples resembling those observed for actinides.

The NEADB test material was prepared as follows. Level widths and energies were produced by Monte Carlo sampling as usual, but not distributed. Instead, they were utilised by P. Ribon to generate Doppler- and resolution-broadened cross sections which were in addition subjected to simulated counting statistics. These "experimental" data (but not the original parameters) were handed over to H. Derrien who tried to recover the resonance parameters by multi-level shape analysis. His extracted resonance energies, neutron widths, spins and parities were then distributed to the participants. They contained thus not only threshold effects due to counting statistics in a very realistic way but also resolution effects in the form of resonance parameters that had been extracted from peaks mistaken for singlets while actually they were doublets and triplets. This latter effect is totally absent in resonance parameters directly obtained by Monte Carlo

sampling. That it was significant can be seen in Table I which shows characteristics of benchmark test material representing almost pure s-wave samples together with STARA results. Strength functions were estimated correctly but level densities were underestimated. One recognises that adding the true numbers of levels lost in unresolved multiplets (disclosed after the benchmark exercise) to the estimated missing-level numbers one gets almost exactly the correct numbers in all three cases. The conclusion is that most of the bias in the STARA results was due to unrecognised multiplets that had been analysed as singlets.

Table I - Characteristics of NEADB benchmark data and STARA results. Numbers in parantheses give STARA results modified by addition of the true number of levels lost in multiplets to the original STARA estimates of missing levels.						
Benchmark Case	S_0 (10^{-4})	$\langle D \rangle$ (eV)	all levels	missing levels	lost in multiplets	origin
5A	2.22 2.23±.30	1.85 2.02±.08 (1.84)	173 158±2 (174)	33 26±2 (42)	16 0 (16)	true STARA (")
5B	2.47 2.52±.25	1.43 1.56±.05 (1.42)	224 204±1 (226)	50 30±1 (52)	22 0 (22)	true STARA (")
5C	1.79 1.81±.25	1.82 1.90±.09 (1.77)	170 162±3 (175)	40 32±3 (45)	13 0 (13)	true STARA (")

Let us now consider the problem that levels are missed not because of a detection threshold but because limited instrumental resolution causes pairs, triples etc. of closely spaced levels to be mistaken for single peaks. We assume that this happens whenever spacings are smaller than some critical separation D_c which of course must be of the order of the instrumental resolution. The fraction of levels lost in unresolved multiplets is then

$$q = \int_0^{D_c} p(D) dD, \quad (41)$$

where $p(D)dD$ is the level spacing distribution. If one assumes that the apparent neutron width extracted from an unresolved multiplet peak is equal to the sum of the true component widths one can show that the observed width distribution is given by [8]

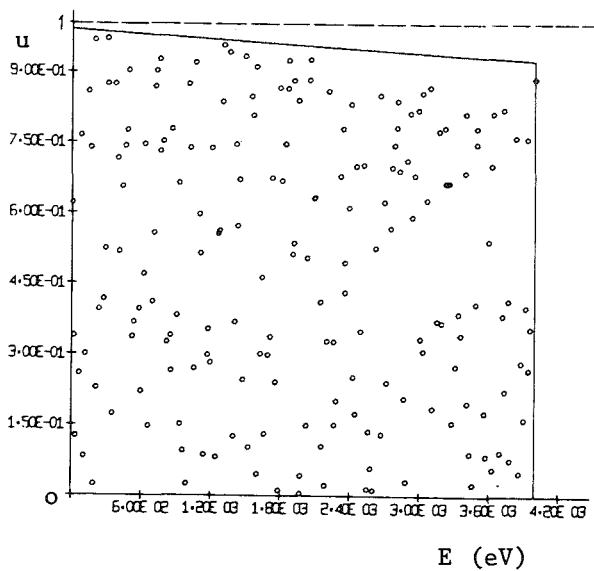
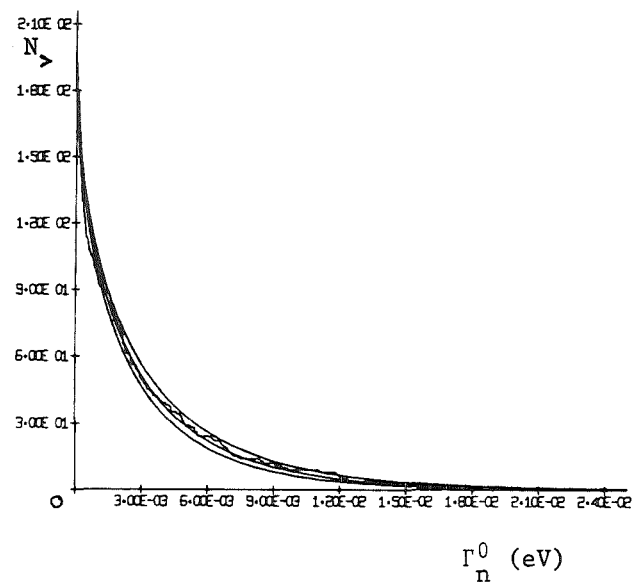
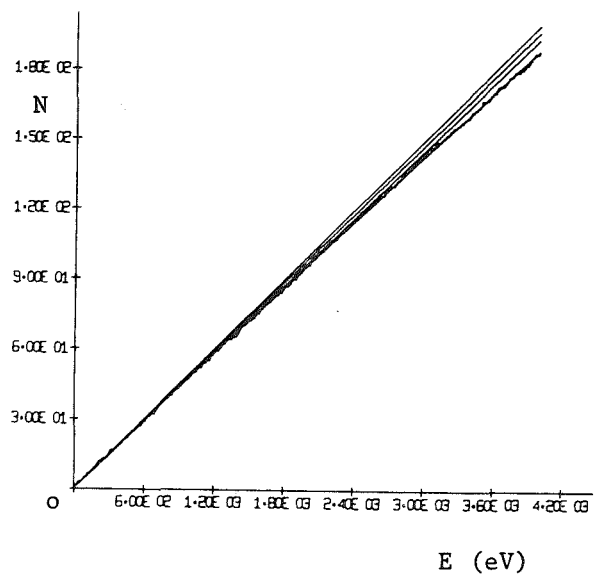


Fig. 5 - STARA results for $^{238}\text{U}+n$.

Top left: Level number staircase curve with parabolic fit and straight lines giving estimated level density and confidence limits (see text).

Top right: Integral Porter-Thomas distribution with confidence limits and data staircase curve showing scarcity of small levels.

Bottom: Uniformly distributed sample points in (E, u) diagram below automatically estimated detection threshold.

(from Ref. 35)

$$p(\Gamma|\langle\Gamma\rangle, q)d\Gamma = (1-q)(1+v) \frac{e^{-x}}{\sqrt{\pi x}} dx, \quad 0 < x \equiv \frac{\Gamma}{2\langle\Gamma\rangle} < \infty \quad (42)$$

with

$$v = \sqrt{\pi} z e^z (1 + \operatorname{erf} z), \quad z = q\sqrt{x} \quad (43)$$

in the case of a single Porter-Thomas distribution. The distortion factor $(1-q)(1+v)$ multiplying the undistorted width distribution reduces the relative frequency of small widths and increases that of large ones as was to be expected (Fig. 6).

It is quite easy to modify the estimators described so far (and the corresponding codes) by replacing the unperturbed Porter-Thomas distribution everywhere by the distorted distribution (42), (43). This analytic treatment of resolution effects is much more convenient than Monte Carlo cross section simulations. It is used in a new version of the STARA code for statistical resonance analysis which gave the improved benchmark results [8] shown in Table II.

Table II - Comparison between NEADB benchmark values and STARA-81 results obtained with analytical estimation of levels lost in unrecognised multiplets.			
Benchmark Case	S_0 (10^{-4})	$\langle D \rangle$ (eV)	origin
5A	2.22 2.20±.30	1.849 1.81±.19	true STARA-81
5B	2.47 2.49±.30	1.428 1.44±.05	true STARA-81
5C	1.79 1.78±.22	1.824 1.86±.09	true STARA-81

5.5. Mixtures of Level Sequences

So far we treated only a single s-wave level sequence as occurs for target nuclei with spin 0. For target nuclei with nonzero spin one has two s-wave level sequences. It is well known that the quantities $g\Gamma$ of the mixed sample (g being the spin factor) are again members of a Porter-Thomas distribution provided that the strength function is the same for both sequences and their level densities can be taken as proportional to $2J+1$, i. e. to g . This means that the methods discussed so far are applicable to all isotopically pure s-wave samples, from both even and odd nuclei.

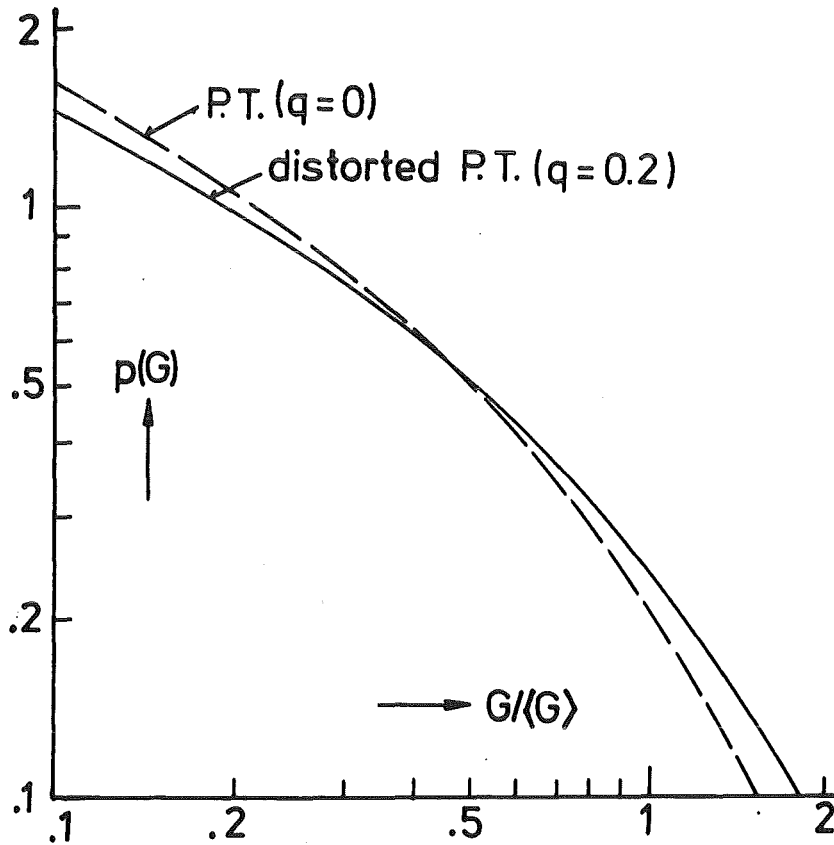


Fig. 6 - Undistorted Porter-Thomas distribution (perfect resolution, $q = 0$) and Porter-Thomas distribution distorted by 20 % missing levels lost in unrecognised multiplets ($q = 0.2$), according to the analytic approximation Eqs. (42), (43).

The problem of p-wave admixture with unidentified level parities is more difficult. One can use artificial thresholds to reject practically all p-wave levels (which usually have very small widths) as is done in ESTIMA [33], MISDO [345] and in the original version of STARA [35], or one can estimate the p-wave strength function together with the s-wave strength function and the level density, as is done in Stefanon's CAVE code [37] where the maximum of the likelihood function is determined by a simple grid search procedure. We shall look first at the simplest possible estimation problem involving an s-wave distribution $p_0(G|G^0)$ and a p-wave distribution $p_1(G|G^1)$ of neutron widths, where we use the notation

$$G \equiv g\Gamma_n \sqrt{1 \text{ eV}/E} (= g\Gamma_n^\ell v_\ell(E)), \quad G^\ell \equiv \langle g\Gamma_n^\ell \rangle \quad (44), (45)$$

g is the statistical spin factor, Γ_n the neutron width and v_ℓ the centrifugal-barrier penetrability (equal to 1 for the s-wave). As we assume that spins and parities are not or not always known we cannot calculate reduced widths from the $g\Gamma_n$ -values which resonance analysis yields (because this would require division by v_ℓ which depends on parity). For s-wave levels G is, however, just the reduced neutron width times the spin factor. For zero target spin both p_0 and p_1 are Porter-Thomas distributions (p_1 at least in good approximation) and we can write

$$p(G_i, E_i | G^0, G^1) dG_i dE_i = \left(w_0 \frac{e^{-G/(2G^0)}}{\sqrt{2\pi GG^0}} + w_1 \frac{e^{-G/(2G v_\ell(E_i))}}{\sqrt{2\pi GG^1 v_\ell(E_i)}} \right) \frac{dG_i dE_i}{E_b - E_a} \quad (46)$$

where w_0, w_1 are the a-priori probabilities that a given resonance is excited by the s- or the p-wave, viz.

$$w_0 = \begin{cases} \frac{\rho_0}{\rho_0 + \rho_1} \\ 1 \\ 0 \end{cases}, \quad w_1 = \begin{cases} \frac{\rho_1}{\rho_0 + \rho_1} \\ 0 \\ 1 \end{cases} \quad \text{for } \begin{cases} \text{unknown parity} \\ \text{s-wave level} \\ \text{p-wave level} \end{cases} \quad (47)$$

where ρ_0, ρ_1 are the densities of s- and p-wave levels ($\rho_1 = 3 \rho_0$ for target spin zero and approximate $(2J+1)$ -dependence of the level densities). The likelihood function becomes maximal for

$$G^0 = \langle g\Gamma_n^0 \rangle = \frac{\sum_i \tilde{w}_{0i} G_i}{\sum_i \tilde{w}_{0i}}, \quad G^1 = \langle g\Gamma_n^1 \rangle = \frac{\sum_i \tilde{w}_{1i} G_i / v_\ell(E_i)}{\sum_i \tilde{w}_{1i}} \quad (48)$$

where \tilde{w}_0, \tilde{w}_1 are the a-posteriori probabilities that a level with given E_i and G_i belongs to the s- or the p-wave part,

$$\tilde{w}_0 = \frac{w_0 \rho_0}{w_0 \rho_0 + w_1 \rho_1}, \quad \tilde{w}_1 = \frac{w_1 \rho_1}{w_0 \rho_0 + w_1 \rho_1} \quad (49)$$

Both estimated parameters occur in the a-posteriori weights so that the eqs. (48) are coupled and must be solved iteratively. For a pure s-wave

sample ($\rho_1 = 0$) the weighted average for $l = 0$ reduces to the unweighted sample average (14). Since we estimate scale parameters, the maximum-likelihood solution is rigorous and the probability distribution for them is just the likelihood function, from which confidence limits (and the covariance) can be calculated.

Eqs. (48) suggest a general approach for samples of mixed parity: Start with guess values for the parameters, calculate the a-posteriori probabilities for each member of the sample and go through the estimation procedure for pure s- and pure p-wave samples separately, with weighted G-values weighted by w_0 and w_1 , respectively. This yields improved estimates for $\langle g\Gamma_n^0 \rangle$ and $\langle g\Gamma_n^1 \rangle$ with which improved posterior probabilities can be calculated. Repeat the process until convergence is achieved. Moore adopted this prescription to generalise his missing-level estimator to mixed parities. The generalised estimator is implemented in the code BAYESZ, available from the neutron data centres. BAYESZ handles also resolution effects in a simple approximation.

It should be clear by now how the formulae derived for single Porter-Thomas distributions can be generalised. We shall only state the result for given, energy-dependent threshold: The maximum-likelihood equations to be solved for the two parameters $\langle g\Gamma_n^0 \rangle$ and $\langle g\Gamma_n^1 \rangle$ are ($l=0, 1$)

$$G^l = \langle g\Gamma_n^l \rangle = \frac{\sum_i \tilde{w}_{li} G_i / v_l(E_i)}{\sum_i \tilde{w}_{li}} \left(1 + \frac{1}{\sum_i \tilde{w}_{li}} \frac{2}{\sqrt{\pi}} \sum_i \frac{w_{li} \exp(-x_{cl}) \sqrt{x_{cl}}}{w_{0i} \operatorname{erfc} \sqrt{x_{c0}} + w_{1i} \operatorname{erfc} \sqrt{x_{c1}}} \right)^{-1} \quad (50)$$

where

$$x_{cl} = \frac{G_c(E)}{2 \langle g\Gamma_n^l \rangle v_l(E)} \quad (51)$$

It is not clear at present how much better the more rigorous Bayesian and maximum-likelihood methods are compared to ad hoc techniques such as Moore's missing-level estimator or the simple approach of finding $\langle g\Gamma_n^0 \rangle$ and the s-wave level density from a least-squares fit to the upper, unperturbed part of the width distribution, then subtracting the extrapolated s-wave distribution from the lower part and fitting the remainder with an average p-wave width. For small samples differences may become noticeable. In any case the more rigorous methods give clearer recipes for error estimation.

6. SUMMARY

Level density estimation methods have been reviewed with emphasis on the mathematical and statistical aspects. A new rigorous solution is given for the problem of simultaneous estimation of mean width and level density (or true number of levels) for a Porter-Thomas distribution affected by a detection threshold with known energy dependence but unknown height.

Furthermore, a new analytical treatment of resolution effects for s-wave levels is presented which can replace Monte Carlo simulation in many cases. The generalisation to mixed (s- and p-wave) resonance samples is also indicated briefly.

A number of conclusions can be drawn from experience with experimental data and benchmark test material:

- Estimators based on level energies (ladder statistics) are not useful except with extremely pure samples.
- Estimators based on the reduced-width (Porter-Thomas) distribution work well. Rigorous solutions for the parameter estimation problem can be given for simple models (known sharp detection threshold, sharp threshold with known energy dependence but unknown height), maximum-likelihood solutions are possible also for more complex models (diffuse threshold, p-level admixture).
- Resolution effects (levels missed in unresolved multiplets) can be treated analytically at least for pure (or almost pure) s-wave samples.
- Estimators should be tested with the NEADB benchmark test material (available from the neutron data centres). Simple tests with Monte Carlo generated resonance parameters are not sufficiently sensitive to resolution effects.
- New estimators could also be compared with well tested and documented codes such as BAYESZ, ESTIMA and MISDO (all available from the neutron data centres).

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