STATISTICAL ASSIGNMENT OF NEUTRON ORBITAL ANGULAR MOMENTUM TO A RESONANCE

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ABSTRACT

We have derived formulae for suggesting the neutron orbital angular momentum quantum number (l) to each neutron resonance if it is not identified experimentally. This suggestion is based on the probability that a resonance having a certain value of $g\Gamma_n$ is an l-wave resonance. The probability is calculated from the Bayes' theorem on conditional probability. For each l, the probability density function (pdf) of $g\Gamma_n$ was derived from the χ^2 distribution proposed by Porter and Thomas. The pdf takes into account two possible channel spins that result in the same total spin for a given l larger than zero. In addition, we suggest adopting the level density as the prior probability in the Bayesian approach regardless of the resolution of measurement. As a sample problem, we presented the result of l-assignment for ^{109}Ag resonances. The SUGGEL code, in which the methodology is incorporated, correctly assigned l's for 67 among 70 resonances of which l's had been determined experimentally. The other test for ^{27}Al showed the applicability of the code as a pre-analysis tool, even though such applicability is limited to a certain extent for light nuclides. The use of the code SUGGEL is expected to reduce the number of repeated runs of a fitting code such as SAMMY, thus to reduce time and effort for the extraction of resonance parameters from measurements.

1. INTRODUCTION

In most neutron cross section measurements, the cross sections are obtained as a function of incident neutron energy after a processing of raw measured data. Then, especially in the resolved resonance energy region, the resonance parameters are subsequently deduced from the point-wise cross sections. A few number of parameters for a resonance, in conjunction with a physics model such as the multi-level Breit-Wigner formula, substitutes for a huge amount of point-wise cross sections.

A set of resonance parameters for each resonance consists of the resonance energy, partial resonance widths such as Γ_n, Γ_γ and Γ_f, and quantum numbers such as the orbital angular momentum l and total spin J. However, it is not always possible to deduce all individual parameters unless several measurements for different kinds of cross sections are available together. This is the major reason why we often find integral quantities such as $g\Gamma_n$ or reaction areas in the literature instead of individual, separate parameters such as the statistical spin factor g (which is equivalent to J), Γ_n and Γ_γ.

The computer code SAMMY[1] is one of the most comprehensive and widely used tools in deducing resonance parameters from measured cross sections. However, there is a limitation: The user, so-called an evaluator, must specify the spin group of each resonance before the code is run. The spin group, which is identified by l, J, and channel spin s, cannot be adjusted automatically within the code. The current practice is as follows. An evaluator assigns spin groups as a part of input at his or her discretion, runs the code, investigates whether the fitted widths are satisfactory, then modifies the spin groups for some resonances, re-runs the code, and so on. This trial-and-error method is time and effort consuming. In addition, it requires the evaluator to make "judgment calls" based on his/her experience. Thus a tool that assigns the spin group in a rather automatic way is requested to reduce the number of trial-and-error runs. Among three quantum numbers for a spin group, the value of l is the primary concern.

We have developed a computer code SUGGEL[2], in which the Bayesian approach is adopted for suggesting the l value of a resonance. The Bayesian approach itself has been used in several analyses[3~8] since Bollinger and Thomas introduced the method in distinguishing p-wave resonance from s-wave resonance of ^{238}U[3]. In this paper, we focus on the formulae incorporated in the method. In addition, discussed are choice of the prior probability and interpretation of resulting posterior probability.

2. FORMULAE FOR BAYESIAN APPROACH

2.1. CONDITIONAL PROBABILITY FORMULATION

The problem being addressed is the determination of l of a resonance with known resonance energy E_r and $g\Gamma_n$. Note that we deal with $g\Gamma_n$, instead of Γ_n, because $g\Gamma_n$ is the quantity usually available from measurements.

From the Bayes' theorem on the conditional probability[9], the probability that a resonance having a certain value of $g\Gamma_n$ is an l-wave resonance is given by

$$P(l \mid g\Gamma_n) = \frac{P(g\Gamma_n \mid l)P(l)}{\sum_{l'} P(g\Gamma_n \mid l')P(l')} . \quad (1)$$

$P(l)$ is the prior (or *a priori*) probability that a resonance is an l-wave resonance and $P(g\Gamma_n \mid l)$ is the probability density function (pdf) of $g\Gamma_n$ of l-wave resonances. $P(l \mid g\Gamma_n)$ is the posterior (*a posteriori*) probability that we want to calculate. For practical application, it would be enough to consider up to d-wave (*i.e.*, $l = 2$; it is called s-wave when $l = 0$ and p-wave when $l = 1$).

2.2. CHOICE OF PRIOR PROBABILITY

It is somewhat subjective and ambiguous what the value of prior probability $P(l)$ should be. Most analyses using the Bayesian approach have adopted the l-dependent level density, in approximated and appropriately normalized form, as the prior probability. By contrast, some others[5,6] adopted a constant value regardless of l: Possibly, lack of information with respect to the prior probability for a 'detected' resonance with the finite resolution of a measuring device might request so-called non-informative, constant prior.

Regarding the choice of prior probability, there could be a lot of more discussions. Nevertheless, as argued in the Appendix, we suggest adopting both theoretical prior and pdf regardless of the

resolution of a measurement. In the code SUGGEL, the prior probability (hereafter we use the notation P_l instead of $P(l)$ for convenience) is assumed to be proportional to the level density such that

$$1/P_l = \overline{D_l} \sum_{l'} 1/\overline{D_{l'}} \,. \tag{2}$$

Here $\overline{D_l}$ is the average level spacing of l-wave resonances, which is computed from J-dependent average spacings as

$$1/\overline{D_l} = \sum_J 1/\overline{D_{lJ}} \,. \tag{3}$$

As emphasized by Gyulassy and Perkins[10], the summation goes over every possible J only once. On the other hand, with an assumption that the level spacing is independent of the incident neutron energy in the energy region of interest, the J-dependent average spacing can be calculated from the Fermi-gas formula approximated as[11]

$$1/\overline{D_{lJ}} = C \cdot (2J+1) \exp\left\{-(J+1/2)^2/2\sigma^2\right\}. \tag{4}$$

The proportional constant C and spin cutoff parameter σ^2 might be obtained[12] from the s-wave average spacing which is well known for most nuclides. Note that Eq. (4) reduces to so-called $(2J+1)$ law if σ is sufficiently large, *i.e.*,

$$1/\overline{D_{lJ}} \propto (2J+1) \,. \tag{4'}$$

2.3. PROBABILITY DENSITY FUNCTION

We have derived the probability density function (pdf) of l-wave neutron width, $P(g\Gamma_n|l)$, from the χ^2 distribution proposed by Porter and Thomas[13]. The probability that the magnitude of neutron width of an l-wave resonance lies in the interval $[g\Gamma_n, g\Gamma_n+d(g\Gamma_n)]$ is obtained by weighted superposition of partial probabilities corresponding to each J values, $p_{lJ}(g\Gamma_n)$. It is given by

$$P(g\Gamma_n|l)\,d(g\Gamma_n) = \sum_J w_{lJ}\, p_{lJ}(g\Gamma_n)\,d(g\Gamma_n) \,,$$

where the weight w_{lJ} is defined as

$$w_{lJ} = \overline{D_l}/\overline{D_{lJ}} \,. \tag{5}$$

Porter and Thomas proposed[13] that the reduced neutron widths obey the following χ^2 distribution:

$$p(x)dx = \frac{e^{-x/2}}{\sqrt{2\pi x}}dx \quad \text{for } \mu = 1, \text{ and}$$

$$p(x)dx = e^{-x}dx \quad \text{for } \mu = 2,$$

where $x = \Gamma_n^l/\overline{\Gamma_n^l}$. The degree-of-freedom, μ, is the number of exit channels and is equal to the multiplicity of J.

Now we replace the reduced width with $g\Gamma_n$ and neutron strength function. Here are necessary relations[14]: the neutron reduced width

$$\Gamma_n^l = \sqrt{\frac{1}{E_r}}\frac{\Gamma_n}{v_l} \quad (E_r \text{ in eV});$$

the penetrability v_l such that

$$v_0 = 1, \quad v_1 = \frac{(kR)^2}{1+(kR)^2}, \text{ and } \quad v_2 = \frac{(kR)^4}{9+3(kR)^2+(kR)^4},$$

where k and R are the neutron wave number and scattering radius, respectively; and the neutron strength functions

$$S_l = \frac{\overline{g\Gamma_n^l}}{(2l+1)\overline{D_l}} \quad \text{and} \quad S_{lJ} = \frac{\overline{\Gamma_n^l}}{\overline{D_{lJ}}}.$$

Then, with the aid of an assumption[14] such that

$$S_{lJ} = \mu_{lJ} S_l,$$

where μ_{lJ} is the multiplicity of J, the partial pdf's are written as follows.

$$p_{lJ}(g\Gamma_n) = \sqrt{w_{lJ}} \frac{\exp\left(-\frac{w_{lJ} g\Gamma_n}{2 g_J T_l}\right)}{\sqrt{2\pi g\Gamma_n g_J T_l}} \quad \text{for } J \text{ values with } \mu_{lJ} = 1, \text{ and}$$

$$p_{lJ}(g\Gamma_n) = w_{lJ} \frac{\exp\left(-\frac{w_{lJ} g\Gamma_n}{2 g_J T_l}\right)}{2 g_J T_l} \quad \text{for } J \text{ values with } \mu_{lJ} = 2,$$

where $T_l = \overline{D_l} S_l \sqrt{E_r} v_l$ and $g_J = (2J+1)/2(2I+1)$ for a target nuclide of spin I. Two possible channel spins for the same J are taken into account in the latter partial pdf. Then we obtain the pdf for Eq. (1) as

$$P(g\Gamma_n \mid l) = \sum_J \left(\frac{w_{lJ}^{3/2}(2-\mu_{lJ})}{\sqrt{2\pi g\Gamma_n g_J T_l}} + \frac{w_{lJ}^2(\mu_{lJ}-1)}{2 g_J T_l} \right) \exp\left(-\frac{w_{lJ} g\Gamma_n}{2 g_J T_l}\right). \quad (6)$$

Applying Eqs. (2)~(6) to Eq. (1), we can calculate the posterior probability to be l-wave. The code SUGGEL independently calculates $P(l=0 \mid g\Gamma_n)$ and $P(l=1 \mid g\Gamma_n)$ using Eq. (1).

2.4. APPROXIMATION WITH THE (2*J*+1) LAW

Gunsing *et al.*[8] presented a formula for the Bayesian approach with the same idea of weighted superposition of partial pdf's. Assuming the (2J+1) law for the average level spacing (See Eq. (4')), we can reproduce their formula as well as formulae found in other works[3~6] from Eq. (6).

Under the (2J+1) law, the weight becomes

$$w_{lJ} = g_J / G_l, \text{ where } \quad G_l \equiv \sum_J g_J,$$

and $\overline{D_l}$ is computed from the s-wave average spacing as

$$\overline{D_l} = \overline{D_0} \cdot G_0 / G_l.$$

Then Eq. (6) is simplified, with $G_0 = 1$ for any I, as

$$P(g\Gamma_n \mid l) = \left(\frac{\alpha_l}{\sqrt{2\pi\, g\Gamma_n\, T_l^*}} + \frac{1-\alpha_l}{2\,T_l^*} \right) \exp\left(-\frac{g\Gamma_n}{2\,T_l^*} \right), \tag{7}$$

where $T_l^* = \overline{D_0}\, S_l \sqrt{E_r}\, \nu_l$. In addition, the prior probability becomes

$$P_l = G_l / \sum_{l'} G_{l'} \,. \tag{8}$$

Table I shows values of G_l and α_l which depend on the target spin. Note that $\alpha_l \cdot G_l$ is the partial sum of g_J's corresponding to $\mu_{lJ} = 1$.

Table I. Sums and Fractions of Statistical Factors under (2*J*+1) Law

Target Spin, *I*	*l* = 0		*l* = 1		*l* = 2	
	G_0	α_0	G_1	α_1	G_2	α_2
0	1	1	3	1	5	1
1/2	1	1	9/4	2/3	15/4	2/3
1	1	1	2	1/2	20/6	1/2
3/2	1	1	2	1/2	25/8	2/5
≥ 2	1	1	2	1/2	3	1/3

Now suppose a problem of distinguishing *s*- and *p*-wave resonances: no detectable *d*-wave resonance is expected. It is a problem we often encounter for medium-heavy nuclides. Applying Eqs. (7) and (8) to Eq. (1) results in

$$P(l=1 \mid g\Gamma_n) = \left[1 + \frac{1}{G_1} \sqrt{\frac{S_1 \nu_1}{S_0 \nu_0}} \frac{\exp\left\{ \frac{g\Gamma_n}{2\overline{D_0}\sqrt{E_r}} \left(\frac{1}{S_1 \nu_1} - \frac{1}{S_0 \nu_0} \right) \right\}}{\alpha_1 + (1-\alpha_1) \sqrt{\frac{\pi\, g\Gamma_n}{2\,\overline{D_0} S_1 \sqrt{E_r}\, \nu_1}}} \right]^{-1} . \tag{9}$$

This formula, which is basically same to those already used in several works[3,5,6,8], should be practical with constants in Table I. We can derive a similar formula for a problem of distinguishing *d*-wave from *p*-wave resonances.

2.5. INTERPRETATION OF CALCULATED POSTERIOR PROBABILITY

The Bayesian approach is a statistical method. Hence there is an area of concern. The orbital momentum could, in fact, be *l'* regardless of how large is the calculated posterior probability to be *l*. Nevertheless, if there is no indication other than the calculated probability, the value suggested by the statistical model is an appropriate choice.

Meanwhile, there is a question regarding how large the calculated, posterior probability should be to assign a specific *l* value. In distinguishing *p*-wave from *d*-wave resonances of ^{206}Pb, Mizumoto *et al.*[4] regarded a resonance as a 'certain' *p*-wave if the probability is greater than 0.99 and as 'uncertain but probably' *p*-wave if the probability is in between 0.33 and 0.99. By contrast, Frankle *et al*.[5] adopted a different criterion in distinguishing the *s*-wave from the *p*-wave resonances of ^{113}Cd. Assuming prior probabilities of $P_0 = P_1 = 0.5$, they assigned a *p*-wave if $P(l=1 \mid g\Gamma_n)$ is greater than

0.69. In brief, the interpretation is different from researcher to researcher, although they have the same method of calculation.

Actually this issue of interpretation is closely related to the choice of prior probability and we may need a long discussion to resolve such an ambiguity as well as that on the prior probability. Nonetheless, with the justification of adopting a theoretical prior regardless of the measurement resolution, yet it seems reasonable to suggest the l value showing greatest posterior probability.

2.6. FEATURES OF SUGGEL

The most important function of the code SUGGEL is to assign l values. The other function is to assign J values by either the Bayesian approach or random assignment method. A formula was derived to calculate $P(J \mid g\Gamma_n, l)$. Concerning J assignment, however, the random method is preferable because the Bayesian approach has an intrinsic limitation[2]. The SUGGEL also includes the missing level estimator[15] to estimate the strength functions and level spacing. A user would utilize the results of missing level estimator to confirm that the input S_l and $\overline{D_0}$ values are reasonable. However, recall that the values of S_1 and S_2 are less confident because the number of measured $l \geq 1$ resonances is usually insufficient.

3. SAMPLE PROBLEMS

3.1. ^{109}Ag

An attempt was made to assign l values for ^{109}Ag resonances. The resonance energies and values of l and $g\Gamma_n$ for 70 resonances up to 1.383 keV were adopted from the compilation of Sukhoruchkin *et al.*[16] The quantum numbers were determined from the analysis of capture gamma-ray spectra[17]. This test case would validate the SUGGEL.

The code correctly assigned l's for 67 resonances among 70 (reference: 53 s-wave and 17 p-wave resonances). It calculated d-wave probabilities as zero for all resonances. The p-wave probabilities for several selected resonances are listed in Table II. The code assigned two s-wave resonances at 106.3 and 327.8 eV as p-waves and a p-wave at 681.5 eV as an s-wave. It seems that the mis-assignment for the first two cannot be avoided because their p-wave probabilities are so large. The Bayesian calculation of Lowie *et al.*[6] revealed the same problem. This shows the potential danger of the Bayesian approach. The third one, however, needs careful investigation because its p-wave probability, 0.45, is not distinctive. Another s-wave resonance at 300.9 eV also shows indistinctive p-wave probability of 0.43.

Table II. Calculated p-wave Probabilities and l Assignment for Selected Resonances of ^{109}Ag

Resonance Energy (eV)	p-wave Probability		l	
	$\sigma = 4.68$	$(2J+1)$ law	Ref.[16]	Assigned
106.3	0.94	0.94	0	1
169.8	0.79	0.74	1	1
300.9	0.43	0.29	0	0
327.8	0.83	0.80	0	1
681.5	0.45	0.34	1	0
949.3	0.04	0.02	0	0

Now let's consider the effect of the (2J+1) law. The spin of ^{109}Ag is 1/2. Adopting the law does not alter posterior probabilities significantly if the probabilities are close to zero or unity. However, the effect is rather strong for indistinctive cases, *e.g.*, resonances at 300.9 and 681.5 eV as shown in Table II. Since these indistinctive cases require additional review anyhow, the approximation with the (2J+1) law seems good enough from the practical point of view.

3.2. ^{27}Al

The resonance energies and $g\Gamma_n$'s of 12 s, 22 p, and 12 d-wave resonances were adopted from Sukhoruchkin *et al*.[16] The first resonance is at 5.905 keV and the last at 726.8 keV. Note that the resonance energies of light nuclides like ^{27}Al are very high.

The SUGGEL correctly assigned l's for 32 resonances, about 2/3 of total. However, the calculated probabilities are indistinctive for so many resonances. For instance, there are only 8 resonances of which the greatest probability among s-, p- and d-wave probabilities is greater than 0.85. Table III shows several extremely indistinctive cases as well as most distinctive ones. Of course, a distinctive probability does not guarantee a correct l assignment.

Table III. Calculated Posterior Probabilities and l Assignment for Selected Resonances of ^{27}Al

Resonance Energy (keV)	Probability			l	
	s-wave	p-wave	d-wave	Ref.[16]	Assigned
420.7	0.34	0.37	0.29	0	1
495.2	0.33	0.34	0.33	1	1
707.7	0.31	0.31	0.38	2	2
716.5	0.34	0.35	0.31	0	1
34.8	0.91	0.09	0.00	0	0
360.7	0.07	0.07	0.86	1	2
429.5	0.03	0.97	0.00	0	1
572.0	0.11	0.89	0.00	1	1

The deficiency of indistinctive probabilities stems from the large penetrability of high l wave neutrons at high energy. Therefore, the Bayesian approach may loose its capability of distinguishing l values for resonances at high energy region or, equivalently, for resonances of light nuclides. Even so, from the viewpoint that SUGGEL is a pre-analysis tool, the suggested assignment could be a good initial guess for a detailed analysis using SAMMY.

4. CONCLUDING REMARK

The use of SUGGEL is expected to reduce time and effort in the evaluation procedure, since the number of repeated runs of the resonance parameter fitting code might be reduced. An effective procedure would be to run three codes RSAP[18], SUGGEL, and then SAMMY. In this procedure, the RSAP's function of peak search of the measured total or scattering cross sections will first provide approximate resonance energy and $g\Gamma_n$ values. Then SUGGEL will generate a prior parameter file for SAMMY with suggested spin group identifications. Finally, SAMMY will be used to perform the detailed analysis.

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APPENDIX.
CHOICE OF PRIOR PROBABILITY FOR MEASUREMENT WITH FINITE RESOLUTION

In general, the neutron resonance width of high l resonance is smaller than that of low l resonance. Therefore, it is less plausible to detect, say, p-wave than to detect s-wave resonance and the degree of plausibility depends on the resolution. For example, if the resolution is very poor so that only very large resonances are detectable, the prior probabilities for p- and d-wave could be set to zero. This is the reason why we concern the resolution of measurements. However, here we justify that both theoretical prior and probability density function, regardless of the resolution of a measurement, are applicable to Eq. (1) in Section 2.1.

Actually what we want to know is $P(l \mid g\Gamma_n, D)$, the probability that a 'detected' (or resolved as a) resonance of $g\Gamma_n$ is an l-wave, instead of $P(l \mid g\Gamma_n)$ in the left hand side of Eq. (1). From the Bayes' theorem, the probability is calculated as

$$P(l \mid g\Gamma_n, D) = \frac{P(l \mid D)\, P(g\Gamma_n \mid l, D)}{P(g\Gamma_n \mid D)}.$$

Thus we need the prior probability $P(l \mid D)$, as well as the pdf $P(g\Gamma_n \mid l, D)$, for which the resolution of measurement must be taken into account. Fortunately, however, the multiplied form of $P(l \mid D)P(g\Gamma_n \mid l, D)$ can be substituted with $P(l)P(g\Gamma_n \mid l)$ as follows. With the aid of further relations from the Bayes' theorem again such that

$$P(l \mid D) = \frac{P(D \mid l)\, P(l)}{P(D)} \quad \text{and}$$

$$P(g\Gamma_n \mid l, D) = \frac{P(g\Gamma_n \mid l) P(D \mid g\Gamma_n, l)}{P(D \mid l)},$$

$P(l \mid g\Gamma_n, D)$ is written as

$$P(l \mid g\Gamma_n, D) = \frac{P(D \mid g\Gamma_n, l)}{P(g\Gamma_n \mid D) P(D)} P(l) P(g\Gamma_n \mid l).$$

Here we pay attention to an understanding that $P(D \mid g\Gamma_n, l)$, the probability to detect an existing l-wave resonance of $g\Gamma_n$, depends on the magnitude of $g\Gamma_n$, but not on l. Then we reach a conclusion

$$P(l \mid g\Gamma_n, D) \propto P(l) P(g\Gamma_n \mid l),$$

with which $P(l \mid g\Gamma_n)$ in Eq. (1) in the text is regarded to actually stand for $P(l \mid g\Gamma_n, D)$. The importance of the above is such that, in the multiplied form of a prior and a pdf, we can adopt both theoretical prior and pdf for the Bayesian approach presented in Eq. (1). Note also that the ratio of prior probabilities for different l's is important in Eq. (1).