

SUGGEL: A PROGRAM SUGGESTING THE  
ORBITAL ANGULAR MOMENTUM OF A  
NEUTRON RESONANCE FROM THE  
MAGNITUDE OF ITS NEUTRON WIDTH

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**SUGGEL: A Program Suggesting the Orbital  
Angular Momentum of a Neutron Resonance from  
the Magnitude of its Neutron Width**

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**February 2001**

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## ABSTRACT

The SUGGEL computer code has been developed to suggest a value for the orbital angular momentum of a neutron resonance that is consistent with the magnitude of its neutron width. The 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 by using Bayes' theorem on the conditional probability. The probability density functions (pdf's) of  $g\Gamma_n$  for up to  $d$ -wave ( $l=2$ ) have been derived from the  $\chi^2$  distribution of Porter and Thomas. The pdf's take two possible channel spins into account.

This code is a tool which evaluators will use to construct resonance parameters and help to assign resonance spin. The use of this tool is expected to reduce time and effort in the evaluation procedure, since the number of repeated runs of the fitting code (*e.g.*, SAMMY) may be reduced.



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# 1. Introduction

In most neutron cross section measurements in the resolved-resonance region, the quantity obtained after preliminary processing will be, for example, the total cross section as a function of energy. Then the experimenter or evaluator deduces individual resonance parameters for every resonance; these parameters include the channel radius, the resonance energy, the partial reaction widths ( $\Gamma_n$ ,  $\Gamma_\gamma$ ,  $\Gamma_f$ , and competition reaction width if any), and the angular momentum quantum numbers (orbital  $l$  and total  $J$ ) for each resonance.<sup>1</sup> These quantities compose a complete set of resonance parameters that should be provided to the evaluated library, specifically File 2 in the ENDF format. Any of several methodologies may be applicable to obtaining the resonance parameters from the measurements [for instance, Ha70, Mu80]; nevertheless it is still not a simple task to deduce values for all relevant parameters if a complete set of measurements is not available.<sup>2</sup> This is the major reason why we often find  $g\Gamma_n$  or reaction areas instead of individual values of  $g$  (equivalent to  $J$ ),  $\Gamma_n$  and  $\Gamma_\gamma$  in the literature.

Let us assume a situation in which an evaluator is deducing a complete set of resonance parameters for every resonance in a particular nuclide, starting from a known set of energy-dependent cross sections. The computer code SAMMY [La00], which is one of the most comprehensive and widely used tools in obtaining resonance parameters from measured data, could be used for this purpose. The evaluator must specify the values of  $l$  and  $J$  before the code<sup>3</sup> is run, because these values cannot be automatically adjusted (fitted) within the code. The current practice is as follows: The evaluator assigns values as a part of input at his/her discretion, runs the code, investigates whether the fitted widths are satisfactory, then modifies the assignments of the quantum numbers for some resonances, and reruns the code, and so on. This trial-and-error method, in addition to consuming time and effort, requires the evaluator to make “judgment calls” based on his experience alone.

In this report we describe a method, and its implementation, for suggesting appropriate values for the quantum numbers for each resonance from the resonance’s known  $g\Gamma_n$  in a rather automatic way.

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<sup>1</sup> The ENDF-6 format for the Reich-Moore formula has been recently revised [La99] to identify the channel spin ( $s$ ). So the channel spin is an additional quantity to be identified in case of adopting the Reich-Moore formalism.

<sup>2</sup> For instance, the quantity obtained from the transmission measurement is  $g\Gamma_n$  (thin sample) or  $g\Gamma_n \Gamma$  (thick sample), while the parameters to be provided in an evaluated library are  $l$ ,  $J$  (from which  $g$  may be derived),  $\Gamma_n$ ,  $\Gamma_\gamma$ , etc. If a measurement of scattering area (which is proportional to  $g\Gamma_n^2/\Gamma$ ) or capture area (proportional to  $g\Gamma_n\Gamma_\gamma/\Gamma$ ) is available as a supplement to the thin and thick sample transmission measurements, one can deduce values for each of  $g$ ,  $\Gamma_n$ , and  $\Gamma_\gamma$  for a non-fissile nuclide.

<sup>3</sup> Actually, each resonance is identified by the spin group in SAMMY. The spin group is defined by  $l$ ,  $s$  (channel spin), and  $J$ .

The resulting values could be a good initial assignment, thus saving time and effort for the evaluator. Chapter 2 describes the method. Chapter 3 describes the computer program SUGGEL; a description of the input is provided, along with some of the models used for calculating basic parameters such as the spin dispersion parameter. Also presented are examples using resonances of  $^{109}\text{Ag}$ ,  $^{27}\text{Al}$  and  $^{235}\text{U}$ . A conclusion and a discussion of future works are found in the final chapter. The derivation of the probability density functions is found in Appendix A. The program source list of SUGGEL is provided in Appendix B, and a brief description for the program LADDER in Appendix C.

## 2. Bayesian Approach for the Identification of $l$ and $J$

### 2.1. Formula of Conditional Probability

The Bayesian approach can be used to calculate a probability that a resonance with a known neutron width is an  $l$ -wave resonance. In spite of a potential danger of incorrect assignment of  $l$  [Mu80, Ga82], this approach has been used quite frequently. Bollinger and Thomas introduced this method in distinguishing  $p$ -wave resonances from  $s$ -wave resonances for  $^{238}\text{U}$  [Bo68]. Mizumoto *et al.* used the same concept in distinguishing  $d$ -wave from  $p$ -wave resonances for  $^{206}\text{Pb}$  [Mi79]. There are other cases such as the analyses for  $^{113}\text{Cd}$  of Frankle *et al.* [Fr94] and for  $^{107}\text{Ag}$  and  $^{109}\text{Ag}$  of Lowie *et al.* [Lo97]. A recent evaluation of fission products also adopted the method with refined formulae [Oh00].

The problem being addressed is the determination of  $l$  of a resonance at energy  $E_n$  from its known  $g\Gamma_n$  value. The neutron width multiplied by the statistical factor  $g$  ( $g\Gamma_n$ ) is called the neutron width hereafter for convenience. The formula for determination of  $J$  is easily derived and will be presented later. According to Bayes' theorem of conditional probability [Sm91], the probability that this resonance is an  $l$ -wave resonance is given by

$$P(l | g\Gamma_n) = \frac{P(g\Gamma_n | l) P_l}{\sum_{l'} P(g\Gamma_n | l') P_{l'}},$$

where  $P_l$  is the *a priori* probability that the resonance is an  $l$ -wave resonance.  $P(g\Gamma_n | l)$  is the probability that an  $l$ -wave resonance has the neutron width of  $g\Gamma_n$ . If the analysis is restricted to values of  $l \leq 2$  ( $d$ -wave), the above equation reduces to

$$P(l | g\Gamma_n) = \frac{P(g\Gamma_n | l) P_l}{\sum_{l'=0}^2 P(g\Gamma_n | l') P_{l'}} = \frac{P(g\Gamma_n | l)}{\sum_{l'=0}^2 P(g\Gamma_n | l') \frac{P_{l'}}{P_l}}. \quad (1)$$

Implicit in these equations is the assumption that the contribution of higher  $l$  values to the width  $\Gamma_n$  of a low- $l$  resonance is negligible. For instance,  $g\Gamma_n$  of a resonance identified as an  $s$ -wave may, in fact, include the  $d$ -wave contribution; however, the contribution is neglected by considering the small penetrability of high- $l$  neutrons especially in a low energy region. As a result, each resonance is assumed to be characterized by a single  $l$  value.

## 2.2. A Priori Probability

The *a priori* probability is assumed to be proportional to the level density, so that the ratio is given by

$$P_{l'}/P_l = \langle D_l \rangle / \langle D_{l'} \rangle,$$

where  $\langle D_l \rangle$  is the average level spacing of  $l$ -wave resonances. The level spacing is calculated from the Bethe formula for the level density [Be36], with an assumption that the level spacing is independent of the incident neutron energy in the energy range of interest.<sup>4</sup> Hence the level spacing is given by the formula

$$\frac{1}{\langle D_l \rangle} = C \cdot \sum_j (2J_{l_j} + 1) \exp\left\{-\left(J_{l_j} + 1/2\right)^2 / 2\sigma^2\right\}, \quad (2)$$

where  $j$  is the index for possible  $J$  values of given  $l$ -wave resonance and  $\sigma^2$  is the spin cutoff parameter. Generally, it is not necessary to know the proportionality constant  $C$  because only the ratio of level spacing is required in Eq. (1). When a value for the proportional constant is needed, it can be calculated from the  $s$ -wave average level spacing that is well known for most nuclides. A description of the calculation of the spin cutoff parameter and the proportionality constant  $C$  is in Chapter 3.

Due to the finite resolution of measurements, many weak (especially higher than  $s$ -wave) resonances may not be detected. Thus, for resonances readily detected, it is reasonable to adopt the *a priori* probability from the ‘measurable’ number of resonances, not from ‘theoretically expected’ numbers. In fact, this consideration is a formality only, because the effect of the *a priori* probability on the Bayesian *a posteriori* probability is much smaller than those of penetrability, which depends on the resonance energy, and the magnitude of  $g\Gamma_n$  itself. Moreover, in practice, the parameter values for the level density formula are obtained from measured resonance data. However, even if it is not important from the practical point of view, an option is provided in the program SUGGEL to modify the code-calculating *a priori* probabilities based on Eq. (2).

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<sup>4</sup> It is assumed that the energy of resolved resonance region is much lower than the magnitude (several MeV) of the neutron separation energy of a compound nucleus.

### 2.3. The Probability Density Functions

The probability density functions (pdf),  $P(g\Gamma_n|l)$ ,  $l = 0, 1$ , and  $2$ , have been derived from the  $\chi^2$  distribution proposed by Porter and Thomas [Po56]. The derivation, as well as assumptions incorporated in the derivation, is presented in the Appendix A. The results are:

for  $s$ -wave,

$$P(g\Gamma_n|l=0) = \sum_{j=1,2} w_{0j}^{3/2} \frac{\exp\left(-\frac{w_{0j}}{2g_{0j}S_0\langle D_0\rangle} \frac{g\Gamma_n}{\sqrt{EV_0}}\right)}{\sqrt{2\pi} g_{0j} S_0 \langle D_0 \rangle \sqrt{EV_0} g\Gamma_n}, \quad (3)$$

for  $p$ -wave,

$$P(g\Gamma_n|l=1) = \sum_{j=1,4} w_{1j}^{3/2} \frac{\exp\left(-\frac{w_{1j}}{2g_{1j}S_1\langle D_1\rangle} \frac{g\Gamma_n}{\sqrt{EV_1}}\right)}{\sqrt{2\pi} g_{1j} S_1 \langle D_1 \rangle \sqrt{EV_1} g\Gamma_n} + \sum_{j=2,3} w_{1j}^2 \frac{\exp\left(-\frac{w_{1j}}{2g_{1j}S_1\langle D_1\rangle} \frac{g\Gamma_n}{\sqrt{EV_1}}\right)}{2 g_{1j} S_1 \langle D_1 \rangle \sqrt{EV_1}}, \quad (4)$$

and for  $d$ -wave,

$$P(g\Gamma_n|l=2) = \sum_{j=1,6} w_{2j}^{3/2} \frac{\exp\left(-\frac{w_{2j}}{2g_{2j}S_2\langle D_2\rangle} \frac{g\Gamma_n}{\sqrt{EV_2}}\right)}{\sqrt{2\pi} g_{2j} S_2 \langle D_2 \rangle \sqrt{EV_2} g\Gamma_n} + \sum_{j=2}^5 w_{2j}^2 \frac{\exp\left(-\frac{w_{2j}}{2g_{2j}S_2\langle D_2\rangle} \frac{g\Gamma_n}{\sqrt{EV_2}}\right)}{2 g_{2j} S_2 \langle D_2 \rangle \sqrt{EV_2}}. \quad (5)$$

The index  $j$  again identifies distinct  $J$  values. The weight  $w_{lj}$  is defined as the ratio of the number of  $l$ -wave resonances for which the total spin is  $J_{lj}$  to the total number of  $l$ -wave resonances; thus it represents the *a priori* probability that the total spin of an  $l$ -wave resonance is  $J_{lj}$ . Other quantities appearing in the above equations are defined in Appendix A.

The first terms on the right-hand side of Eqs. (4) and (5) are those for the  $J$ -values for which the multiplicity is 1, and represent the Porter-Thomas distribution, *i.e.*, the  $\chi^2$  distribution with the degree-of-freedom of 1. The second terms are for  $J$ 's with the multiplicity of 2. The above formulae all include the possibility of two channel spins for one  $J$  value. Depending on the value of target spin, some weights  $w_{lj}$  may take the value of zero. For  $I = 0$  nuclides, for instance, weights for  $j = 1$  or  $2$  (but not both) of  $l = 0$ , for  $j = 2$  and  $3$  of  $l = 1$ , and for  $j = 2$  to  $5$  of  $l = 2$  become zero, in which case the pdf's reduce to forms rather similar to the traditional Porter-Thomas distribution.

## 2.4. Interpretation of Calculated Probability

The Bayesian approach is a statistical method. Hence, there is a potential area of concern: a resonance could, in fact, have orbital angular momentum  $l'$  regardless of how large is the probability that the orbital angular momentum is  $l$ . Nevertheless, if there is no indication other than the calculated probability, the value suggested by the statistical model is an appropriate choice.

There is a question regarding how large the calculated probability should be for a suggested  $l$  value. For instance, in distinguishing  $p$ -wave from  $d$ -wave resonances of  $^{206}\text{Pb}$ , Mizumoto *et al.* [Mi79] regarded a resonance as a ‘certain’  $p$ -wave if the probability to be  $p$ -wave is greater than 0.99, and as ‘uncertain but probably’  $p$ -wave if the probability is between 0.33 and 0.99. Frankle *et al.* [Fr94], in distinguishing  $s$ -wave from  $p$ -wave resonances of  $^{113}\text{Cd}$ , suggested  $p$ -wave if the probability is greater than 0.69.<sup>5</sup> In spite of the ambiguity, it seems reasonable to suggest the  $l$  value showing greatest *a posteriori* probability.

The program SUGGEL suggests the  $l$  value with the maximum probability among the three probabilities (for  $s$ -,  $p$ -, and  $d$ -waves). However, as described in the next chapter, a user can specify a minimum probability for  $l$ -value alteration via an input variable ‘pcut’; if the maximum probability is less than this value, the original  $l$  value is maintained.

## 2.5. Further Consideration

In addition to the intrinsic limitation originating from the statistical approach, a second type of limitation exists. This is best described by an example. Consider a simplified problem of distinguishing  $s$ - and  $p$ -wave resonances for zero-spin target nuclides. According to the  $(2J+1)$  law for the level density, the probability for a resonance to be a  $p$ -wave is as follows:

$$P(l=1 | g\Gamma_n) = \left[ 1 + \frac{1}{3} \sqrt{\frac{S_1 V_1}{S_0 V_0}} \exp \left\{ \frac{g\Gamma_n}{2\langle D_0 \rangle \sqrt{E}} \left( \frac{1}{S_1 V_1} - \frac{1}{S_0 V_0} \right) \right\} \right]^{-1}.$$

See Eq. (A10) of Appendix A. This formula was used by Bollinger and Thomas.[Bo68]

Consider an extreme case in which the equality  $S_1 V_1 = S_0 V_0$  holds. Here, regardless of the magnitude of  $g\Gamma_n$ , the probability  $P(l=1 | g\Gamma_n)$  becomes 0.75, which is equal to the *a priori* probability. This suggests that, in a situation for which  $S_1 V_1$  is approximately equal to  $S_0 V_0$ , the Bayesian approach

may lose its ability to distinguish between different  $l$ -waves. In general, the strength functions of  $s$ -,  $p$ -, and  $d$ -wave are within an order of magnitude. In addition, because the penetrabilities of  $p$ - and  $d$ -wave neutrons increase to unity as the neutron energy increases,<sup>6</sup> it is expected that the applicability of the Bayesian approach should diminish in the high-energy region.<sup>7</sup>

The following example shows the limitation of the Bayesian approach for resonances in higher energy region from the other point of view. Figs. 1 and 2 show the magnitude of  $g\Gamma_n$ 's of resonances of  $^{27}\text{Al}$  and  $^{109}\text{Ag}$ , respectively. Those resonances were adopted from a recent compilation of Sukhoruchkin *et al.* [Su98] (See sample cases 1 and 3 in Section 3.3). In Fig. 1, for which the energy range is below 800 keV,  $g\Gamma_n$ 's of each  $l$ -value are intermixed, so that it would be impossible to say which one belongs to which  $l$ -value if there were no legend. This is in contrast to Fig. 2, for which the energy range is below 1.5 keV. Note that the  $g\Gamma_n$ 's are well separated for each wave. The difference between Figs. 1 and 2, *i.e.* the degree of separation, is due to the variation of the penetrability with the incident neutron energy. As presented in Section 3.3, the Bayesian approach for resonances correctly predicted  $l$  values for 67 of 70 resonances for  $^{109}\text{Ag}$ , but only 32 of 46 resonances for  $^{27}\text{Al}$ . In conclusion, the magnitude of  $g\Gamma_n$  should be distinguishable wave by wave for the Bayesian approach to work. However, that is not the case in a high energy region, say above several hundred keV, so the approach might be applicable only to low energy resonances.

---

<sup>5</sup> Frankle, et al. wrote that the *a priori* probabilities for  $s$ - and  $p$ -wave were assumed equal. However, their probability calculation formula readily includes adequate *a priori* probabilities, 4/9 and 5/9. The same problem is found in the work of Lowie *et al.*[Lo97]

<sup>6</sup> For example, the  $p$ -wave penetrability, with a scattering radius of 5 fm, is about 0.5 at 1 MeV, 0.18 at 100 keV, and 0.001 at 1 keV.

<sup>7</sup> Thus the approach should have its limitation for the resonances of light nuclides.

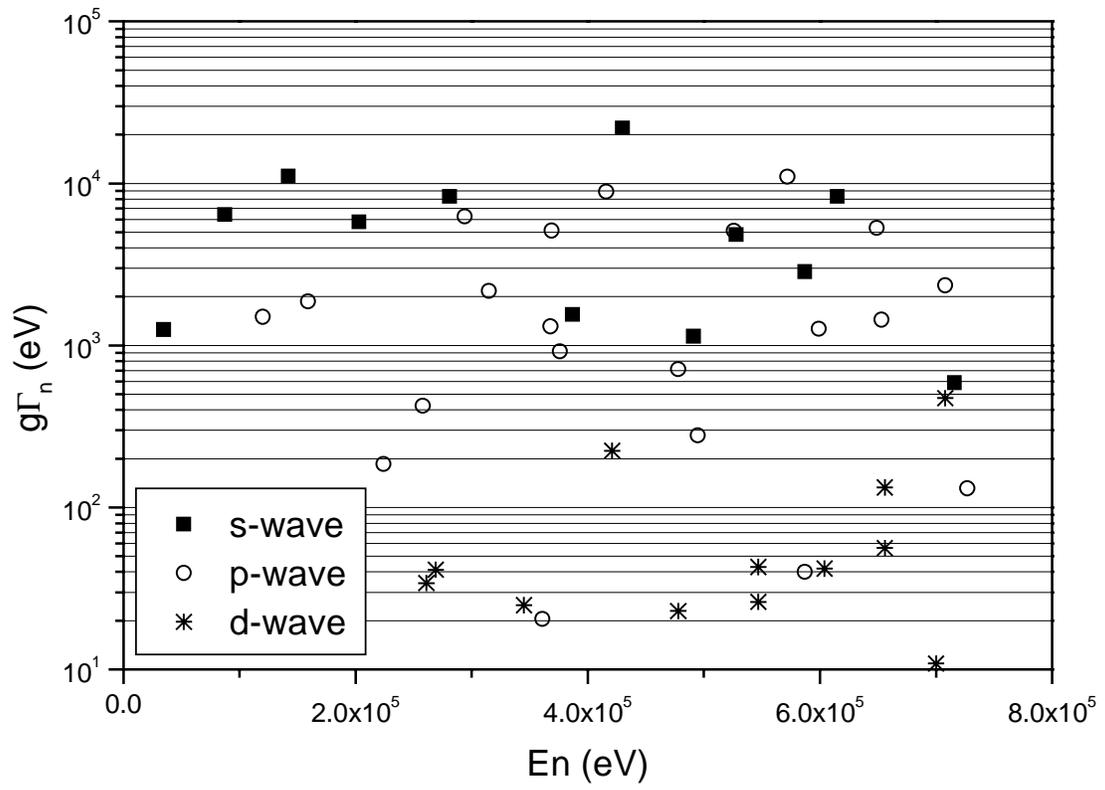


Fig. 1.  $g\Gamma_n$  Values of  $^{27}\text{Al}$  Resonances

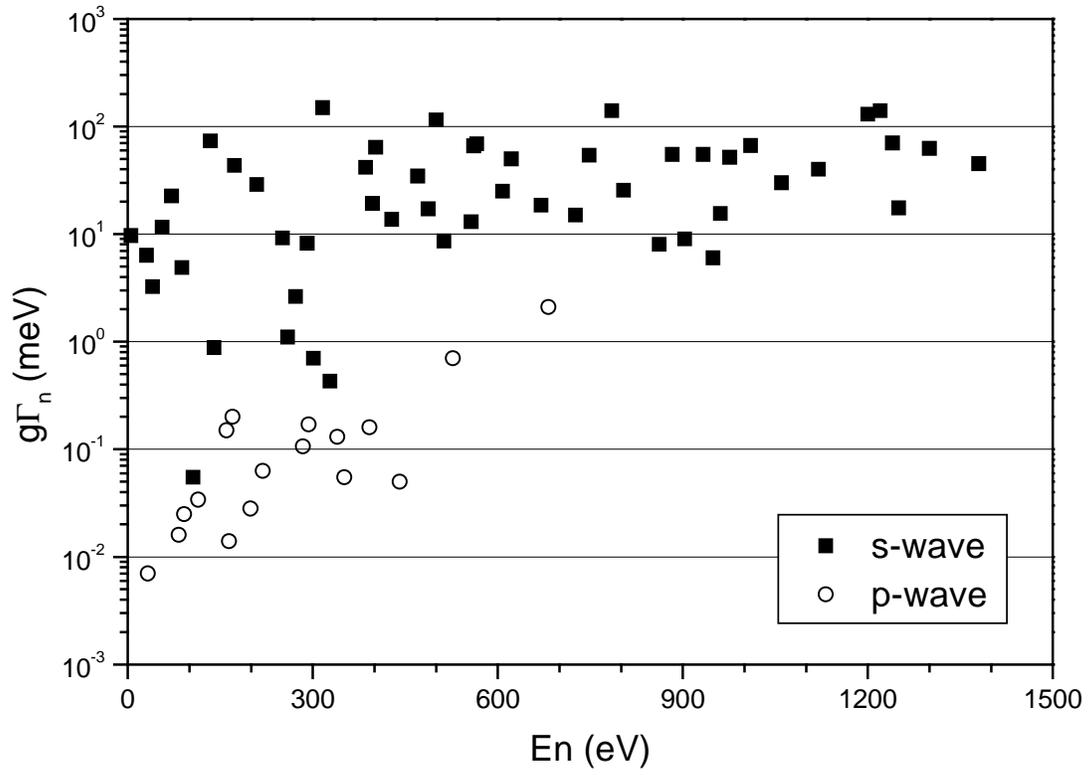


Fig. 2.  $g\Gamma_n$  Values of  $^{109}\text{Ag}$  Resonances

## 2.6. Identification of $J$

After the decision of  $l$ , the resonance spin ( $J$ ) is determined using a similar method. Below is an example for an  $s$ -wave resonance in a non-zero target spin nuclide. Applying each term in Eq. (3) to the Bayesian theorem, the *a posteriori* probability that  $J$  is to be  $(I - 1/2)$  is written as

$$P(J = I - \frac{1}{2} | g\Gamma_n) = \left[ 1 + \frac{1-w}{w} \sqrt{\frac{1-w}{w} \frac{I}{I+1}} \exp \left\{ \frac{(2I+1)g\Gamma_n}{2S_0 \langle D_0 \rangle \sqrt{E}} \left( \frac{w}{I} - \frac{1-w}{I+1} \right) \right\} \right]^{-1},$$

where  $w$  is a *a priori* probability that  $J = I - 1/2$ .

Here is a deficiency similar to that presented in the previous section. With the  $(2J+1)$  law,  $w = I/(2I+1)$ , thus the *a posteriori* probability becomes  $w$ , exactly same as the *a priori* probability. Because  $w$  is less than 0.5 for any  $I$ , the resulting  $J$  must be  $I+1/2$  always. This implies that the calculation is useless in distinguishing  $J = I-1/2$  from  $J = I+1/2$  from the magnitude of  $g\Gamma_n$ . Since the difference between *a posteriori* probability using  $(2J+1)$  law and the probability taking into account the exponential term in Eq. (2) is negligible in most cases,<sup>8</sup> the deficiency seldom is removed. The same situation occurs for  $p$ - or  $d$ -wave resonances.

The program SUGGEL provides two options on the  $J$  assignment. One is a deterministic method for which the most probable  $J$ -value, *i.e.* the value of  $J$  having the maximum probability from the Bayesian calculation. The other is a random assignment method for which the cumulative distribution function is obtained from the *a priori* probabilities [Oh00]. Users are advised to use the former method.

---

<sup>8</sup> Especially for nuclides with a large spin cutoff parameter and/or with a large spin.

## 3. Program SUGGEL

### 3.1. General Description

The program SUGGEL is written in FORTRAN 77. This program produces a “suggested value” for the orbital angular momentum ( $l$ ) of a resonance from the magnitude of its  $g\Gamma_n$ . SUGGEL also either suggests the most probable resonance spin ( $J$ ), or assigns the spin value randomly, according to user preference. The suggested value is based on the probability calculated by using the Bayesian approach as described in the previous chapter. The source listing for SUGGEL is found in Appendix B.

The physics models and assumptions are summarized as follows.

- Each resonance is identified by  $l$  and  $J$ .<sup>9</sup>
- The distribution of reduced neutron widths,  $g\Gamma_n^l$ , follows the  $\chi^2$  distribution as described in Appendix A. For an  $l > 0$  resonance of a non-zero spin nuclide, the pdf contains two terms, one with the degree-of-freedom (dof) equal to two and the other with dof equal to one. With this pdf, two channel spins,  $s = I \pm 1/2$ , are allowed for a resonance.
- The neutron strength function of ( $l, J$ ) resonances is assumed to be  $S_{l,J} = \mu_{l,J} \cdot S_l$ , where  $\mu_{l,J}$  is the degree-of-freedom for resonances with quantum numbers ( $l, J$ ).
- The level density is assumed to be constant over the energy range under consideration, and is given by Eq. (2).

The program requires two input files and generates two output files. The basic data, as well as some control options, for the calculation are included in a file named in “suggel.inp”, while sets of resonance energy and neutron widths are provided in the other input file. One of the output files shows calculation results; the other output file contains resonance parameters in SAMMY.PAR format [La00].

### 3.2. Input Description

The file “suggel.inp” is prepared in the name-list format. This file consists of:

The first card (or “record” or “line”): “&indata” from column 2 to 8,

The second to the last-but-one cards: data section with the name-list keywords (each card shall have the first column blank), and

---

<sup>9</sup> In SAMMY, a resonance is usually identified with  $l, J$ , and  $s$  (the channel spin) for dealing with the Reich-Moore formula.

The last card: “&end” from column 2 to 5. Notes can be added after this card for the user’s convenience.

**Table 1 Variables Appearing in the “suggel.inp” File**

Keyword	Unit	Description
parin		Input resonance parameter data file name. In the file, the resonance energy is given in eV and $\Gamma_n$ (or $g\Gamma_n$ ) in meV.
partyp		Type of neutron width in ‘parin’ file. If partyp=0, the parin file is in SAMMY.PAR file format and $\Gamma_n$ ’s are given; otherwise, the file is in rsap.gamma format and $g\Gamma_n$ ’s are given. Concerning the rsap.gamma file, see the text following this table.
fout		Output list file name.
parout		File name of the output resonance parameter file, which is in SAMMY.PAR format.
awri		Atomic mass of target nuclide.
spin		Spin of the target nuclide (I).
scattr	fm	Scattering radius (R’). If scattr=0., the program calculates it as $R' = 0.123 (awri)^{1/3} + 0.08 [10^{-12} \text{ cm}]$
disp		Square root of spin cutoff parameter (spin dispersion parameter, $\sigma$ ). If disp=0., the program calculates the value. A very large value for ‘disp’ (e.g. 999) indicates that the $(2J+1)$ law is to be used, for which the level density is proportional to $2J+1$ .
sigcon		Constant for the calculation of spin cutoff parameter. See further discussion for ‘disp’ and ‘sigcon’ in the text following this table.
bn	MeV	Neutron separation energy of (A+1) nuclide
pair	MeV	Pairing energy
denpar	MeV <sup>-1</sup>	Level density parameter
eini	eV	Lower energy boundary under the analysis
efin	eV	Upper energy boundary under the analysis

**Table 1 Variables Appearing in the “suggel.inp” File**

Keyword	Unit	Description
pcut		Probability cutoff. The suggested orbital angular momentum is adopted for a resonance for which the probability is higher than this value. When the probability is lower than this value, the value for $l$ is not altered from its original assignment as given in ‘parin’ file. When the rsap.gamma file is used for input, the suggested orbital angular momentum value is always adopted.
optj		Method of $J$ assignment. If optj=0, the most probable $J$ value is adopted; otherwise, the $J$ value is assigned randomly. However, if the original $l$ value is retained due to the probability cutoff, then the $J$ value is also not altered. See Section 2.6.
stn(i), i=1,2,3	$10^{-4}$	Neutron strength functions for $s$ -, $p$ -, and $d$ -wave, respectively
dzero	eV	Average level spacing of $s$ -wave resonance. Level spacings of $p$ - and $d$ -wave are calculated in the program.
frac(i), i=1,2,3		<i>A priori</i> probability correction factors for $s$ -, $p$ -, and $d$ -wave, respectively. See Section 2.2.
lsam(i), i=1~max.18		$l$ value of spin group $i$ in ‘parin’ file. This definition shall be kept in subsequent SAMMY run. The number of spin groups can be more than 18 in a SAMMY run (as is often the case when more than one nuclide is included), but is limited to 18 in SUGGEL.
ajsam(i), i=1~max.18		$J$ value of spin group $i$ in ‘parin’ file. This definition shall be kept in subsequent SAMMY run.

One of the features of the program RSAP [Sa00] is the ability to do a “peak search” from the measured total cross section in the resonance region. The results of this peak search, the resonance energy and  $g\Gamma_n$ , are listed in a file ‘rsap.gamma’. This search can be the initial step in a resonance parameter evaluation; the resulting energies and widths could be compiled into the *a priori* parameter file as one of SAMMY input files.

The spin cutoff parameter,  $\sigma^2$ , is calculated in the program (if disp=0) as

$$\sigma^2 = C \cdot \sqrt{aU} A^{2/3},$$

where  $a$  is the level density parameter,  $U$  the effective excitation energy, and  $A$  is compound nucleus mass. The program calculates  $U$  as  $U = B_n + (eini+efin)/2 - E_{pair}$ , where all four parameters are input quantities. The theoretical value of  $C$  ('sigcon' in the input file) has been known as  $6/\pi^2 \times 0.24 = 0.146$  [Fa68], however, a value of 0.0888 is also used traditionally. In addition, there is the other possibility; Mughabghab obtained a value of 0.0494 via fittings [Mu98]. One has to pay attention to the choice of  $C$  value, because the values of level density parameter and pairing energy are strongly connected to  $C$ . For instance, when a user wants to adopt the pairing energy and level density parameter from [Mu98], the value of  $C$  must be 0.0494.

It should be noted that the value of  $g\Gamma_n$ , rather than the value of  $\Gamma_n$ , is conserved in 'parin' and 'parout' file. If the newly assigned  $J$  value differs from the original value,  $\Gamma_n$  in 'parout' must be different from that in 'parin' in order to conserve the reaction area.

### 3.3. Sample Cases

#### Case 1: $^{109}\text{Ag}$ resonances

An attempt was made to assign  $l$  and  $J$  values for  $^{109}\text{Ag}$  resonances. The resonance energies,  $l$  and  $J$ , and  $g\Gamma_n$  values for 70 resonances up to 1.383 keV were adopted from the recent compilation of Sukhoruchkin *et al.*[Su98]. The resonance parameters in the compilation, except those for only one resonance at 5.145 eV, came from the measurements of Corvi *et al.*[Co97], in which they determined quantum numbers from the analysis of capture gamma-ray spectra. Lowie *et al.*[Lo97] also reported the measurement with  $l$  and  $J$  assignment using the Bayesian approach, and their  $g\Gamma_n$  values are almost identical to those in the compilation of Sukhoruchkin.

Table 2 shows the input file, 'suggel.inp'. The sources of values are summarized at the end of input file. (It is not a part of input.)  $J$  values will be assigned per the calculated probabilities. Table 3 lists the standard output. The calculated *a priori* probabilities (0.157 for  $s$ , 0.334 for  $p$ , and 0.509 for  $d$ -wave) differ from those assuming the  $(2J+1)$  law (0.143, 0.321, and 0.536 for  $s$ -,  $p$ -, and  $d$ -wave, respectively).

The code failed in the assignment of  $l$  for only 3 resonances at 106.2, 327.8, and 681.5 eV among 70 resonances.<sup>10</sup> It seems that the mis-assignment for the first two resonances cannot be avoided because their probabilities to be  $p$ -wave are so large. This shows the potential danger of the Bayesian approach. The resonance at 681.5 eV, however, needs careful investigation because its  $s$ -wave probability is rather far from both ends, zero and unity. A user may pay attention to the resonances at 169.8 and 300.9 eV as well.

Concerning the  $J$  assignment, the results reveal the deficiency described in section 2.6: The code assigned  $J = 1.0$  to all  $s$ -wave and most  $p$ -wave resonances. These suggested  $J$  values are dubious as a whole, and might be used just as the starting guess of spin groups for a detailed analysis with SAMMY.

The information below the “New assignment” section in the output is based on the missing level estimation (MLE) [Mo78, Ga82] for each wave. In integrating theoretical quantities for the MLE, the pdf’s derived in this work have been used. For the  $s$ -wave MLE, the range of integration is 0.25 to infinity in units of  $g\Gamma_n^0 / \langle g\Gamma_n^0 \rangle$ . The range is set to 0.25 to 5.0 for  $p$ - and  $d$ -wave MLEs, respectively. By using a finite upper limit, the possible contamination of lower  $l$ -wave resonances is presumably removed. The relative inherent uncertainty in  $\langle D_l \rangle$  is given as of  $\sqrt{0.52^2/N}$ , where  $N$  is the number of resonances, from the Wigner’s surmise [Wi57] and that in  $\langle g\Gamma_n^l \rangle$  is  $\sqrt{2/N}$  from the Porter-Thomas distribution [Po56]. The relative uncertainty of strength function is calculated as  $\sqrt{0.52^2/N_D + 2/N_W}$ , in which the number of resonances for calculating average reduced width,  $N_W$ , could be different from that for calculating average level spacing. For the  $^{109}\text{Ag}$  case, the  $s$ -wave MLE resulted in the strength function of  $(0.67 \pm 0.14) \times 10^{-4}$  and  $\langle D_0 \rangle$  of  $17.4 \pm 1.0$  eV, which are consistent with  $S_0 = (0.75 \pm 0.08) \times 10^{-4}$  and  $\langle D_0 \rangle = 15.1 \pm 1.4$  eV recommended in the RIPL [Re98] within their associated uncertainties.<sup>11</sup>

The MLE for each wave could provide information to help a user determine whether the input values are reasonable or not. Unfortunately in a real situation, however, it may not provide good values for high  $l$  resonances due to insufficient number of measured resonances. If the input strength functions and  $s$ -wave level spacing are quite different from those from the MLE, iteration with the new values is recommended. Actually values of  $S_0$  and  $D_0$  in the input for  $^{109}\text{Ag}$  (Table 2) came from the  $s$ -wave MLE in the initial run with  $S_0 = 1.0$  and  $D_0 = 15.1$  eV. Note that the input  $S_0$  and that from the MLE are same in Table 3.

---

<sup>10</sup> Lowie’s calculation using the Bayesian approach [Lo97] showed very similar results. Of course, the *a posteriori* probabilities of Lowie are different, even if it is not significant, from those in Table 3.

<sup>11</sup> However, the  $s$ -wave strength function is much lower than  $1.0 \times 10^{-4}$  of Lowie.

**Table 2. Input for Sample Case 1**

```

&indata
parin="ag109.par", partyp=0, fout="ag109.out", parout="ag109new.par",
awri=108.905, spin=0.5, scattr=0.00,
disp=0., sigcon=0.0888, bn=6.809, pair=-0.1, denpar=16.95,
eini=0., efin=1400., pcut=0., optj=0,
stn(1)=0.674, 3.900, 1.000, dzero=17.4,
frac(1)=1.000, 1.000, 1.000,
lsam(1)=0, 0, 1, 1, 1, 2, 2, 2,
ajsam(1)=0., 1., 0., 1., 2., 1., 2., 3.
&end

NOTES
level density parameter= 16.95 (calc. from Su Zongdi 85)
pairing energy = -0.44+0.34 (from Su Zongdi 85)
S2=S0 assumed (not affect anyhow)
resonance parameters from Sukhoruchkin 98 compilation
S0=1.00, S1=3.9 from Lowie 97
D0=17.5 from RIPL Ch.3
S0 and D0 adopted from the s-wave MLE

```

**Table 3. Output of Sample Case 1**

```

-----
*** PROGRAM SUGGEL v.1.0 ***
-----

* Input (En, Gn) data file name = ag109.par

* Input Variables:
  Energy range under consideration [eV] = 0.0000E+00 to 1.4000E+03
  n. strength function (s,p,d) [1E-04] = 0.674 3.900 1.000
  s-wave avg level spacing [eV] = 1.7400E+01
  target spin = 0.500
  atomic weight (AWRI) = 107.969
  probability cutoff for renewal of L = 0.000
  J assignment = most probable

* Calculated Quantities from the input:
  scattering radius (AP) [fm] = 6.657
  spin dispersion parameter (sigma) = 4.682
  A priori probabilities, s, p, and d = 0.157 0.334 0.509
  p & d level spacing, relative to s = 0.470 0.308

```

nres	En (eV)	Reduced Gn (eV)	Probability			L		J	
			s	p	d	old	new	old	new
1	5.1450E+00	5.6726E-03	1.000	0.000	0.000	0	0	1.0	1.0
2	3.0600E+01	1.5257E-03	1.000	0.000	0.000	0	0	1.0	1.0
3	3.2700E+01	2.3776E-02	0.024	0.976	0.000	1	1	1.0	1.0
4	4.0300E+01	6.8050E-04	1.000	0.000	0.000	0	0	1.0	1.0
5	5.5800E+01	2.0741E-03	1.000	0.000	0.000	0	0	0.0	1.0
6	7.1000E+01	3.5683E-03	1.000	0.000	0.000	0	0	1.0	1.0
7	8.2500E+01	8.1377E-03	0.026	0.974	0.000	1	1	2.0	2.0
8	8.7700E+01	6.9337E-04	1.000	0.000	0.000	0	0	1.0	1.0
9	9.1500E+01	1.8144E-02	0.032	0.968	0.000	1	1	2.0	1.0
10	1.0630E+02	3.1878E-02	0.060	0.940	0.000	0	1 *	0.0	1.0
11	1.1350E+02	1.7862E-02	0.035	0.965	0.000	1	1	2.0	1.0

12	1.3390E+02	8.4576E-03	1.000	0.000	0.000	0	0	1.0	1.0
13	1.3960E+02	9.9304E-05	1.000	0.000	0.000	0	0	1.0	1.0
14	1.6030E+02	4.6954E-02	0.135	0.865	0.000	1	1	1.0	1.0
15	1.6430E+02	2.5340E-03	0.028	0.972	0.000	1	1	2.0	2.0
16	1.6980E+02	5.7427E-02	0.208	0.792	0.000	1	1	0.0	1.0
17	1.7310E+02	4.3881E-03	1.000	0.000	0.000	0	0	1.0	1.0
18	1.9900E+02	3.8023E-03	0.032	0.968	0.000	1	1	1.0	2.0
19	2.0920E+02	2.6595E-03	1.000	0.000	0.000	0	0	1.0	1.0
20	2.1920E+02	7.4006E-03	0.039	0.961	0.000	1	1	2.0	2.0
21	2.5120E+02	7.7398E-04	1.000	0.000	0.000	0	0	1.0	1.0
22	2.5900E+02	9.1134E-05	0.988	0.012	0.000	0	0	0.0	1.0
23	2.7240E+02	2.1247E-04	1.000	0.000	0.000	0	0	1.0	1.0
24	2.8400E+02	8.4445E-03	0.047	0.953	0.000	1	1	2.0	2.0
25	2.9060E+02	6.4217E-04	1.000	0.000	0.000	0	0	1.0	1.0
26	2.9330E+02	2.1508E-02	0.063	0.937	0.000	1	1	1.0	1.0
27	3.0090E+02	5.3805E-05	0.574	0.426	0.000	0	0	0.0	1.0
28	3.1620E+02	1.1210E-02	1.000	0.000	0.000	0	0	1.0	1.0
29	3.2780E+02	4.6046E-02	0.175	0.825	0.000	0	1	*	1.0
30	3.4020E+02	7.9002E-03	0.050	0.950	0.000	1	1	2.0	2.0
31	3.5140E+02	3.1840E-03	0.041	0.959	0.000	1	1	2.0	2.0
32	3.8620E+02	2.8150E-03	1.000	0.000	0.000	0	0	1.0	1.0
33	3.9160E+02	7.8740E-03	0.053	0.947	0.000	1	1	1.0	2.0
34	3.9730E+02	1.2823E-03	1.000	0.000	0.000	0	0	1.0	1.0
35	4.0170E+02	4.2510E-03	1.000	0.000	0.000	0	0	0.0	1.0
36	4.2790E+02	8.8626E-04	1.000	0.000	0.000	0	0	1.0	1.0
37	4.4100E+02	2.0592E-03	0.044	0.956	0.000	1	1	1.0	2.0
38	4.6970E+02	2.1225E-03	1.000	0.000	0.000	0	0	0.0	1.0
39	4.8700E+02	1.0338E-03	1.000	0.000	0.000	0	0	1.0	1.0
40	4.9980E+02	6.8406E-03	1.000	0.000	0.000	0	0	1.0	1.0
41	5.1260E+02	5.0646E-04	1.000	0.000	0.000	0	0	0.0	1.0
42	5.2670E+02	3.6819E-02	0.149	0.851	0.000	1	1	1.0	1.0
43	5.5720E+02	7.3429E-04	1.000	0.000	0.000	0	0	1.0	1.0
44	5.6070E+02	3.7164E-03	1.000	0.000	0.000	0	0	0.0	1.0
45	5.6550E+02	3.8688E-03	1.000	0.000	0.000	0	0	1.0	1.0
46	6.0810E+02	1.3517E-03	1.000	0.000	0.000	0	0	1.0	1.0
47	6.2240E+02	2.6722E-03	1.000	0.000	0.000	0	0	1.0	1.0
48	6.6950E+02	9.5333E-04	1.000	0.000	0.000	0	0	1.0	1.0
49	6.8150E+02	1.0726E-04	0.547	0.453	0.000	1	0	*	2.0
50	7.2610E+02	7.4222E-04	1.000	0.000	0.000	0	0	1.0	1.0
51	7.4760E+02	2.6333E-03	1.000	0.000	0.000	0	0	1.0	1.0
52	7.8470E+02	6.6638E-03	1.000	0.000	0.000	0	0	1.0	1.0
53	8.0380E+02	1.1992E-03	1.000	0.000	0.000	0	0	1.0	1.0
54	8.6180E+02	3.6336E-04	0.999	0.001	0.000	0	0	1.0	1.0
55	8.8300E+02	2.4679E-03	1.000	0.000	0.000	0	0	1.0	1.0
56	9.0280E+02	3.9938E-04	0.999	0.001	0.000	0	0	1.0	1.0
57	9.3300E+02	2.4008E-03	1.000	0.000	0.000	0	0	1.0	1.0
58	9.4930E+02	2.5965E-04	0.956	0.044	0.000	0	0	1.0	1.0
59	9.6100E+02	6.6667E-04	1.000	0.000	0.000	0	0	0.0	1.0
60	9.7600E+02	2.1980E-03	1.000	0.000	0.000	0	0	1.0	1.0
61	1.0090E+03	2.7914E-03	1.000	0.000	0.000	0	0	0.0	1.0
62	1.0570E+03	1.2303E-03	1.000	0.000	0.000	0	0	1.0	1.0
63	1.0620E+03	1.2274E-03	1.000	0.000	0.000	0	0	0.0	1.0
64	1.1160E+03	1.5965E-03	1.000	0.000	0.000	0	0	1.0	1.0
65	1.2040E+03	4.9953E-03	1.000	0.000	0.000	0	0	1.0	1.0
66	1.2190E+03	5.3465E-03	1.000	0.000	0.000	0	0	1.0	1.0
67	1.2360E+03	2.6548E-03	1.000	0.000	0.000	0	0	1.0	1.0
68	1.2540E+03	6.5890E-04	1.000	0.000	0.000	0	0	1.0	1.0
69	1.3000E+03	2.3112E-03	1.000	0.000	0.000	0	0	1.0	1.0
70	1.3830E+03	1.6134E-03	1.000	0.000	0.000	0	0	0.0	1.0

\* : L has been altered from the original assignment.  
? : L should be altered, but the probability is too low.

Energy range has been adjusted to 3.7801E+00 ~ 1.3844E+03 eV.

		s	p	d
		-----	-----	-----
Original assignment:				
Number of resonances	=	53	17	0
Strength function [1E-04]	=	0.654	0.694	0.000
New assignment:				
Number of resonances	=	52	18	0
Strength function [1E-04]	=	0.654	0.699	0.000
From the Missing Level Estim.,				
Avg. g*red.width [eV]	=	1.171E-03	1.099E-03	0.000E+00?
Expected no. of resonances	=	79	39	1?
Based on the "s"-wave MLE:				
Number of resonances	=	79	169	258
Strength function [1E-04]	=	0.673	0.449	1.000
Measurement efficiency	=	0.655	0.107	0.000
Avg. level spacing [eV]	=	1.738E+01	8.170E+00	5.355E+00
Recommended frac (as the input)	=	1.000	0.163	0.000

### Case 2: $^{235}\text{U}$ pseudo-resonances

A pseudo-resonance parameter file for  $^{235}\text{U}$  was generated using the program LADDER (see Appendix C). The input strength functions for this LADDER run were 1.0, 1.2, and  $0.5 \times 10^{-4}$  for  $s$ -,  $p$ -,  $d$ -wave, respectively; nevertheless, those of the actually-generated resonances are 0.99, 1.03, and  $0.51 \times 10^{-4}$ . (These slight differences indicate the statistical accuracy of the method.) In the energy range from 100 to 200 eV, the number of resonances generated by LADDER is 197 for  $s$ -waves, 380 for  $p$ -waves, and 577 for  $d$ -waves. However, weak resonances were eliminated from the LADDER output, so the file 'case1r.par' contains 193  $s$ -wave, 108  $p$ -wave, and 0  $d$ -wave resonances in 100~200 eV energy region.

Table 4 shows the input file and Table 5 gives the output from the SUGGEL run (omitting the 6<sup>th</sup> through the 296<sup>th</sup> resonance). Because there are large differences between the values of  $g\Gamma_n$ 's for  $s$ - and  $p$ -wave resonances in this example, SUGGEL has correctly suggested the  $l$  values of 293 resonances among the total of 301. Meanwhile, the  $s$ -wave strength function and level spacing generated using the MLE agree well with values provided to the original LADDER run which generated these resonances. Similarly, the number of  $p$ -wave resonances estimated using the MLE agrees well with the actual number, while the expected strength function ( $0.83 \times 10^{-4}$ ) is rather small comparing with  $1.2 \times 10^{-4}$  for the LADDER run.

**Table 4. Input for Sample Case 2**

```

&indata
parin="caselr.par", partyp=0, fout="caselr.out", parout="suglr.par",
awri=233.03, spin=3.5, scattr=0.,
disp=999., sigcon=0.0888, bn=0., pair=0., denpar=0.,
eini=100.,efin=200., pcut=0., optj=1,
stn(1)=1.00,1.20,0.50, dzero=0.50, frac=1.00,0.35,0.00,
lsam(1)=2*0,4*1,6*2,
ajsam(1)=3.,4., 2.,3.,4.,5., 1.,2.,3.,4.,5.,6.
&end
Test with pseudo par file generated by using ladder
Set as S0=1.0, S1=1.2, S2=0.5, D0=0.5 eV
Small resonances were removed from casel.par

```

**Table 5. Output of Sample Case 2**

```

-----
*** PROGRAM SUGGEL v.1.0 ***
-----

* Input (En, Gn) data file name = caselr.par

* Input Variables:
Energy range under consideration [eV] = 1.0000E+02 to 2.0000E+02
n. strength function (s,p,d) [1E-04] = 1.000 1.200 0.500
s-wave avg level spacing [eV] = 5.0000E-01
target spin = 3.500
atomic weight (AWRI) = 233.030
probability cutoff for renewal of L = 0.000
J assignment = random
spin dispersion parameter (sigma) = 999.000

* Calculated Quantities from the input:
scattering radius (AP) [fm] = 8.369
A priori probabilities, s, p, and d = 0.588 0.412 0.000
p & d level spacing, relative to s = 1.429 99.000

-----
nres      En      Reduced Gn      Probability      L      J
          (eV)      (eV)      s    p    d    old new    old new
-----
  1  1.0052E+02  4.4001E-04  1.000 0.000 0.000  0  0    3.0 4.0
  2  1.0112E+02  5.2106E-05  1.000 0.000 0.000  0  0    4.0 3.0
  3  1.0174E+02  3.2304E-05  1.000 0.000 0.000  0  0    4.0 3.0
  4  1.0189E+02  1.5629E-06  1.000 0.000 0.000  0  0    3.0 4.0
  5  1.0202E+02  1.4167E-04  1.000 0.000 0.000  0  0    4.0 4.0
  ...
297 1.9793E+02  3.8945E-04  0.099 0.901 0.000  1  1    4.0 3.0
298 1.9839E+02  1.5046E-05  1.000 0.000 0.000  0  0    3.0 3.0
299 1.9890E+02  3.0790E-04  0.068 0.932 0.000  1  1    3.0 2.0
300 1.9903E+02  1.2077E-04  1.000 0.000 0.000  0  0    3.0 3.0
301 1.9963E+02  4.3334E-04  0.083 0.917 0.000  1  1    2.0 2.0

* : L has been altered from the original assignment.
? : L should be altered, but the probability is too low.

Energy range has been adjusted to 1.0047E+02 ~ 1.9968E+02 eV.

                               s           p           d
-----

```

Original assignment:				
Number of resonances	=	193	108	0
Strength function [1E-04]	=	0.995	0.699	0.000
New assignment:				
Number of resonances	=	189	112	0
Strength function [1E-04]	=	0.995	0.706	0.000
From the Missing Level Estim.,				
Avg. g*red.width [eV]	=	5.229E-05	6.436E-05	0.000E+00?
Expected no. of resonances	=	187	383	1?
Based on the "p"-wave MLE:				
Number of resonances	=	202	383	527
Strength function [1E-04]	=	1.065	0.829	0.500
Measurement efficiency	=	0.936	0.292	0.000
Avg. level spacing [eV]	=	4.913E-01	2.588E-01	1.884E-01
Recommended frac (as the input)	=	1.000	0.312	0.000

### Case 3: <sup>27</sup>Al resonances

For <sup>27</sup>Al resonances, the resonance energies,  $l$  and  $J$ , and  $g\Gamma_n$  values for 46 resonances were adopted from the recent compilation of Sukhoruchkin *et al.*[Su98] The number of resonances are: 12 ( $s$ -wave), 22 ( $p$ ), and 12 ( $d$ ), respectively, in an energy range 0 to 726.8 keV. Table 6 shows the input file and the sources of values are summarized at the end of input file. Due to insufficient number of measured resonances,  $\langle D_0 \rangle$  and strength functions have very large uncertainties. An arbitrary value of 0.5 was adopted for 'pcut'.

Table 7 shows the output list. The  $l$  values for about 2/3 of resonances were assigned correctly. However, such assignments are more or less dubious because the calculated probabilities are scattered among the various values of  $l$ . For instance, the  $p$ -wave probabilities for resonances at 478.29 ( $\Gamma_n = 1.22$  keV) and 490.82 keV ( $\Gamma_n = 1.95$  keV) are around 0.55, which are not significantly large, and the suggested  $l$  values are 1 for both resonances. Note that the correct  $l$  values are 1 and 0, respectively. More ambiguous example is the resonance at 495.18 keV; the probabilities are around 1/3 for each wave, so one could not rely on the calculated probabilities in determining  $l$  value at all.

The above deficiency stems from large penetrabilities of high  $l$  wave neutrons in the high energy region. The Bayesian approach may lose its capability of distinguishing  $l$  values for resonances at high energy region, especially for the 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 of the spin group for a detailed analysis using SAMMY.

**Table 6. Input for Sample Case 3**

```

&indata
parin="al27.par", partyp=0, fout="al27.out", parout="al27new.par",
awri=26.982, spin=2.5, scattr=0.00,
disp=0.0 ,sigcon=0.0888, bn=7.725, pair=0.0, denpar=4.102,
eini=0., efin=730000., pcut=0.5, optj=0,
stn(1)=0.500, 2.600, 0.500, dzero=45000.,
frac(1)=1.000, 1.000, 1.000,
lsam(1)=2*0, 4*1, 6*2,
ajsam(1)=2.,3., 1.,2.,3.,4., 0.,1.,2.,3.,4.,5.
&end

NOTES
level density parameter= 4.102 (calc. from Su Zongdi 85)
pairing energy = 0.0 (from Su Zongdi 85, odd-odd)
resonance parameters from Sukhoruchkin 98 compilation
S0=0.5 read from Mughabghab 81, Fig.2
S1=2.6+-1.0 from Mughabghab 81
S2=S0 assumed
D0=45+-15 keV from RIPL Ch.3

```

**Table 7. Output of Sample Case 3**

```

-----
*** PROGRAM SUGGEL v.1.0 ***
-----

* Input (En, Gn) data file name = al27.par

* Input Variables:
  Energy range under consideration [eV] = 0.0000E+00 to 7.3000E+05
  n. strength function (s,p,d) [1E-04] = 0.500 2.600 0.500
  s-wave avg level spacing [eV] = 4.5000E+04
  target spin = 2.500
  atomic weight (AWRI) = 26.750
  probability cutoff for renewal of L = 0.500
  J assignment = most probable

* Calculated Quantities from the input:
  scattering radius (AP) [fm] = 4.479
  spin dispersion parameter (sigma) = 2.165
  A priori probabilities, s, p, and d = 0.207 0.364 0.429
  p & d level spacing, relative to s = 0.568 0.481

-----
nres      En      Reduced Gn      Probability      L      J
          (eV)      (eV)      s    p    d    old new    old new
-----
  1  5.9050E+03  2.4386E+01  0.125 0.875 0.000  1  1  1.0 2.0
  2  3.4750E+04  1.1495E+01  0.906 0.094 0.000  0  0  2.0 3.0
  3  8.7300E+04  3.7229E+01  0.729 0.271 0.000  0  0  3.0 3.0
  4  1.1975E+05  7.6422E+01  0.381 0.619 0.000  1  1  2.0 3.0
  5  1.4210E+05  3.4593E+02  0.342 0.658 0.000  0  1 * 3.0 4.0
  6  1.5860E+05  6.4364E+01  0.341 0.659 0.000  1  1  3.0 3.0
  7  2.0335E+05  1.4240E+02  0.271 0.729 0.000  0  1 * 2.0 3.0
  8  2.2419E+05  9.3136E+00  0.392 0.579 0.029  1  1  2.0 1.0
  9  2.5762E+05  1.7815E+01  0.385 0.610 0.005  1  1  3.0 1.0
 10  2.6094E+05  2.0246E+01  0.159 0.174 0.667  2  2  4.0 3.0
 11  2.6870E+05  2.2851E+01  0.182 0.199 0.619  2  2  4.0 3.0

```

12	2.8073E+05	1.3341E+02	0.178	0.822	0.000	0	1	*	3.0	3.0
13	2.9360E+05	9.4653E+01	0.207	0.793	0.000	1	1		2.0	3.0
14	3.1510E+05	4.1966E+01	0.307	0.693	0.000	1	1		1.0	2.0
15	3.4543E+05	1.0613E+01	0.083	0.077	0.840	2	2		5.0	2.0
16	3.6069E+05	7.8355E+00	0.073	0.065	0.862	1	2	*	1.0	2.0
17	3.6771E+05	2.0835E+01	0.357	0.642	0.002	1	1		2.0	2.0
18	3.6866E+05	8.1074E+01	0.220	0.780	0.000	1	1		4.0	2.0
19	3.7647E+05	1.4175E+01	0.383	0.609	0.007	1	1		2.0	2.0
20	3.8677E+05	2.3201E+01	0.348	0.651	0.001	0	1	*	3.0	2.0
21	4.1643E+05	8.6523E+01	0.144	0.856	0.000	1	1		2.0	3.0
22	4.2073E+05	3.3087E+01	0.338	0.369	0.292	2	2	?	4.0	4.0
23	4.2953E+05	2.0689E+02	0.032	0.968	0.000	0	1	*	2.0	3.0
24	4.7783E+05	7.5472E+00	0.077	0.062	0.861	2	2		1.0	1.0
25	4.7829E+05	1.3707E+01	0.405	0.533	0.063	1	1		3.0	1.0
26	4.9082E+05	1.2724E+01	0.391	0.587	0.022	0	1	*	3.0	2.0
27	4.9518E+05	5.1191E+00	0.328	0.342	0.330	1	1		1.0	1.0
28	5.2607E+05	5.2584E+01	0.229	0.771	0.000	1	1		3.0	2.0
29	5.2822E+05	4.9581E+01	0.237	0.763	0.000	0	1	*	3.0	2.0
30	5.4672E+05	6.1716E+00	0.092	0.072	0.835	2	2		1.0	2.0
31	5.4711E+05	6.2656E+00	0.084	0.064	0.852	2	2		4.0	1.0
32	5.7203E+05	7.3092E+01	0.114	0.886	0.000	1	1		3.0	3.0
33	5.8709E+05	2.5855E+01	0.319	0.676	0.005	0	1	*	3.0	2.0
34	5.8717E+05	8.1430E+00	0.092	0.070	0.838	1	2	*	4.0	1.0
35	5.9935E+05	1.8697E+01	0.393	0.557	0.050	1	1		4.0	1.0
36	6.0390E+05	8.0051E+00	0.094	0.071	0.836	2	2		4.0	1.0
37	6.1533E+05	7.1486E+01	0.159	0.841	0.000	0	1	*	3.0	2.0
38	6.4932E+05	4.2929E+01	0.236	0.763	0.001	1	1		3.0	2.0
39	6.5346E+05	1.9271E+01	0.388	0.555	0.057	1	1		2.0	1.0
40	6.5578E+05	5.3218E+00	0.101	0.076	0.823	2	2		5.0	2.0
41	6.5627E+05	1.2551E+01	0.147	0.120	0.734	2	2		4.0	2.0
42	7.0023E+05	1.4836E+00	0.117	0.077	0.806	2	2		5.0	1.0
43	7.0770E+05	2.0957E+01	0.313	0.307	0.380	2	2		4.0	4.0
44	7.0825E+05	1.7237E+01	0.356	0.616	0.027	1	1		2.0	2.0
45	7.1649E+05	1.6658E+00	0.340	0.348	0.312	0	0	?	2.0	2.0
46	7.2682E+05	9.8464E+00	0.136	0.106	0.758	1	2	*	2.0	2.0

\* : L has been altered from the original assignment.  
 ? : L should be altered, but the probability is too low.

Energy range has been adjusted to 1.2552E+03 ~ 7.3147E+05 eV.

		s	p	d
		-----	-----	-----
Original assignment:				
Number of resonances	=	12	22	12
Strength function [1E-04]	=	1.997	1.712	0.235
New assignment:				
Number of resonances	=	3	28	15
Strength function [1E-04]	=	0.399	4.527	0.261
From the Missing Level Estim.,				
Avg. g*red.width [eV]	=	6.062E+00	2.943E+01	3.792E+00
Expected no. of resonances	=	5	31	21
Based on the "p"-wave MLE:				
Number of resonances	=	17	31	36
Strength function [1E-04]	=	1.440	4.104	0.374
Measurement efficiency	=	0.173	0.916	0.416
Avg. level spacing [eV]	=	4.210E+04	2.390E+04	2.026E+04
Recommended frac (as the input)	=	1.000	1.000	0.454

## 4. Concluding Remarks

The SUGGEL computer code has been developed and tested on both resonance parameters taken from actual evaluations and on artificially-generated parameters. Test results show that SUGGEL is capable of providing a reasonable first estimate for the orbital angular momentum quantum numbers for many resonances. By using SUGGEL as a pre-analysis tool before running SAMMY, the analyst can expect a reduction in the time and effort required for proper spin group assignments.

This Bayesian approach is unfortunately not appropriate for some resonances at high energy region, higher than ~hundred keV, where the magnitudes of  $g\Gamma_n$ 's of  $s$ -wave and higher  $l$ -waves are comparable. This was anticipated initially, and is observed in a test for  $^{27}\text{Al}$  with SUGGEL. There is another kind of deficiency: The Bayesian approach fails in distinguishing the total angular momentum. However, in spite of deficiencies in the  $l$  assignment for higher energy resonances as well as in the  $J$  assignment, SUGGEL is still effective in providing a good initial guess of spin group for a detailed analysis.

The method (as well as the calculation of the probability density functions) could be incorporated into the SAMMY code. An effective alternate procedure would be to run the three codes RSAP, SUGGEL, and then SAMMY. In this procedure, the RSAP 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 priori parameter file with suggested spin group identification. Finally, SAMMY will be used to perform the detailed analysis.

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## Appendix A. Probability Density Function of Neutron Width

### A.1. Derivation of the Probability Density Functions

According to Porter and Thomas [Po56], the reduced neutron widths (represented as  $x = \Gamma_n^l / \langle \Gamma_n^l \rangle$ ) obey the following distribution:

$$p(x)dx = \frac{1}{\sqrt{2\pi x}} e^{-x/2} dx \text{ for } \nu = 1, \text{ and} \quad (\text{A1})$$

$$p(x)dx = e^{-x} dx \text{ for } \nu = 2. \quad (\text{A2})$$

Here  $\nu$ , the degree of freedom (dof), is the number of exit channels and is equal to the multiplicity of  $J$ .

The neutron reduced width,  $\Gamma_n^l$ , is defined herein as

$$\Gamma_n^l = \sqrt{\frac{1 \text{ eV}}{E} \frac{\Gamma_n}{V_l}}, \quad (\text{A3})$$

where  $E$  is the resonance energy and the penetrability  $V_l$  is given by

$$V_0 = 1,$$

$$V_1 = \frac{(kR)^2}{1 + (kR)^2}, \text{ and}$$

$$V_2 = \frac{(kR)^4}{9 + 3(kR)^2 + (kR)^4}$$

for  $l = 0, 1, \text{ and } 2$  ( $s, p, \text{ and } d$ -waves) respectively. Here  $k$  and  $R$  are the neutron wave number and scattering radius, respectively.

If one then makes the change of variable from  $x = \Gamma_n^l / \langle \Gamma_n^l \rangle$  in Eqs. (A1) and (A2) to  $y = g\Gamma_n^l / \langle g\Gamma_n^l \rangle$ , applies  $p(x)dx = p(y)dy$ , and re-arranges so that the integration variable is  $g\Gamma_n$ , then the equations take the form

$$p_{l_j}(g\Gamma_n) d(g\Gamma_n) = \frac{\exp\left(-\frac{g\Gamma_n^l}{2g_j\langle\Gamma_{nj}^l\rangle}\right)}{\sqrt{\frac{2\pi g\Gamma_n^l}{g_j\langle\Gamma_{nj}^l\rangle}}} d\left(\frac{g\Gamma_n^l}{g_j\langle\Gamma_{nj}^l\rangle}\right) = \frac{\exp\left(-\frac{g\Gamma_n}{2g_j\langle\Gamma_{nj}^l\rangle\sqrt{EV_l}}\right)}{\sqrt{2\pi g\Gamma_n g_j\langle\Gamma_{nj}^l\rangle\sqrt{EV_l}}} d(g\Gamma_n), \quad (\text{A1}')$$

$$\begin{aligned} p_{l_j}(g\Gamma_n) d(g\Gamma_n) &= \exp\left(-\frac{g\Gamma_n^l}{g_j\langle\Gamma_{nj}^l\rangle}\right) d\left(\frac{g\Gamma_n^l}{g_j\langle\Gamma_{nj}^l\rangle}\right) \\ &= \exp\left(-\frac{g\Gamma_n}{g_j\langle\Gamma_{nj}^l\rangle\sqrt{EV_l}}\right) \frac{d(g\Gamma_n)}{g_j\langle\Gamma_{nj}^l\rangle\sqrt{EV_l}}, \end{aligned} \quad (\text{A2}')$$

in which the subscript  $j$  is an index representing the resonance spin  $J_j$ , and  $g_j$  is the statistical factor. Note that  $g\Gamma_n$  is treated here as a single quantity. Also recall that above equations are for resonances of the same  $J_j$ .

Consider now the quantity  $\langle\Gamma_{nj}^l\rangle$ . This term, unlike  $\langle g\Gamma_n^l\rangle$ , is generally not known from measurements because statistical factors for all resonances are not determined experimentally.<sup>12</sup> From the definition of the neutron strength function,

$$S_{l_j} = \frac{\langle\Gamma_{nj}^l\rangle}{\langle D_{lj}\rangle} \text{ and } S_l = \frac{\langle g\Gamma_n^l\rangle}{(2l+1)\langle D_l\rangle},$$

and an assumption [A1] that

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

where  $\mu_{l_j}$  is the multiplicity of  $J_j$ ,  $\langle\Gamma_{nj}^l\rangle$  is found to have the form

$$\langle\Gamma_{nj}^l\rangle = \langle D_l\rangle \frac{\langle D_{lj}\rangle}{\langle D_l\rangle} \mu_{l_j} S_l = \frac{\langle D_l\rangle}{w_{l_j}} \mu_{l_j} S_l. \quad (\text{A4})$$

---

<sup>12</sup> Actually, this is the reason to deal with  $g\Gamma_n$ , instead of  $\Gamma_n$ , as a single quantity.

The average level spacing can be calculated from a theoretical model with empirical model parameters such as the level density parameter. The model is described in Section 2.2 in the text. The determination of  $w_{lj}$  is described below; see Eq. (A6).

The pdf for  $l$ -wave resonances, in which all possible  $J$  values for the specific  $l$ -wave are taken into account, is derived as follows by weighting pdf's for each  $J_j$  given by Eq. (A1') or (A2'). The probability that the magnitude of neutron width of an  $l$ -wave resonance lies in between  $g\Gamma_n$  and  $g\Gamma_n + d(g\Gamma_n)$  is obtained as

$$P(g\Gamma_n | l) d(g\Gamma_n) = \sum_j w_{lj} p_{lj}(g\Gamma_n) d(g\Gamma_n), \quad (\text{A5})$$

where the weight  $w_{lj}$  is the probability that the total spin of a certain  $l$ -wave resonance is  $J_j$ . The weight is calculated as the ratio of number of  $l$ -wave resonances of which resonance spin is  $J_j$  to the total number of  $l$ -wave resonances;

$$w_{lj} \equiv \frac{N_{lj}}{N_l} = \frac{\langle D_l \rangle}{\langle D_{lj} \rangle}. \quad (\text{A6})$$

The sum over  $j$  in Eq. (A5) is the sum for all distinct  $J_j$ 's only once, regardless of its multiplicity.

The following paragraphs indicate the derivation of the detailed form of the pdf for  $p$ -wave resonances. Pdf's for  $s$ - and  $d$ -wave can be derived in analogous fashion; results are given in the text in Eqs. (3) and (5).

For the  $p$ -wave, at most four different  $J$  values are permitted. For convenience, we consider  $J$  values sorted in ascending order. Table A1 shows this convention and the multiplicity.

**Table A 1. Target Spin Dependent Multiplicity of J for p-wave Resonances**

Target Spin	Channel Spin	Possible $J$				Multiplicity				Note
		$j = 1$	$j = 2$	$j = 3$	$j = 4$	$j = 1$	$j = 2$	$j = 3$	$j = 4$	
0	1/2	1/2			3/2	1	0	0	1	$w_{12} = w_{13} = 0$
1/2	0 1	0	1 1		2	1	2	0	1	$w_{13} = 0$
1	1/2 3/2		1/2 1/2	3/2 3/2	5/2	0	2	2	1	$w_{11} = 0$
$\geq 3/2$	I-1/2 I+1/2	I-3/2	I-1/2 I-1/2	I+1/2 I+1/2	I+3/2	1	2	2	1	

By applying Eq. (A1') for  $j = 1$  and 4 and (A2') for  $j = 2$  and 3, and using Eq. (A4) through Eq. (A5), we find that the pdf for p-waves takes the form

$$\begin{aligned}
P(g\Gamma_n | l=1) = & w_{11} \frac{\exp\left(-\frac{w_{11}}{2g_{11}S_1\langle D_1 \rangle} \frac{g\Gamma_n}{\sqrt{EV_1}}\right)}{\sqrt{2\pi} g_{11} \frac{S_1\langle D_1 \rangle}{w_{11}} \sqrt{EV_1} g\Gamma_n} + w_{12} \frac{\exp\left(-\frac{w_{12}}{g_{12}2S_1\langle D_1 \rangle} \frac{g\Gamma_n}{\sqrt{EV_1}}\right)}{g_{12} \frac{2S_1\langle D_1 \rangle}{w_{12}} \sqrt{EV_1}} \\
& + w_{13} \frac{\exp\left(-\frac{w_{13}}{g_{13}2S_1\langle D_1 \rangle} \frac{g\Gamma_n}{\sqrt{EV_1}}\right)}{g_{13} \frac{2S_1\langle D_1 \rangle}{w_{13}} \sqrt{EV_1}} + w_{14} \frac{\exp\left(-\frac{w_{14}}{2g_{14}S_1\langle D_1 \rangle} \frac{g\Gamma_n}{\sqrt{EV_1}}\right)}{\sqrt{2\pi} g_{14} \frac{S_1\langle D_1 \rangle}{w_{14}} \sqrt{EV_1} g\Gamma_n}.
\end{aligned}$$

## A.2. Approximation

If the  $(2J+1)$  law of the level density such that

$$\frac{1}{\langle D(J) \rangle} \propto (2J + 1)$$

is assumed, the weight of Eq. (A6) becomes

$$w_{lj} = \frac{\langle D_l \rangle}{\langle D_{lj} \rangle} = \frac{(2J_{lj} + 1)}{\sum_{j'} (2J_{lj'} + 1)} = \frac{g_{lj}}{G_l}, \quad G_l \equiv \sum_j g_{lj}. \quad (\text{A6}')$$

From the same concept, the  $l$ -wave average level spacing is calculated as  $\langle D_l \rangle = \langle D_l \rangle \cdot G_l / G_l$ , and especially,  $\langle D_l \rangle = \langle D_0 \rangle / G_l$  because  $G_0 = 1$  regardless of the value of target spin. The values of  $G_l$  are given in Table A2.

**Table A 2. Sum of Statistical Factors**

$I$	$l=0$	$l=1$		$l=2$	
	$G_0$	$G_1$	$(g_{11}+g_{14})/G_1$	$G_2$	$(g_{21}+g_{26})/G_2$
0	1	3	1	5	1
1/2	1	9/4	2/3	15/4	2/3
1	1	2	1/2	20/6	1/2
3/2	1	2	1/2	25/8	2/5
$\geq 2$	1	2	1/2	3	1/3

Applying the weight of Eq. (A6') to each pdf's results in

$$P(g\Gamma_n | l=0) = \frac{\exp\left(-\frac{g\Gamma_n}{2S_0\langle D_0\rangle\sqrt{EV_0}}\right)}{\sqrt{2\pi} S_0\langle D_0\rangle\sqrt{EV_0} g\Gamma_n}, \quad (\text{A7})$$

$$\begin{aligned} P(g\Gamma_n | l=1) &= \frac{1}{G_1} \left( \frac{g_{11} + g_{14}}{\sqrt{2\pi} G_1 S_1 \langle D_1 \rangle \sqrt{EV_1} g\Gamma_n} + \frac{g_{12} + g_{13}}{2 G_1 S_1 \langle D_1 \rangle \sqrt{EV_1}} \right) \exp\left(-\frac{g\Gamma_n}{2 G_1 S_1 \langle D_1 \rangle \sqrt{EV_1}}\right) \\ &= \left( \frac{(g_{11} + g_{14}) / G_1}{\sqrt{2\pi} S_1 \langle D_0 \rangle \sqrt{EV_1} g\Gamma_n} + \frac{1 - (g_{11} + g_{14}) / G_1}{2 S_1 \langle D_0 \rangle \sqrt{EV_1}} \right) \exp\left(-\frac{g\Gamma_n}{2 S_1 \langle D_0 \rangle \sqrt{EV_1}}\right), \text{ and} \quad (\text{A8}) \end{aligned}$$

$$\begin{aligned} P(g\Gamma_n | l=2) &= \frac{1}{G_2} \left( \frac{g_{21} + g_{26}}{\sqrt{2\pi} G_2 S_2 \langle D_2 \rangle \sqrt{EV_2} g\Gamma_n} + \frac{g_{22} + g_{23} + g_{24} + g_{25}}{2 G_2 S_2 \langle D_2 \rangle \sqrt{EV_2}} \right) \exp\left(-\frac{g\Gamma_n}{2 G_2 S_2 \langle D_2 \rangle \sqrt{EV_2}}\right) \\ &= \left( \frac{(g_{21} + g_{26}) / G_2}{\sqrt{2\pi} S_2 \langle D_0 \rangle \sqrt{EV_2} g\Gamma_n} + \frac{1 - (g_{21} + g_{26}) / G_2}{2 S_2 \langle D_0 \rangle \sqrt{EV_2}} \right) \exp\left(-\frac{g\Gamma_n}{2 S_2 \langle D_0 \rangle \sqrt{EV_2}}\right). \quad (\text{A9}) \end{aligned}$$

### A.3. Distinguishing $s$ - and $p$ -wave resonances with $(2J+1)$ law

Consider a simplified problem of distinguishing  $s$ - and  $p$ -wave resonances. Applying Eqs. (A7) and (A8) to Eq. (1) in the text, the probability for a  $p$ -wave may be written as:

$$P(l=1 | g\Gamma_n) = \left[ 1 + \frac{1}{G_1} \sqrt{\frac{S_1 V_1}{S_0 V_0}} \frac{\exp\left\{ \frac{g\Gamma_n}{2\langle D_0 \rangle \sqrt{E}} \left( \frac{1}{S_1 V_1} - \frac{1}{S_0 V_0} \right) \right\}}{\alpha + (1-\alpha) \sqrt{\frac{\pi g\Gamma_n}{2\sqrt{E} \langle D_0 \rangle S_1 V_1}}} \right]^{-1}, \quad (\text{A10})$$

where  $G_1 = 3$ ,  $\alpha = 1$  for  $I = 0$  nuclide,  $G_1 = 9/4$ ,  $\alpha = 2/3$  for  $I = 1/2$ , and  $G_1 = 2$ ,  $\alpha = 1/2$  for  $I \geq 1$ .

## Reference Appendix A

- [A1] McLane, V. *et al.*, Ed., "ENDF-102: Data Formats and Procedures for the Evaluated Nuclear Data File ENDF-6," Appendix D, BNL-NCS-44945, Rev.2/97, Brookhaven National Lab. (1997)

## Appendix B. Source Listing of SUGGEL

```
program suggel
c
c GENERAL DESCRIPTION:
c 1.This program suggests the orbital angular momentum (l) of a resonance
c   from the magnitude of its g*Gamma_n.
c 2.Such suggestion is based on the probability that a resonance with gGn
c   is an l-wave. The probability is calculated by using the Bayesian
c   theorem on the conditional probability.
c 3.Physics Models and Assumptions:
c   - Each resonance is characterized by l and resonance spin (J).
c     Two channels are allowed for some J's for l>0 in case of I>0 target.
c   - Reduced neutron widths (gGn^l) follow the Chi-square distribution
c     (dof=1 for multiplicity(mu)=1 and dof=2 for mu=2).
c   - The neutron strength function of (l,J) resonances is assumed as
c     S_lJ = mu_lJ*S_l, and
c   - Bethe level density formula is adopted:
c     the level density is proportional to (2J+1)*exp{-(J+1/2)^2/2sigma^2},
c     the density is assumed to be constant over energy.
c 4.To take the finite resolution of measurement into account, this program
c   adjusts a priori probabilities via an input variable "frac".
c   - The measurement efficiency, as one of the output, may be considered
c     as "frac" in the input that corrects a priori probabilities. It is
c     obtained from the missing level estimation (MLE).
c   - The MLE is performed for every wave.
c
c INPUT:
c   unit 5: standard input in the namelist format:
c           First line contains " &indata", and last line " &end".
c   unit 2: if partyp=0, a file containing (En,Gn) data in SAMMY.PAR format
c           otherwise, a file containing (En,gGn) data in RSAP.GAMMA format
c OUTPUT:
c   unit 3: standard output list
c   unit 4: a file containing (En,Gn,spin group) data in SAMMY.PAR format
c
c Written by S-Y. Oh (syoh@kaeri.re.kr), KAERI.
c Last modification: Aug. 22, 2000
c
parameter (nrs=10000)
common /data1/ spin,awri,rr,sigsq
common /data2/ dd(3),stn(3),vv(3),pcut
common /tbl/ aj(12),g(12),wt(12),wtl(3)
common /ajseed/ seed
dimension probl(3),frac(3),priori(3),dth(3),nth(3),effi(3)
dimension sumggn(3),nr(3),stnew(3),stnm(3),lsam(18),ajsam(18)
dimension ggnl(nrs,3),anth(3),avggn(3),nmle(3)
dimension sumold(3),nrold(3),stno(3)
integer partyp,optj
character*24 parin,fout,parout
character*13 assj(2)
character*1 flagl,flagg,txt(65),txt2(15),wave(3),flgmle(3)
data pi/3.141593/,eps/0.00001/,wave/'s','p','d'/
data assj/'most probable','random'/
namelist /indata/parin,partyp,fout,parout,eini,efin,awri,spin,pcut
* ,optj,scatter,disp,sigcon,bn,pair,denpar,stn,dzero,frac,lsam
* ,ajsam
data pi/3.141593/,eps/0.00001/,wave/'s','p','d'/
data assj/'most probable','random'/
```

```

c
c parin = input (En, Gn or gGn) data file name [En in eV, Gn or gGn in meV]
c partyp = type of the neutron width in parin file:
c           if 0, Gn in SAMMY.PAR format; otherwise, g*Gn in rsap.gamma format
c fout = standard output file name
c parout = output resonance parameter file name in SAMMY.PAR format
c eini [eV] = lower energy boundary to be analyzed
c efin [eV] = upper energy boundary to be analyzed
c pcut = probability cutoff: L will be altered for a resonance of which prob.
c         is higher than pcut.
c optj = option for J assignment: If optj = 0, most probable J is assigned,
c         otherwise, J is assigned randomly.
c awri = atomic mass of target nuclide
c spin = spin of the target nuclide
c scattr [fm] = scattering radius
c disp = spin dispersion parameter (sigma):
c         if = 0, calculate it with parameters such as bn, pair, and denpar
c         if (2J+1) law is wanted, enter a large number (e.g., 999)
c sigcon = constant for the calculation of spin dispersion parameter,
c           sigma^2=sigcon*sqrt(denpar*U)*awri^(2/3)
c bn [MeV] = neutron separation energy for calculating disp
c pair [MeV] = pairing energy
c denpar [1/MeV] = level density parameter
c stn(3) [1.E-04] = neutron strength functions of s-, p-, and d-wave
c dzero [eV] = s-wave avg level spacing
c frac(3) = fraction of number of measured resonances to the theoretical
c           number of resonances for each l
c lsam(i) = l value of spin group i (i= 1 to max. 18) in SAMMY.PAR file
c ajsam(i) = J value of spin group i (i= 1 to max. 18) in SAMMY.PAR file
c
c       open(5,file='suggel.inp',status='old')
c       read(5,indata)
c       close(5)
c
c       awri=awri/1.008665
c       rr=scattr*0.1                               ! R' in 1.E-12
c       if(rr.le.eps) then
c         rr=0.123*awri**0.33333+0.08
c       end if
c       sigsq=disp*disp
c       if(disp.le.eps) then
c         sigsq=denpar*(bn+(eini+efin)/2000000.-pair)
c         sigsq=sigcon*sqrt(sigsq)*(awri+1.)**(2./3.)
c       sigsq=0.0494*sqrt(sigsq)*(awri+1.)**(2./3.) ! From Mughabghab 98
c       sigsq=0.146*sqrt(sigsq)*(awri+1.)**(2./3.) ! From Facchini 68
c       end if
c       ck=0.002196771*rr*awri/(awri+1.)           ! for wave number calc.
c       vv(1)=1.                                     ! s-wave penetrability
c       do i=1,3
c         stn(i)=stn(i)*0.0001                       ! in null dimension
c       end do
c       flagg= ' '
c       if(partyp.ne.0) flagg='g'
c       if(optj.ne.0) optj=1
c       seed=19
c
c       open(2,file=parin,status='old')
c       open(3,file=fout,status='unknown')
c       open(4,file=parout,status='unknown')
c
c       Preparing table of weights for each term identified by l and J

```

```

c
call calcg(spin,sigsq)
sumwtl=0.
do i=1,3
  frac(i)=amax1(eps,frac(i))
  priori(i)=wtl(i)                ! keep theoretical
  wtl(i)=priori(i)*frac(i)
  sumwt=sumwt+wtl(i)
  dd(i)=dzero*priori(1)/priori(i) ! use theoretical <D>
end do
do i=1,3
  wtl(i)=wtl(i)/sumwt
end do

c
write(3,300)
* flagg,parin,eini,efin,stn*10000,dd(1),spin,awri,pcut,assj(optj+1)
if(scattr.ge.eps) then
  write(3,302) scattr
  if(disp.ge.eps) write(3,304) disp
  write(3,306)
  if(disp.lt.eps) write(3,304) sqrt(sigsq)
else
  if(disp.ge.eps) write(3,304) disp
  write(3,306)
  write(3,302) rr*10.
  if(disp.lt.eps) write(3,304) sqrt(sigsq)
end if
write(3,308)
* wtl,amin1(wtl(1)/wtl(2),1000.),amin1(wtl(1)/wtl(3),1000.)
300 format(' -----'/
*      ' *** PROGRAM SUGGEL v.1.0 ***'/
*      ' -----'//
*      ' * Input (En,',a1,'Gn) data file name = ',a12//
*      ' * Input Variables:/'
*      '      Energy range under consideration [eV] = ',1pe11.4,
*      ' to',e11.4/
*      '      n. strength function (s,p,d) [1E-04] = ',0p3f7.3/
*      '      s-wave avg level spacing [eV] = ',1pe11.4/
*      '      target spin = ',0pf7.3/
*      '      atomic weight (AWRI) = ',f7.3/
*      '      probability cutoff for renewal of L = ',f7.3/
*      '      J assignment = ',a13)
302 format('      scattering radius (AP) [fm] = ',f7.3)
304 format('      spin dispersion parameter (sigma) = ',f7.3)
306 format('/' * Calculated Quantities from the input:')
308 format('      A priori probabilities, s, p, and d = ',3f7.3/
1      '      p & d level spacing, relative to s = ',2f7.3//
2' -----',
3' -----'/ ' nres      En      Reduced ',
4'Gn      Probability      L      J'/
4'      (eV)      (eV)      s      p      d      old new',
4'      old new'/
5' -----',
5' --- ---')

c
write(*,610) priori
610 format('A priori probabilities with infinitesimal resolution = '
*      ',3f6.3)
ifirst=1
nres=0
do i=1,3

```

```

        nr(i)=0
        sumggn(i)=0.
        nroid(i)=0
        sumold(i)=0.
    end do
    enmax=0.0
    enmin=1.0E+7
910 continue                ! continue for the next resonance
    flagl=' '
    nres=nres+1
c
c Now read (En,Gn) file:
c If partyp=0, read Gamma_n from "parin" file and calculate g*G_n
c otherwise, read g*Gamma_n from rsap.gamma
c
    if(partyp.eq.0) then
        call samr(eini,efin,en,gn,ids,txt,txt2,endflg)
        lold=lsam(ids)
        ajold=ajsam(ids)
        width=gn*(2.*ajold+1.)/(2.*(2.*spin+1.))           ! width = g*Gn in eV
    else
        call rsapr(eini,efin,en,gn,gamgam,ifirst,endflg)
        width=gn                                           ! originally gn = gGn
        ifirst=0
        lold=0
    end if
    if(endflg.ge.999.) go to 990
    enmax=amax1(en,enmax)
    enmin=amin1(en,enmin)
    vv(2)=penet(ck,en,1)
    vv(3)=penet(ck,en,2)
c
c The main calculation
c
    call bayes(en,width,optj,lnew,ajnew,probl)             ! width = g*G_n
c
    if(partyp.ne.0) then
        lold=lnew
        ajold=ajnew
    end if
    if(lnew.ne.lold.and.probl(lnew+1).lt.pcut) then
        lnew=lold
        ajnew=ajold
        flagl='?'
    end if
    if(lnew.ne.lold) flagl='*'
    redw=1./sqrt(en)/vv(lnew+1)                            ! in eV
    nr(lnew+1)=nr(lnew+1)+1
    ggnl(nr(lnew+1),lnew+1)=width*redw
    sumggn(lnew+1)=sumggn(lnew+1)+width*redw
    gnew=(2.*ajnew+1.)*0.5/(2.*spin+1.)
    Gn=width/gnew                                         ! Conserve gGn instead of Gn
    Gn1=Gn*redw                                           ! Now G_n^1
    nroid(lold+1)=nroid(lold+1)+1
    sumold(lold+1)=sumold(lold+1)+width/sqrt(en)/vv(lold+1)
c
    write(3,310)
    * nres,en,Gn1,(probl(i),i=1,3),lold,lnew,flagl,ajold,ajnew
310 format(i4,1x,1p2e11.4,1x,0p3f6.3,2i4,1x,a1,2x,2f4.1)
c
    idsnew=99

```

```

do i=1,18
  if(lnew.eq.lsam(i).and.ajnew.eq.ajsam(i)) idsnew=i
end do
if(flagl.eq."?") idsnew=ids
if(partyp.eq.0) then
  write(4,410) (txt(i),i=1,22),Gn*1000.,(txt(i),i=34,65),idsnew
410  format(22a1,1pe11.4,32a1,i2)
  else
    write(4,420) en,gamgam*1000.,Gn*1000.,idsnew
420  format(1p3e11.4,22x,' 0 0 0 0 0',i2)
  end if
c
c  Now move to the next resonance
c
  go to 910
c
990  continue
  dtheo=dzero*priori(1) ! = 1/(1/D0+1/D1+1/D2)
  efin=enmax+dtheo/2.
  eini=enmin-dtheo/2.
  write(3,320) eini,efin
320  format
* (' * : L has been altered from the original assignment.'
*  '/' ? : L should be altered, but the probability is too low.'
*  '/' Energy range has been adjusted to',1pe11.4,' ~',e11.4,' eV.'
*  //33x,14x,'s',10x,'p',10x,'d'/
*  33x,4x,' -----')
c
  do i=1,3
    stnm(i)=sumggn(i)/(efin-eini)/(2*i-1)
    stno(i)=sumold(i)/(efin-eini)/(2*i-1)
c    avgggn(i)=stn(i)*dd(i)*(2*i-1) ! use input stn for MLE
    avgggn(i)=stnm(i)*dd(i)*(2*i-1) ! use new stn for MLE
  end do
  write(3,330)
  write(3,332) nrold,stno*10000.
  write(3,334)
  write(3,332) nr,stnm*10000.
330  format(' Original assignment:')
332  format(' Number of resonances = ',3i11/
*  ' Strength function [1E-04] = ',3f11.3)
334  format('/' New assignment:')
c
c  Missing Level Estimation: Avg. gG_n^1 from MLE's for every wave.
c  However, <D> and S are based on the results for a certain wave.
c  If(max. meas. effi. ge.1.0), ref. wave is the wave showing max. effi.
c  Otherwise, s-wave is the ref.
c
  if(nr(1).ge.nrs.or.nr(2).ge.nrs.or.nr(3).ge.nrs) then
    write(*,('...Warning...No. of resonances exceeds the array "
*  , "size. Reduce the energy interval.))
    stop
  end if
c
  call missl(ggnl,nr,anth,avgggn,flgmle)
c
  do i=1,3
    nmle(i)=anth(i)+0.5
  end do
  iii=1
  rr2=anth(2)*priori(1)/priori(2)

```

```

rr3=anth(3)*priori(1)/priori(3)
if(anth(1).lt.rr2) iii=2
if(rr2.lt.rr3) iii=3
do i=1,3
  dth(i)=(efin-eini)/anth(iii)*priori(iii)/priori(i)
  ann=(efin-eini)/dth(i)
  nth(i)=ann+0.5
  effi(i)=nr(i)/ann
  frac(i)=aminl(1.,effi(i))
  stnew(i)=avgggn(i)/dth(i)/(2.*i-1.)
  if(flgmle(i).eq.'?') stnew(i)=stn(i)
end do
effimx=effi(1)
fff=frac(1)
jjj=1
do i=2,3
  if(effi(i).gt.effimx) then
    effimx=effi(i)
    fff=frac(i)
    jjj=i
  end if
end do
do i=1,3
  frac(i)=frac(i)/fff
end do
if(jjj.ge.2) then
  frac(1)=1.
  if(jjj.eq.3) frac(2)=1.
end if
c
  write(3,340)
* (avgggn(i),flgmle(i),i=1,3),(nmle(i),flgmle(i),i=1,3),wave(iii)
write(3,332) nth,stnew*10000.
write(3,342) effi,dth,frac
340 format('/ From the Missing Level Estim.,'/
*      ' Avg. g*red.width [eV]           = ',1p3(e10.3,a1)/
*      ' Expected no. of resonances      = ',3(i10,a1)//
*      ' Based on the "',a1,'" -wave MLE:')
342 format(' Measurement efficiency      = ',3f11.3/
*      ' Avg. level spacing [eV]         = ',1p3e11.3//
*      ' Recommended frac (as the input) = ',0p3f11.3)
c
  stop
  end
c.....
subroutine calcg(spin,sigsq)
c
c For neutron up to d-wave.
c Each group (i) is identified by l and J:
c   i= 1 and 2 for s-wave, i= 3~6 for p-wave, and i= 7~12 for d-wave;
c   J in ascending order
c Calculated quantities are:
c   aj(12) = J of lj group
c   g(12)  = g (statistical factor)
c   wt(12) = weight (a priori probability to belong to lj group)
c   wtl(3) = a priori probability to belong to l-wave
c           (assuming infinitesimal resolution in this subroutine)
c
common /tbl/ aj(12),g(12),wt(12),wtl(3)
data eps/0.01/
dens(x,y)=(2.*x+1.)*exp(-(x+0.5)*(x+0.5)*0.5/y)

```

```

c s-wave
  aj(1)=spin-0.5
  aj(2)=spin+0.5
c p-wave
  aj(3)=abs(spin-1.)-0.5
  aj(6)=spin+1.5
  do i=4,5
    aj(i)=aj(i-1)+1.
  end do
  do i=4,5
    if(aj(i).ge.aj(6)-eps) aj(i)=-0.5           ! makes weight = 0.
  end do
c d-wave
  ajmin=abs(abs(spin-2.)-0.5)
  aj(7)=ajmin
  if(spin.eq.2.) aj(7)=-0.5
  aj(12)=spin+2.5
  do i=8,11
    aj(i)=aj(i-1)+1.
  end do
  do i=8,11
    if(aj(i).ge.aj(12)-eps) aj(i)=-0.5
  end do
c
  denom=0.5/(2.*spin+1.)
  do i=1,12
    g(i)=(2.*aj(i)+1.)*denom
    wt(i)=dens(aj(i),sigsg)
    if(aj(i).le.-eps) g(i)=1.                   ! to avoid "divided by zero"
  end do
  sumwts=wt(1)+wt(2)
  sumwtp=wt(3)+wt(4)+wt(5)+wt(6)
  sumwtd=wt(7)+wt(8)+wt(9)+wt(10)+wt(11)+wt(12)
  sumwt=sumwts+sumwtp+sumwtd
  wtl(1)=sumwts/sumwt
  wtl(2)=sumwtp/sumwt
  wtl(3)=sumwtd/sumwt
  do i=1,2
    wt(i)=wt(i)/sumwts
  end do
  do i=3,6
    wt(i)=wt(i)/sumwtp
  end do
  do i=7,12
    wt(i)=wt(i)/sumwtd
  end do
c
  return
end
c.....
  subroutine samr(eini,efin,en,width,ids,txt,txt2,endflg)
c .PAR file could be out of sorting in energy
  character*1 txt(65),txt2(15)
  endflg=1.
910  continue
  read(2,205,end=990) txt,txt2
205  format(65a1,15a1)
  if(txt(5).ne.' ') then
    backspace 2
    read(2,210) en,gn,ids
210  format(f11.3,11x,e11.4,22x,10x,i2)

```

```

        width=gn*0.001                                ! in eV
        if(en.lt.eini.or.en.gt.efin) then
            write(4,205) txt,txt2
            go to 910
        end if
    else
911    continue
        write(4,205) txt,txt2
        read(2,205,end=990) txt,txt2
        go to 911
    end if
    return
c
990  endflg=9999.
    return
    end
c.....
    subroutine rsapr(eini,efin,en,gn,gamgam,ifirst,endflg)
    character*7 last
    if(ifirst.eq.0) go to 110
    do i=1,4
        read(2,210) last
210    format(a7)
    end do
    read(2,*) dum,dum,dum,gamgam
    do i=1,8
        read(2,210) last
    end do
110  continue
        read(2,210) last
        if(last.eq." PKFIN") go to 990
        backspace 2
        read(2,*) idum,en,dum,dum,dum,dum,gn
        if(en.lt.eini) go to 110
        if(en.gt.efin) go to 990
        return
990  endflg=999.
    return
    end
c.....
    subroutine bayes(en,ggn,jopt,lnew,ajnew,probl)
c
c Calculating the probability to be a l-wave (probl(3)) and
c                                     to have J (probj(12)), and
c Suggesting new l and J
c
    common /data2/ dd(3),stn(3),vv(3),pcut
    common /tbl/ aj(12),g(12),wt(12),wtl(3)
    common /ajseed/ seed
    dimension cl(12),probl(3),probj(12),term(12),each(12),ppp(3)
    data pi/3.14159/,eps/1.E-19/,alarge/1.E+38/
c
    do i=1,12
        j=1
        if(i.ge.3) j=2
        if(i.ge.7) j=3
        cl(i)=2.*sqrt(en)*vv(j)*stn(j)*dd(j)
    end do
    do i=1,12
        term(i)=wt(i)/cl(i)/g(i)
        each(i)=wt(i)*exp(-term(i))*ggn)

```

```

        if(i.le.3.or.i.eq.6.or.i.eq.7.or.i.eq.12) then      ! for dof=1
            if(term(i).gt.1./eps.and.ggn.lt.eps) then
                each(i)=alarge
            else
                each(i)=each(i)*sqrt(term(i)/pi/ggn)
            end if
        else
            each(i)=each(i)*term(i)                        ! for dof=2
        end if
    end do
c
    ppp(1)=each(1)+each(2)
    ppp(2)=each(3)+each(4)+each(5)+each(6)
    ppp(3)=each(7)+each(8)+each(9)+each(10)+each(11)+each(12)
    pall=ppp(1)*wtl(1)+ppp(2)*wtl(2)+ppp(3)*wtl(3)
    almax=0.
    do i=1,3
        probl(i)=ppp(i)*wtl(i)/pall
        if(probl(i).gt.almax) then
            almax=probl(i)
            lnew=i-1
        end if
    end do
c
    iini=lnew*lnew+lnew+1
    ifin=lnew*lnew+3*lnew+2
    if(jopt.eq.0) then
c
c
c
        Suggest most probable J: for only terms belonged to lnew
c
        ajmax=0.
        do i=iini,ifin
            probj(i)=probl(lnew+1)*each(i)/ppp(lnew+1)
            if(probj(i).gt.ajmax) then
                ajmax=probj(i)
                ajnew=aj(i)
            end if
        end do
        return
    else
c
c
c
        Assign J randomly (instead of deterministic J assignment above)
c
        cdf=0.
        crit=rand(seed)
        do i=iini,ifin
            cdf=cdf+wt(i)
            if(crit.le.cdf) then
                ajnew=aj(i)
                return
            end if
        end do
    end if
    return
end
c.....
function penet(ck,en,l)
rksq=ck*ck*abs(en)
if(l.eq.0) penet=1.
if(l.eq.1) penet=rksq/(1.+rksq)
if(l.eq.2) penet=rksq*rksq/(9.+3.*rksq+rksq*rksq)

```

```

return
end
c.....
subroutine missl(ggnl,nr,anth,avggn,flgmle)
c
c Returns expected (theoretical) no. of resonances and avg. gGn^1
c obtained from the Missing Level Estimation.
c Integration from cut0(=1/4, adjustable) to cut1(=5).
c E.g., for s-wave with (2J+1) law, qth=1.2063, ath=1.5705, cdfth=0.6171
c
parameter (nsr=10000)
dimension ggnl(nsr,3),nr(3),anth(3)
* ,qth(3),ath(3),cdfth(3),avggn(3)
character*1 flgmle(3)
data cut0/0.25/,cut1/5.0/
cut=cut0
cutu=cut1
do i=1,3
flgmle(i)=' '
end do
c
do 100 i=1,3
if(nr(i).lt.2) then
anth(i)=1.
avggn(i)=ggnl(1,i)
flgmle(i)='?'
go to 100
end if
call sort(nr(i),ggnl(1,i))
910 continue
call theo(cut,cutu,qth,ath,cdfth)
qmm=0.
am=0.
mm=0
nskip=0
do 110 j=nr(i),1,-1
if(i.ge.2.and.ggnl(j,i)/avggn(i).gt.cutu) then
nskip=nskip+1
go to 110
end if
am=am+ggnl(j,i)
qmm=qmm+sqrt(ggnl(j,i))
mm=mm+1
qm=mm*am/qmm/qmm
if(qm.ge.qth(i)) go to 900
110 continue
write(*,'(...Warning... Integration for MLE (l="i1,")',
* " will be adjusted to ",f5.2," ~",f5.2)') i-1,cut+0.1,cutu
cut=cut+0.1
if(cut.ge.cutu) then
write(*,'(...Missing Level Estim. for l="i1,
* " is unavailable.")') i-1
anth(i)=nr(i)
cut=cut0
flgmle(i)='?'
pause
go to 100
end if
go to 910
900 anth(i)=mm/cdfth(i)
am=am/mm

```

```

        avggn(i)=am/ath(i)
        cut=cut0
100  continue
      return
      end
c.....
      subroutine theo(cut0,cutu,qth,ath,cdfth)
      common /tbl/ aj(12),g(12),wt(12),wtl(3)
      dimension qth(3),ath(3),cdfth(3),xpt(3),rxpt(3)
      dimension pup(12),xpup(12),rxpup(12)
      dimension tt(12),terf(12),texp(12),p(12),xp(12),rxp(12),mul(12)
      data pi/3.141593/,eps/1.E-20/,mul/3*1,2*2,2*1,4*2,1/
      external erf

c
c   Integrate x_lo(=cut0) to inf. for s-wave
c   Integrate x_lo to x_up(=cutu) for p- and d-wave
c   Integrate x_up to inf. first (ii=1)
c
      cut=cutu
      do ii=1,2
      do i=1,12
          tt(i)=wt(i)/2./g(i)*cut
          if(i.ge.7) tt(i)=tt(i)*5.
          if(i.ge.3.and.i.le.6) tt(i)=tt(i)*3.
          if(tt(i).le.eps) tt(i)=eps
          terf(i)=erf(sqrt(tt(i)))
          texp(i)=exp(-tt(i))
          if(mul(i).eq.1) then
              p(i)=wt(i)*(1.-terf(i))
              xp(i)=wt(i)/tt(i)*cut*
*              ( sqrt(tt(i)/pi)*texp(i)+0.5*(1.-terf(i)) )
              rxp(i)=wt(i)/sqrt(tt(i)/cut*pi)*texp(i)
          else
              p(i)=wt(i)*texp(i)
              xp(i)=wt(i)/tt(i)*cut*(tt(i)+1.)*texp(i)
              rxp(i)=wt(i)*( sqrt(cut)*texp(i)+
*              sqrt(pi/tt(i)*cut)*0.5*(1.-terf(i)) )
          end if
          if(ii.eq.1) then
              if(i.gt.3) then
                  pup(i)=p(i)
                  xpup(i)=xp(i)
                  rxpup(i)=rxp(i)
              else
                  pup(i)=0.
                  xpup(i)=0.
                  rxpup(i)=0.
              end if
          else
              p(i)=p(i)-pup(i)
              xp(i)=xp(i)-xpup(i)
              rxp(i)=rxp(i)-rxpup(i)
          end if
      end do
      cut=cut0
      end do

c
      do i=1,3
          cdfth(i)=0.
          xpt(i)=0.
          rxpt(i)=0.

```

```

        j1=i*i-i+1
        j2=i*i+i
        do j=j1,j2
            cdfth(i)=cdfth(i)+p(j)
            xpt(i)=xpt(i)+xp(j)
            rxpt(i)=rxpt(i)+rxp(j)
        end do
        qth(i)=xpt(i)*cdfth(i)/rxpt(i)/rxpt(i)
        ath(i)=xpt(i)/cdfth(i)
    end do
    return
end

C .....
C (C) Copr. 1986-92 Numerical Recipes Software <=s='%'.
    FUNCTION erf(x)
    REAL erf,x
CU    USES gammp
    REAL gammp
    if(x.lt.0.)then
        erf=-gammp(.5,x**2)
    else
        erf=gammp(.5,x**2)
    endif
    return
    END
C (C) Copr. 1986-92 Numerical Recipes Software <=s='%'.
    FUNCTION gammp(a,x)
    REAL a,gammp,x
CU    USES gcf,gser
    REAL gammpcf,gamser,gln
    if(x.lt.0..or.a.le.0.)pause 'bad arguments in gammp'
    if(x.lt.a+1.)then
        call gser(gamser,a,x,gln)
        gammp=gamser
    else
        call gcf(gammpcf,a,x,gln)
        gammp=1.-gammpcf
    endif
    return
    END
C (C) Copr. 1986-92 Numerical Recipes Software <=s='%'.
    SUBROUTINE gser(gamser,a,x,gln)
    INTEGER ITMAX
    REAL a,gamser,gln,x,EPS
    PARAMETER (ITMAX=100,EPS=3.e-7)
CU    USES gammln
    INTEGER n
    REAL ap,del,sum,gammln
    gln=gammln(a)
    if(x.le.0.)then
        if(x.lt.0.)pause 'x < 0 in gser'
        gamser=0.
        return
    endif
    ap=a
    sum=1./a
    del=sum
    do 11 n=1,ITMAX
        ap=ap+1.
        del=del*x/ap
        sum=sum+del

```

```

        if(abs(del).lt.abs(sum)*EPS)goto 1
11    continue
        pause 'a too large, ITMAX too small in gser'
1    gamser=sum*exp(-x+a*log(x)-gln)
        return
        END
C (C) Copr. 1986-92 Numerical Recipes Software <=s='%'.
        SUBROUTINE gcf(gammcf,a,x,gln)
        INTEGER ITMAX
        REAL a,gammcf,gln,x,EPS,FPMIN
        PARAMETER (ITMAX=100,EPS=3.e-7,FPMIN=1.e-30)
CU    USES gammln
        INTEGER i
        REAL an,b,c,d,del,h,gammln
        gln=gammln(a)
        b=x+1.-a
        c=1./FPMIN
        d=1./b
        h=d
        do 11 i=1,ITMAX
            an=-i*(i-a)
            b=b+2.
            d=an*d+b
            if(abs(d).lt.FPMIN)d=FPMIN
            c=b+an/c
            if(abs(c).lt.FPMIN)c=FPMIN
            d=1./d
            del=d*c
            h=h*del
            if(abs(del-1.).lt.EPS)goto 1
11    continue
        pause 'a too large, ITMAX too small in gcf'
1    gammcf=exp(-x+a*log(x)-gln)*h
        return
        END
C (C) Copr. 1986-92 Numerical Recipes Software <=s='%'.
        FUNCTION gammln(xx)
        REAL gammln,xx
        INTEGER j
        DOUBLE PRECISION ser,stp,tmp,x,y,cof(6)
        SAVE cof,stp
        DATA cof,stp/76.18009172947146d0,-86.50532032941677d0,
*24.01409824083091d0,-1.231739572450155d0,.1208650973866179d-2,
*-.5395239384953d-5,2.5066282746310005d0/
        x=xx
        y=x
        tmp=x+5.5d0
        tmp=(x+0.5d0)*log(tmp)-tmp
        ser=1.000000000190015d0
        do 11 j=1,6
            y=y+1.d0
            ser=ser+cof(j)/y
11    continue
        gammln=tmp+log(stp*ser/x)
        return
        END
c.....
        SUBROUTINE SORT(N,RA)
        DIMENSION RA(N)
        L=N/2+1
        IR=N

```

```

10  CONTINUE
    IF(L.GT.1)THEN
      L=L-1
      RRA=RA(L)
    ELSE
      RRA=RA(IR)
      RA(IR)=RA(1)
      IR=IR-1
      IF(IR.EQ.1)THEN
        RA(1)=RRA
        RETURN
      ENDIF
    ENDIF
    I=L
    J=L+L
20  IF(J.LE.IR)THEN
      IF(J.LT.IR)THEN
        IF(RA(J).LT.RA(J+1))J=J+1
      ENDIF
      IF(RRA.LT.RA(J))THEN
        RA(I)=RA(J)
        I=J
        J=J+J
      ELSE
        J=IR+1
      ENDIF
      GO TO 20
    ENDIF
    RA(I)=RRA
    GO TO 10
  END

```

## Appendix C. Program LADDER

### C.1. Introduction

The program LADDER is used to generate Reich-Moore type pseudo resonance parameters. It produces a parameter file in SAMMY.PAR format. Samplings are performed as follows; these are basically same to the methods used in the program URR [Le90].

- Resonance energy: random sampling from the cumulative Wigner distribution,
- Neutron width and fission width: random sampling from  $\chi^2$  distribution (degree of freedom of one or two) by using the rejection technique, and
- Radiative width: constant.

### C.2. Input Description

Table C1 shows a sample input; input for the generation of pseudo  $^{235}\text{U}$  resonance parameters. Description of input variables follows the table. The input is prepared in free format.

Table C 1. Sample Input of LADDER

```
233.0351
0.,200.
3
2
1.143,3,1.143e-4,1,0.1625,0.1625,3,0.038
0.889,4,0.889e-4,1,0.086,0.086,2,0.038
0.0,0,0.0,0,0.0,0.0,0,0.0
4
1.600,2,1.920e-4,1,0.2115,0.2115,3,0.024
1.143,3,2.743e-4,2,0.0625,0.0625,1,0.024
0.889,4,2.134e-4,2,0.1995,0.1995,3,0.024
0.727,5,0.872e-4,1,0.0625,0.0625,1,0.024
0.0,0,0.0,0,0.0,0.0,0,0.0
6
2.667,1,1.334e-4,1,0.250,0.250,2,0.038
1.600,2,1.600e-4,2,0.250,0.250,2,0.038
1.143,3,1.143e-4,2,0.1625,0.1625,3,0.038
0.889,4,0.889e-4,2,0.0860,0.0860,2,0.038
0.727,5,0.727e-4,2,0.250,0.250,3,0.038
0.615,6,3.075e-5,1,0.250,0.250,2,0.038
0.0,0,0.0,0,0.0,0.0,0,0.0

# Set as S0=1.0, S1=1.2, S2=0.5, D0=0.5, D1=D0/2, D2=D0/3 eV
```

Card 1: mass of the target nuclide

Card 2: lower and upper energy boundary [eV]

Card 3: number of  $l$  states

For each  $l$ ,

Card 4: number of J states

Card 5+ (one card for each J): level spacing [eV], value of J, average reduced neutron width [eV],  
multiplicity of J, average first fission width [eV], average second fission width [eV], number of  
fission channels, average gamma width [eV]

Card next: 0.0 (this card terminates cards set for each  $l$ .)

Repeat above cards set for all  $l$ .

Last card: blank

### C.3. Source Listing

```
      program ladder
c
c This program generates Reich-Moore type resonance parameter in a
c form suitable to the code SAMMY. Parameters are sample according
c to the appropriate probability density function. Level spacings are
c Sample from a Wigner distribution. Level width are sample from
c chi-squared distribution with corresponding degrees of freedom.
c
      character*20 file
      integer*4 seed
c
      parameter (id=150000)
      dimension ds(id), ee(id), gg(id),
*             gn(id), gfl(id), gf2(id), nnn(id),
*             nff(id), gnn(id), gnfl(id), gnf2(id),
*             aj(id), ajj(id), v(3)
c
      common seed
c
      write(6,('Input filename: "$')')
      read(5,'(a)') file
      open(unit=1, file=file,status='unknown')
c
      write(6,('Output filename: "$')')
      read(5,'(a)') file
      open(unit=2, file=file,status='unknown')
c
      seed = 19
      ak0 = 0.002196771
c
c write(*,*) ' Read some pertinente stuff'
c
      read(1,*) awri
c
c write(*,*) 'Enter energy boundaries'
c
      read(1,*) ei, ef
```

```

c
c write(*,*) ' Enter number of l states'
c
c read(1,*) l
c
c write(*,*) ' Enter data for each j state'
c
is = 0
i = 0
do il = 1, l
  read(1,*) js
  ip = 0
1  read(1,*) d, ajl, gnav, nn, gfavg1, gfavg2, nf, ggavg
  if ( d .eq. 0.0) go to 2
  ip = ip + 1
  is = is + 1
  ajj(ip) = is
  ds(ip) = d
  gn(ip) = gnav / nn
  gf1(ip) = gfavg1 / nf
  gf2(ip) = gfavg2 / nf
  gg(ip) = ggavg
  nnn(ip) = nn
  nff(ip) = nf
  go to 1
c
2  continue
  do j = 1, js
    nn = nnn(j)
    nc = nn + nff(j)
    er = ei
    do e = ei, ef, ds(j)
      i = i + 1
c
c Sample d from a Wigner distribution
c
      rr = -alog(amax1(rand(seed), 0.00001))
      x = 1.128379 * ds(j) * sqrt(rr)
      er = er + x
      ee(i) = er
c
c Calculates Penetrabilities
c
      ak = ak0 * sqrt(ee(i)) * awri / (awri + 1.0)
      r = 0.123 * awri ** (1.0/3.0) + 0.08
      rho = ak * r
      rho2 = rho * rho
      rho4 = rho2 * rho2
      v(1) = 1.0
      v(2) = rho2 / (1.0 + rho2)
      v(3) = rho4 / (9.0 + 3.0 * rho2 + rho4)
c
c Ends penetrabilities calculations
c
      gnp = gn(j) * v(il) * sqrt(ee(i))
      gn1 = 0.0
      gf11 = 0.0
      gf12 = 0.0
c
c Gamma width and spin
c

```

```

        gg(i) = gg(j)
        aj(i) = ajj(j)
c
c Sample neutron width from a Porter-Thomas distribution
c
        do inc = 1, nc
3          r1 = -alog(amax1(rand(seed), 0.00001))
            r2 = -alog(amax1(rand(seed), 0.00001))
            if ( 2.0 * r1 .lt. (r2-1) * (r2-1)) go to 3
            if(inc .le. nn) gn1 = gn1 + r2 * r2 * gnp
            if(inc .gt. nn) then
c
c First fission channel
c
                gf11 = gf11 + r2 * r2 * gf1(j)
c
c Second fission channel
c
4          r1 = -alog(amax1(rand(seed), 0.00001))
            r2 = -alog(amax1(rand(seed), 0.00001))
            if ( 2.0 * r1 .lt. (r2-1) * (r2-1)) go to 4
            gf12 = gf12 + r2 * r2 * gf2(j)
            endif
        enddo
c
c Neutron width
c
        gnn(i) = gn1
c
c Sign for the first fission channel
c
        sn = 2.0 * rand(seed) - 1.0
        if (sn .eq. 0.0) then
            sign = 1.0
        else
            sign = sn / abs(sn)
        endif
        gnf1(i) = sign * gf11
c
c Sign for the second fission channel
c
        sn = 2.0 * rand(seed) - 1.0
        if (sn .eq. 0.0) then
            sign = 1.0
        else
            sign = sn / abs(sn)
        endif
        gnf2(i) = sign * gf12
        enddo
    enddo
c
    enddo
    nr = i
    call order(nr, ee, gg, gnn, gnf1, gnf2, aj)
    do i = 1, nr
c
        gg(i) = gg(i) * 1000.0
        gnn(i) = gnn(i) * 1000.0
        gnf1(i) = gnf1(i) * 1000.0
        gnf2(i) = gnf2(i) * 1000.0
        jj = aj(i)

```

```

c
c SAMMY format for .par files
c
    if (ee(i) .lt. 10.0) then
        write(2,1000) ee(i), gg(i), gnn(i), gnfl(i), gnf2(i), jj
    else if (ee(i) .gt. 10.0 .and. ee(i) .lt. 100.0) then
        write(2,1001) ee(i), gg(i), gnn(i), gnfl(i), gnf2(i), jj
    else if (ee(i) .gt. 100.0 .and. ee(i) .lt. 1000.0) then
        write(2,1002) ee(i), gg(i), gnn(i), gnfl(i), gnf2(i), jj
    else if (ee(i) .gt. 1000.0 .and. ee(i) .lt. 10000.0) then
        write(2,1003) ee(i), gg(i), gnn(i), gnfl(i), gnf2(i), jj
    else if (ee(i) .ge. 10000.0 .and. ee(i) .lt. 100000.0) then
        write(2,1004) ee(i), gg(i), gnn(i), gnfl(i), gnf2(i), jj
    else
        write(2,1005) ee(i), gg(i), gnn(i), gnfl(i), gnf2(i), jj
    endif
enddo
c
    stop
1000 format(f11.9, 4(1pelli.4), ' 0 0 0 0 0', i2)
1001 format(f11.8, 4(1pelli.4), ' 0 0 0 0 0', i2)
1002 format(f11.7, 4(1pelli.4), ' 0 0 0 0 0', i2)
1003 format(f11.6, 4(1pelli.4), ' 0 0 0 0 0', i2)
1004 format(f11.5, 4(1pelli.4), ' 0 0 0 0 0', i2)
1005 format(f11.2, 4(1pelli.4), ' 0 0 0 0 0', i2)
    end
c
c Random number generation
c
    function rnmaxf(t)
        integer*4 seed
        common seed
        data ff/0.0/
        u= exprnf(u)
        if(ff) 3, 1, 3
1    r1 = ran(seed)
        r2 = ran(seed)
        r1sq = r1 * r1
        r2sq = r2 * r2
        rsq = r1sq + r2sq
        if(rsq - 1.0) 2, 2, 1
2    w = exprnf(w)/rsq
        ff = 1.0
        rnmaxf = (r2sq * w + u) * t
        go to 4
3    ff = 0.0
        rnmaxf = (r1sq * w + u) * t
4    return
    end
    function exprnf(a)
        real i
        integer*4 seed
        common seed
        i = 0.0
1    x = ran(seed)
        z = x
2    y = ran(seed)
        if(z - y) 5, 5, 3
3    z = ran(seed)
        if(z - y) 2, 4, 4
4    i = i + 1.0

```

```

    go to 1
5   exprnf = x + i
    return
    end
c
c   Order
c
    subroutine order(n, x, y, z, v, w, ay)
c
    dimension x(n), y(n), z(n), v(n), w(n), ay(n)
    n1 = n - 1
    do 2 i = 1, n1
        i1 = i + 1
        do 1 j = i1, n
            if (x(i) .le. x(j)) go to 1
c
                temp = x(i)
                x(i) = x(j)
                x(j) = temp
c
                temp = y(i)
                y(i) = y(j)
                y(j) = temp
c
                temp = z(i)
                z(i) = z(j)
                z(j) = temp
c
                temp = v(i)
                v(i) = v(j)
                v(j) = temp
c
                temp = w(i)
                w(i) = w(j)
                w(j) = temp
c
                temp = ay(i)
                ay(i) = ay(j)
                ay(j) = temp
c
1   continue
2   continue
    return
    end

```

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