2. FILE 2. RESONANCE PARAMETERS

2.1. General Description

The primary function of File 2 is to contain data for both resolved and unresolved resonance parameters. It has only one section, with the reaction type number MT=151. A File 2 is required for incident-neutron evaluations, but it may be omitted in other cases. The use of File 2 is controlled by the parameter LRP (see section 1.1):

LRP=-1 No File 2 is given. Not allowed for incident neutrons.

LRP= 0 No resonance parameters are given except for the scattering radius AP.

AP is included for the convenience of users who need an estimate of the potential scattering cross section. It is not used to calculate a contribution to the scattering cross section, which in this case is represented entirely in File 3.

LRP= 1 Resonance contributions for the total, elastic, fission, and radiative capture cross sections are to be computed from the resonance parameters and added to the corresponding cross sections in File 3[1].

The File 2 resonance contributions should also be added to any lumped reactions included in File 3. For SLBW and MLBW, any other competing reactions in the resonance range must be given in their entirety in File 3 and included in the background for the total cross section. The effects of the competing reactions on the resonance reactions are included using a single competitive width, Γ_x. This width is given explicitly in the unresolved resonance region, and implicitly in the resolved region. In the latter region, it is permissible for the total width to exceed the sum of the neutron,

$$\Gamma_x = \Gamma - \left(\Gamma_n + \Gamma_\gamma + \Gamma_f\right)$$

radiative capture, and fission widths. The difference is interpreted as the competitive width:

For the Reich-Moore or Adler-Adler formalisms competitive reactions are not used.

LRP= 2 Resonance parameters are given in File 2 but are not to be used in calculating cross sections, which are assumed to be represented completely in File 3. Used for certain derived libraries only.

[1] In the unresolved resonance region, the evaluator may, optionally, specify a different procedure, which uses the unresolved resonance parameters in File 2 solely for the purpose of computing an energy-dependent self-shielding factor. This option is governed by a flag, LSSF, defined in Section 2.3.1, and discussed in Section 2.4.21. When this option is specified, File 3 is used to specify the entire infinitely-dilute cross section, and the function of File 2 is to specify the calculation of self-shielding factors for shielded pointwise or multigroup values.

The resonance parameters for a ***material*** are obtained by specifying the parameters for each ***isotope*** in the ***material***. The data for the various ***isotopes*** are ordered by increasing ZAI values (charge-isotopic mass number). The resonance data for each isotope may be divided into several incident neutron energy ranges, given in order of increasing energy. The energy ranges for an isotope should not overlap; each may contain a different representation of the cross sections.

In addition to these parameterized resonance ranges, the full energy range may contain two additional non-resonance ranges, also non-overlapping. Comments on these ranges follow:

1. The low energy region (LER) is one in which the cross sections are tabulated as smooth functions of energy. Doppler effects must be small enough so that the values are essentially zero degrees Kelvin. For light elements, *i.e.*, those whose natural widths far exceed their Doppler widths and hence undergo negligible broadening, the entire energy range can often be represented in this way. For heavier materials, this region can sometimes be used below the lowest resolved resonances. With a good multilevel resonance fit, the LER can often be omitted entirely, and this is preferred. An important procedure for the LER is described in Section 2.4.6.4.
2. The resolved resonance region (RRR) is one in which resonance parameters for individual resonances are given. Usually this implies that experimental resolution is good enough to "see" the resonances, and to determine their parameters by area or shape analysis, but an evaluator may choose to supply fictitious resolved parameters if he so desires. If the evaluator does this, the resonances must have physically-allowed quantum numbers, and be in accord with the statistics of level densities (Appendix D, Section D.2.2). A File 3 background may be given. The essential point is that resonance self-shielding can be accounted for by the user for each resonance individually.
3. The unresolved resonance region (URR) is that region in which the resonances still do not actually overlap, so that self-shielding is still important, but experimental resolution is inadequate to determine the parameters of individual resonances. In this situation, self-shielding must be handled on a statistical basis. A File 3 may be given. The interpretation of this cross section depends on the flag LSSF (see Sections 2.3.1 and 2.4.21). It may be interpreted either as a partial background cross section, to be added to the File 2 contribution, as in the resolved resonance region or it may be interpreted as the entire dilute cross section, in which case File 2 is to be used solely to specify the self-shielding appropriate to this energy region. It is important to choose the boundary between the RRR and the URR so that the statistical assumptions underlying the unresolved resonance treatments are valid. This problem is discussed further in Section 2.4.
4. The high-energy region (HER) starts at still higher energies where the resonances overlap and the cross sections smooth out, subject only to Ericson fluctuations. The boundary between the URR and HER should be chosen so that self-shielding effects are small in the HER.

File 3 may contain "background cross sections" in the resonance ranges resulting from inadequacies in the resonance representation (*e.g.*, SLBW), the effects of resonances outside the energy range, the average effects of missed resonances, or competing cross sections. If these background cross sections are nonzero, there must be double energy points in File 3 corresponding to each resonance range boundary (except 10^{-5}eV). See Section 2.4 for a more complete discussion of backgrounds.

Several representations are allowed for specifying resolved resonance parameters. The flag, LRF, indicates the representation used for a particular energy range:

LRF=1 Single-level Breit-Wigner; (no resonance-resonance interference; one single-channel inelastic competitive reaction is allowed).

LRF=2 Multilevel Breit-Wigner (resonance-resonance interference effects are included in the elastic scattering and total cross sections; one single-channel inelastic competitive reaction is allowed).

LRF=3 Reich-Moore (multilevel multichannel R-matrix; no competitive reactions allowed).

It is possible to define partial widths $\Gamma_{l\,s_1\,J}$ and $\Gamma_{l\,s_2\,J}$ with two different values of the channel spin, as is required when both the target spin and the orbital angular momentum are greater than zero. This is accomplished by setting the resonance spin parameter AJ to a positive value for the larger channel spin ($s = I + 1/2$), and negative for the smaller channel spin ($s = I - 1/2$). (See definition of AJ in 2.2.1.) Older ENDF files have not used this feature, but instead have only positive AJ; in this case, all resonances of a given *l,J* are assumed to have the same channel spin.

For a given resonance, the only rigorously conserved quantities are *J* (total angular momentum) and π (total parity). Nevertheless, this format assumes that both *l* (orbital angular momentum) and *s* (channel spin) are also conserved quantities.

LRF=4 Adler-Adler (level-level and channel-channel interference effects are included in all cross sections via "effective" resonance parameters; usually applied to low-energy fissionable materials; no competitive reactions).

LRF=5 This option is no longer available.

LRF=6 This option is no longer available.

LRF=7 R-Matrix Limited format, which contains all the generality of LRF=3 plus unlimited numbers and types of channels.

Preferred formalisms for evaluation are discussed in Section 2.4.17. Further discussion of the above formalisms is contained in the Procedures Section 2.4.

Each resonance energy range contains a flag, LRU that indicates whether it contains resolved or unresolved resonance parameters. LRU=1 means resolved, LRU=2 means unresolved.

Only one representation is allowed for the unresolved resonance parameters, namely average single-level Breit-Wigner. However, several options are permitted, designated by the flag LRF. With the first option, LRF=1, only the average fission width is allowed to vary as a function of incident neutron energy. The second option, LRF=2, allows the following average parameters to vary: level spacing, fission width, reduced neutron width, radiation width, and a width for the sum of all competitive reactions.

The data formats for the various resonance parameter representations are given in Sections 2.2.1 (resolved) and 2.3.1 (unresolved). Formulae for calculating cross sections from the various formalisms are given in Appendix D.

The following quantities have definitions that are the same for all resonance parameter representations:

NIS Number of isotopes in the material (NIS≤10).

ZAI (Z,A) designation for an isotope.

NER Number of resonance energy ranges for this isotope.

ABN Abundance of an isotope in the material. This is a number fraction, not a ***weight*** fraction, nor a ***percent***.

LFW Flag indicating whether ***average fission widths*** are given in the unresolved resonance region for this isotope:
- LFW=0, average fission widths ***are not*** given;
- LFW=1, average fission widths ***are*** given.

NER Number of resonance energy ranges for isotope.

EL Lower limit for an energy range[2].

EH Upper limit for an energy range[3].

LRU Flag indicating whether this energy range contains data for resolved or unresolved resonance parameters:
- LRU=0, only the scattering radius is given (LRF=0, NLS=0, LFW=0 is required with this option);
- LRU=1, resolved resonance parameters are given.
- LRU=2, unresolved resonance parameters are given.

LRF Flag indicating which representation has been used for the energy range. The definition of LRF depends on the value of LRU:

If LRU=1(resolved parameters), then
- LRF=1, single-level Breit-Wigner (SLBW);
- LRF=2, multilevel Breit-Wigner (MLBW);
- LRF=3, Reich-Moore (RM);
- LRF=4, Adler-Adler (AA);
- LRF=5, no longer available;
- LRF=6, no longer available;
- LRF=7, R-Matrix Limite (RML).

If LRU=2 (unresolved parameters), then
- LRF=1, only average fission widths are energy-dependent;
- LRF=2, average level spacing, competitive reaction widths, reduced neutron widths, radiation widths, and fission widths are energy-dependent.

NRO Flag designating possible energy dependence of the scattering radius:
- NRO=0, radius is energy independent;
- NRO=1 (not allowed in the ENDF/B-VI library)[3].

[2] These energies are the limits to be used in calculating cross sections from the parameters. Some resolved resonance levels, *e.g.*, bound levels, will have resonance energies outside the limits.

[3] Formerly used for radius expressed as a table of energy, radius pairs.

NAPS Flag controlling the use of the two radii, the ***channel radius*** *a* and the ***scattering radius*** AP.

For NRO=0 (AP energy-independent), if:

NAPS=0, calculate *a* from Equation (D.0) given in Appendix D, and read AP as a single energy-independent constant on the subsection CONT (range) record; use *a* in the penetrabilities and shift factors, and AP in the hard-sphere phase shifts;

NAPS=1, do not use Equation (D.0); use AP in the penetrabilities and shift factor as well as in the phase shifts.

For NRO=1 (AP energy-dependent), if:

NAPS=0, calculate *a* from the above equation and use it in the penetrabilities and shift factors. Read AP(E) as a TAB1 quantity in each subsection and use it in the phase shifts;

NAPS=1, read AP(E) and use it in all three places, P_l, S_l, φ_l;

NAPS=2, read AP(E) and use it in the phase shifts. In addition, read the single, energy-independent quantity "AP, see following, and use it in P_l and S_l, overriding the above equation for *a*.

File 2 contains a single section (MT=151) containing subsections for each energy range of each isotope in the material.

The structure of File 2, for the *special case* in which just a scattering radius is specified (no resolved or unresolved parameters are given), is as follows: (such a material is not permitted to have multiple isotopes or an energy-dependent scattering radius)

```
[MAT, 2,151/  ZA, AWR,   0,   0, NIS,    0] HEAD                  (NIS=1)
[MAT, 2,151/ ZAI, ABN,   0, LFW, NER,    0] CONT
                                          (ZAI=ZA,ABN=1.0,LFW=0,NER=1)
[MAT, 2,151/  EL,  EH, LRU, LRF, NRO, NAPS] CONT
                                          (LRU=0,LRF=0,NRO=0,NAPS=0)
[MAT, 2,151/ SPI,  AP,   0,   0, NLS,    0] CONT                  (NLS=0)
[MAT, 2,  0/ 0.0, 0.0,   0,   0,   0,    0] SEND
[MAT, 0,  0/ 0.0, 0.0,   0,   0,   0,    0] FEND
```

If resonance parameters are given, the structure of File 2 is as follows:

```
[MAT, 2,151/  ZA, AWR,   0,   0, NIS,    0] HEAD
[MAT, 2,151/ ZAI, ABN,   0, LFW, NER,    0] CONT                  (isotope)
[MAT, 2,151/  EL,  EH, LRU, LRF, NRO, NAPS] CONT                  (range)
<Subsection for the first energy range for the first isotope>
(depends on LRU and LRF)
[MAT, 2,151/   EL,  EH, LRU, LRF, NRO, NAPS] CONT                 (range)
<Subsection for the second energy range for the first isotope>
  ------------------------------
  ------------------------------
[MAT, 2,151/   EL,   EH, LRU, LRF, NRO, NAPS] CONT                (range)
   <Subsection for the last energy range for the last isotope for this material>
[MAT, 2,  0/ 0.0,  0.0,   0,   0,   0,    0] SEND
```

The data are given for all ranges for a given isotope, and then for all isotopes. The data for each range start with a CONT (range) record; those for each isotope, with a CONT (isotope) record. The specifications for the subsections that include resonance parameters are given in Sections 2.2.1 and 2.3.1, below. A multi-isotope material is permitted to have ***some***, but not all, isotopes specified by a scattering radius only. The structure of a ***subsection*** for such an isotope is:

```
[MAT, 2,151/ SPI,   AP,   0,   0, NLS,    0] CONT                (NLS=0)
```

and as above LFW=0, NER=1, LRU=0, LRF=0, NRO=0, and NAPS=0 for this isotope.

In the case that NRO≠0, the "range" record preceding each subsection is immediately followed by a record giving the energy dependence of the scattering radius, AP.

```
[MAT, 2,151/ 0.0,  0.0,   0,   0,  NR,   NP/ E_int / AP(E)] TAB1
```

If NAPS is 0 or 1 the value of AP on the next record of the subsection should be set to 0.0. If NAPS is 2, it should be set equal to the desired value of the channel radius.

2.2. Resolved Resonance Parameters (LRU=1)

2.2.1.Formats

Six different resonance formalisms are allowed to represent the resolved resonance parameters. Formulae for the various quantities, and further comments on usage, are given in Appendix D. The flag LRU=1, given in the CONT (range) record, indicates that resolved resonance parameters are given for a particular energy range. Another flag, LRF, in the same record specifies which resonance formalism has been used.

The following quantities are defined for use with all formalisms:

SPI Spin, I, of the target nucleus.

AP Scattering radius in units of 10^{-12}cm. For LRF=1-4, it is assumed to be independent of the channel quantum numbers.

NLS Number of *l*-values (neutron orbital angular momentum) in this energy region.
LRF=1-4, a set of resonance parameters is given for each *l*-value.
LRF=5 and 6, NLS is the number of *l*-values required to converge the calculation of the scattering cross section (see Sections 2.4.23 and 2.4.24). Another cutoff, NLSC, is provided for converging the angular distributions. Currently, NLS≤4.

AWRI Ratio of the mass of a particular isotope to that of a neutron.

QX Q-value to be added to the incident particle's center-of-mass energy to determine the channel energy for use in the penetrability factor. The conversion to laboratory system energy depends on the reduced mass in the exit channel. For inelastic scattering to a discrete level, the Q-value is minus the level excitation energy. QX=0.0 if LRX=0.

L Value of *l*.

LRX Flag indicating whether this energy range contains a competitive width:
LRX=0, no competitive width is given, and $\Gamma = \Gamma_n + \Gamma_\gamma + \Gamma_f$ in the resolved resonance region, while $\langle\Gamma_x\rangle=0$ in the unresolved resonance region; LRX must be 0 for LRF=3 or 4;
LRX=1, a competitive width is given, and is an inelastic process to the first excited state. In the resolved region, it is determined by subtraction, $\Gamma_x = \Gamma - [\Gamma_n + \Gamma_\gamma + \Gamma_f]$

NRS Number of resolved resonances for a given *l*-value. (NRS≤600.)

ER Resonance energy (in the laboratory system).

AJ The absolute value of AJ is the floating-point value of J (the spin, or total angular momentum, of the resonance).
When two channel spins are possible, if the sign of AJ is negative, the lower value for the channel spin is implied; if positive, the higher value is implied. When AJ is zero, only one value of channel spin is possible so there is no ambiguity; the channel spin *s* is equal to the orbital angular momentum *l*.

GT Resonance total width, Γ, evaluated at the resonance energy ER.

GN Neutron width evaluated at the resonance energy ER.

GG Radiation width, Γ_γ, a constant.

GF Fission width, Γ_f, a constant.

GX Competitive width, Γ_x, evaluated at the resonance energy ER.
It is not given explicitly for LRF=1 or 2 but is to be obtained by subtraction,
GX = GT – (GN+ GG + GF), if LRX≠0.

a ***Channel*** radius, in 10^{-12} cm. An uppercase symbol is not defined because it is not an independent library quantity. Depending on the value of NAPS, it is either calculated from the equation given earlier (and in Appendix D), or read from the position usually assigned to the ***scattering radius*** AP.

2.2.1.1. SLBW and MLBW (LRU=1, LRF=1 or 2)

The structure of a ***subsection*** is:

```
[MAT, 2,151/  0.0, 0.0,   0,     0,    NR,  NP/ E_int / AP(E)] TAB1
                                                              (if NRO ≠0)
[MAT, 2,151/  SPI,  AP,   0,     0,   NLS,   0] CONT
```

Use AP=0.0, if AP(E) is supplied and NAPS=0 or 1.

```
[MAT, 2,151/ AWRI,  QX,    L,   LRX, 6*NRS, NRS/
             .ER1,  AJ1,  GT1,   GN1,   GG1,  GF1,
             .ER2,  AJ2,  GT2,   GN2,   GG2,  GF2,
            ---------------------------------
             ERNRS, AJNRS, GTNRS,  GNNRS,  GGNRS, GFNRS] LIST
```

The LIST record is repeated until each of the NLS *l*-values has been specified in order of increasing *l*. The values of ER for each *l*-value are given in increasing order.

2.2.1.2. Reich-Moore (LRU=1, LRF=3)

The following additional quantities are defined:

LAD	Flag indicating whether these parameters can be used to compute angular distributions. LAD=0 do not use LAD=1 can be used if desired. Do ***not*** add to file 4.
NLSC	Number of *l*-values which must be used to converge the calculation with respect to the incident *l*-value in order to obtain accurate elastic angular distributions. See Sections D.1.5.and D.1.6.5. (NLSC≥NLS).
APL	*l*-dependent scattering radius. If zero, use APL=AP.
GFA	First partial fission width, a constant.
GFB	Second partial fission width, a constant.

GFA and GFB are signed quantities, their signs being determined by the relative phase of the width amplitudes in the two fission channels. In this case, the structure of a subsection is similar to LRF=1 and 2, but the total width is eliminated in favor of an additional partial fission width. GFA and GFB can both be zero, in which case, Reich-Moore reduces to an R-function.

The structure for a subsection is:

```
[MAT, 2,151/  0.0, 0.0,   0,   0,    NR,   NP/ E_int / AP(E)] TAB1
                                                              (if NRO≠0)
[MAT, 2,151/  SPI,  AP, LAD,   0,   NLS, NLSC] CONT
[MAT, 2,151/ AWRI, APL,   L,   0, 6*NRS,  NRS/
              ER1,  AJ1,  GN1, GG1,  GFA1, GFB1,
              ER2,  AJ2,  GN2, GG2,  GFA2, GFB2,
             ------------------------------
              ERNRS,AJNRS, GNNRS,GGNRS,GFANRS,GFBNRS] LIST
```

The LIST record is repeated until each of the NLS *l*-values has been specified in order of increasing *l*. The values of ER for each *l*-value are given in increasing order.

2.2.1.3. Adler-Adler (LRU=1,LRF=4)

For the case of (LRU=1, LRF=4) additional quantities are defined:

LI Flag to indicate the kind of parameters given:
- LI=1, total widths only
- LI=2, fission widths only
- LI=3, total and fission widths
- LI=4, radiative capture widths only
- LI=5, total and capture widths
- LI=6, fission and capture widths
- LI=7, total, fission, and capture widths.

NX Number of sets of background constants given. There are six constants per set. Each set refers to a particular cross section type. The background correction for the ***total*** cross section is calculated by using the six constants in the manner following .

σ_T Background $= \left[C/\sqrt{E}\left(AT_1 + AT_2/E + AT_3/E^2 + AT_4/E^3 + BT_1E + BT_2E^2 \right) \right]$

where $C = \pi\lambda\!\!\!^{-2} = \pi/k^2$ and k is defined in Appendix D.

The background terms for the ***fission*** and ***radiative capture*** cross sections are calculated in a similar manner.
- NX=2, background constants are given for the total and capture cross sections.
- NX=3, background constants are given for the total, capture, and fission cross sections.

NJS Number of sets of resolved resonance parameters (each set having its own J-value) for a specified *l*.

NLJ Number of resonances for which parameters are given, for a specified AJ and L.

AT_1, AT_2, AT_3, AT_4, BT_1, BT_2 Background constants for the total cross section.

AF_1, AF_2, AF_3, AF_4, BF_1, BF_2 Background constants for the fission cross section.

AC_1, AC_2, AC_3, AC_4, BC_1, BC_2 Background constants for the radiative capture cross section.

DET_r [4]Resonance energy, (μ), for the total cross section. Here and below, the subscript r denotes the r^{th} resonance.

DEF_r [5]Resonance energy, (μ), for the fission cross section.

DEC_r [5]Resonance energy, (μ), for the radiative capture cross section.

DWT_r [5]Value of Γ/2, (v), for the total cross section.

DWF_r [5]Value of Γ/2, (v), for the fission cross section.

DWC_r [5]Value of Γ/2, (v), for the radiative capture cross section.

GRT_r Symmetrical total cross section parameter, G_r^T.

GIT_r Asymmetrical total cross section parameter, H_r^T.

GRF_r Symmetrical fission parameter, G_r^f.

GIF_r Asymmetrical fission parameter, H_r^f.

GRC_f Symmetrical capture parameter, G_r^γ.

GIC_r Asymmetrical capture parameter, H_r^γ.

---

[4] Note: DET_r=DEF_r=DEC_r and DWT_r=DWF_r=DWC_r. The redundancy is an historical carryover.

The structure of a subsection for LRU=1 and LRF=4 depends on the value of NX (the number of sets of background constants). For the most general case (NX=3) the structure is

```
[MAT, 2,151/ 0.0,  0.0, 0, 0, NR, NP/ E_int / AP(E)] TAB1
```
optional record for energy-dependent scattering radius.
```
[MAT, 2,151/  SPI,   AP,   0,    0,   NLS,    0] CONT
[MAT, 2,151/ AWRI,  0.0,  LI,    0,  6*NX,   NX/
              AT1,  AT2,  AT3,  AT4,   BT1,   BT2,
              AF1, --------------------,   BF2,
              AC1, --------------------,   BC2] LIST
[MAT, 2,151/ 0.0,  0.0,   L,    0,    NJS,    0] CONT(l)
[MAT, 2,151/  AJ,  0.0,   0,    0, 12*NLJ,  NLJ/
             DET1, DWT1, GRT1, GIT1,   DEF1,  DWF1,
             GRF1, GIF1, DEC1, DWC1,   GRC1,  GIC1,
             DET2, DWT2, ----------------------
             --------------------------,  GIC2,
              DET3,-----------------------------
              ---------------------------------
            ------------------------------, GICNLJ] LIST
```

The last LIST record is repeated for each J-value (there will be NJS such LIST records). A new CONT (*l*) record will be given which NJS LIST records will follow. Note that if NX=2 then the quantities AF_1, ---BF_2 will not be given in the first LIST record. Also, if LI≠7 then certain of the parameters for each level may be set to zero, *i.e.*, the fields for parameters not given (depending on LI) will be set to zero.

The format has no provision for giving Adler-Adler parameters for the scattering cross section. The latter is obtained by subtracting the capture and fission cross sections from the total.

Although the format allows separation of the resonance parameters into J-subsets, no use is made of J in the A-A formalism. There is no analog to the resonance-resonance interference term of the MLBW formalism. Such interference is represented implicitly by the asymmetric terms in the fission and capture cross sections.

2.2.1.4. (LRU=1, LRF=5) no longer available
2.2.1.5. (deleted)
2.2.1.6. (LRU=1, LRF=6) no longer available

2.2.1.7 R-Matrix Limited format (LRU=1,LRF=7)

In R-matrix scattering theory, a channel is defined by the two particles inhabiting that channel and by the quantum numbers for the combination. The two particles are hereafter referred to as a particle-pair (PP), and are defined by their properties: neutron (or other particle) plus target nuclide (in ground or excited state), with individual identifiers such as mass, spin, parity, and charge. The additional quantum numbers defining the channel include orbital angular momentum *l*, channel spin *s* and associated parity, and total spin and parity J^{π}.

NOTE: This format is NOT restricted to one neutron (entrance) channel and two exit channels. There may be several entrance channels and a multitude of exit channels. Charged-particle exit channels are not excluded.

The term "spin group" may be used to define the set of resonances with the same channels and quantum numbers. For any given spin group, only total spin and parity are constant; there may be several entrance channels and/or several reaction channels (and, hence, several values of *l* or *s*, etc.) contributing to the spin group.

The "R-Matrix Limited" (RML) format was designed to accommodate the features of R-Matrix theory as implemented in analyses codes being used for current evaluations. In this format, relevant parameters appear only once. Particle-pairs are given first: the masses, spins and parities, and charges for the two particles are specified, as well as the Q-value and the MT value (which defines whether this particle-pair represents elastic scattering, fission, inelastic, capture, etc.). Two particle-pairs will always be present: gamma + compound nucleus, and neutron + target nucleus in ground state. Other particle-pairs are included as needed.

The list of resonance parameters is ordered by J^{π}, which (as stated above) is the only conserved quantity for any spin group. For each spin group, the channels are first specified in the order in which they will occur in the list of resonances. For each channel, the particle-pair number and the values for *l* and *s* are given, along with the channel radii.

2.2.1.7.1 Formats for the basic RML subsection

Additional quantities are defined (or, in some cases, re-defined):

KRM Flag to specify which formulae for the R-matrix are to be used. KRM = 1 for single-level Breit-Wigner, KRM = 2 for multilevel Breit-Wigner, KRM = 3 for Reich Moore, KRM = 4 for full R-matrix. (Others may be added at a later date.)

KRL Flag is zero for non-relativistic kinematics, 1 for relativistic.

NJS Number of values of J^{π} to be included.

NPP Total number of particle-pairs.

IA Spin (and parity, if non-zero) of one particle in the pair (the neutron or projectile, if this is an incident channel).

IB Spin of the other particle in the pair (target nuclide, if this is an incident channel). IB is set to zero and ignored if the first particle is a photon.

PA Parity for first particle in the pair, used only in the case where IA is zero and the parity is negative. (Value = +1.0 if positive, -1.0 if negative.)

PB Parity for second particle, used if IB= 0 and parity is negative.

MA Mass of first particle in the pair (in units of neutron mass).

MB Mass of second particle (in units of neutron mass).

ZA Charge of first particle.

ZB Charge of second particle.

QI Q-value for this particle-pair. (See Sect. 3.3.2 for details)

PNT Flag is 1 if penetrability is to be calculated, -1 if not (default depends on number; MT=108 implies PNT = -1, others are generally PNT = +1)

SHF Flag is 1 if shift factor is to be calculated, -1 if not (default = not)

MT Reaction type associated with this particle-pair; see Appendix B.

AJ Floating point value of *J* (spin); sign indicates parity.

PJ Parity (used only if AJ = 0.0).
NCH Number of channels for the given J^{π}.
IPP Particle-pair number for this channel (written as floating-point number).
L Orbital angular momentum (floating-point value).
SCH Channel spin (floating-point value).
BND Boundary condition for this channel (needed when SHF=+1)
APE Effective channel radius (scattering radius), used for calculation of phase shift only. Units are 10^{-12} cm.
APT True channel radius (scattering radius), used for calculation of penetrability and shift factors. Units are 10^{-12} cm.
KBK Non-zero if background R-matrix exists; sees Subsect. 2.2.1.7.2. (Often set to 0.)
KPS Non-zero if non-hard-sphere phase shift are to be specified. (Often set to 0.)
NRS Number of resonances for the given J^{π}.
NX Number of lines required for all resonances for the given J^{π}, assuming each resonance starts on a new line; equal to (NCH/6+1)*NRS. If there are no resonances for a spin group, then NX = 1.
ER Resonance energy in eV.
IFG Flag is 0 if GAM is channel width in eV, 1 if reduced-width amplitude in $eV^{1/2}$.
GAM Channel width in eV or reduced-width amplitude in $eV^{1/2}$.

NOTE: For IFG = 0, the input quantity GAM is the width at the energy of the resonance; reduced width amplitudes are calculated from Eq. (7) of D.1.7, with E set to E_λ. (For negative-energy dummy resonances, the convention is that the input quantity is the width evaluated at the absolute value of the resonance energy.) In all cases, if the value GAM given in File 2 for the partial width is negative, the standard convention is assumed: the negative sign is to be associated with the reduced width amplitude $\gamma_{\lambda c}$ rather than with $\Gamma_{\lambda c}$ (since $\Gamma_{\lambda c}$ is always a positive quantity). More specifically, $\Gamma_{\lambda c} = |\mathrm{GAM}|$ and $\gamma_{\lambda c} = \mathrm{sign}(\mathrm{GAM}) \times \sqrt{\mathrm{GAM}/2\,\mathrm{P}}$, with P evaluated at the energy of the resonance.

If IFG =1, the input quantity is the reduced width amplitude $\gamma_{\lambda c}$.

Formats are as follows:

```
[MAT,2,151/   0.0,     0.0,     IFG,     KRM,      NJS,          KRL        ]
                                                                 CONT
```

(The following record provides all particle-pair descriptions. For KRM=1,2, or 3, the first particle-pare is the gamma plus compound nucleus pair.)

```
[MAT,2,151/   0.0,    0.0,    NPP,    0,      12*NPP,    2*NPP/
              MA1,    MB1,    ZA1,    ZB1,    IA1,       IB1,
              Q1,     PNT1,   SHF1,   MT1,    PA1,       PB1,
              MA2,    MB2,    ZA2,    ZB2,    IA2,       IB1,
              Q2,     PNT2,   SHF2,   MT2,    PA2,       PB1,
              ----------------------------------------------
              MANPP,  MBNPP,  ZANPP,  ZBNPP,  IANPP,     IBNPP,
              QNPP,   PNTNPP, SHFNPP, MTNPP,  PANPP,     PBNPP ] LIST
```

The following record provides the channel descriptions for one spin group.)

```
[Mat,2,151/   AJ,     PJ,     KBK,    KPS,    6*NCH,     NCH/
              IPP1,   L1,     SCH1,   BND1,   APE1,      APT1,
              IPP2,   L2,     SCH2,   BND2,   APE2,      APT2,
              ----------------------------------------------
              IPPNCH, LNCH,   SCHNCH, BNDNCH, APENCH,    APTNCH] LIST
```

(The following record gives the values for resonance energy and widths for each resonance in this spin group.)

```
[Mat,2,151/   0.0,    0.0,     0,       NRS,       6*NX,     NX/
              ER1,    GAM1,1,  GAM2,1   GAM3,1,    GAM4,1,   GAM5,1,
              GAM6,1, GAMNCH,1,
              ER2,    GAM1,2,  GAM2,2,  GAM3,2,    GAM4,2,   GAM5,2,
              GAM6,2, …,       GAMNCH,2,
              ----------------------------------------------
              ERNRS,  GAM1,NRS,GAM2,NRS,  GAM3,NRS,  GAM4,NRS, GAM5,NRS,
              GAM6,NRS,…,GAMNCH,NRS                                ] LIST
```

(If the number of resonances is zero for a spin group, then NRS = 0 but NX =1 in this record.)

Other records may be included here, as described below in Sect. 2.2.1.7.2. If KBK is greater than zero, a "background R-matrix" is given. If KPS is greater than zero, tabulated values exist for phase shifts. If KBK = 0 and KPS = 0, no additional records are needed.

The above records, beginning with "channel descriptions," are repeated until each of the NJS J^{π} spin groups has been fully specified.

2.2.1.7.2 Formats for optional extensions to the RML

The formats described in the previous section are sufficient for most evaluations currently (2003) available (using KRM = 3, KBK = 0, and KPS = 0). For the sake of generality, and to accommodate expected future developments in R-matrix analysis codes, additional capabilities are included in the RML format.

2.2.1.7.2.1 Different R-Matrix formulations (KRM = 1,2,4)

Equations given in Appendix D.1.7 are relevant to the Reich-Moore approximation to R-Matrix theory. The format, however, can also be used for single-level Breit-Wigner (KRM = 1), multilevel Breit-Wigner (KRM = 2), R-Matrix without approximations (KRM = 4). Equations for KRM = 1 or 2 will be written up if/when the need arises. Equations for KRM = 4 are identical to those given in Appendix D.1.7 with the elimination of the imaginary term in the denominator of Eq. (6), and the inclusion of each gamma-channel on a equal basis with all other channels.

2.2.1.7.2.2 Background R-matrix (KBK > 0):

As described in Appendix D (D.1.7.7), a background R-Matrix can be defined in a variety of different methods.

For KBK = 0, Option 0 is used everywhere (that is, for all channels for this spin group) for the background R-Matrix. No additional formats are required and no additional records need to be written; the dummy resonances are included along with the physical resonances in the list record described above.

For KBK > 0, one LIST record (and two TAB1 records, for tabulated values) is included for each channel of the current spin group, a total of NCH records. The particular option to be used for the channel is identified by parameter **LBK**. The formats for the four options are as follows:

Option 0. Dummy resonances (**LBK** = 0)

No additional information is conveyed in this record, other than LBK = 0. No terms are added to the R-matrix for this channel.

```
[Mat,2,151/ 0.0,   0.0,    0,      0,      LBK,     1/
            0.0,   0.0,    0.0,    0.0,    0.0,     0.0 ] LIST
```

Option 1. Tabulated complex function of energy (**LBK** = 1)

Notation:

RBR Value of real part of tabulated function
RBI Value of imaginary part of tabulated function

```
[Mat,2,151/ 0.0,   0.0,   0,     0,     LBK,    1/
            0.0,   0.0,   0.0,   0.0,   0.0,    0.0] LIST
[Mat,2,151/ 0.0,   0.0,   0,     0,     NR,     NP/ Eint / RBR(E) / TAB1
[Mat,2,151/ 0.0,   0.0,   0,     0,     NR,     NP/ Eint / RBR(E) / TAB1
```

(Recall that NR and NP are parameters, which define the interpolation scheme for TAB1 records, as defined in Section 0.7.7. Energy values given by E_{int} are in units of eV.)

Option 2. SAMMY's logarithmic parameterization (**LBK** = 2)

Notion (See Eq. (47) of Sect. D.1.7.7 for meanings of these quantities):

R0	$\overline{R}_{com,c}$	**S0**	$\overline{s}_{com,c}$
R1	$\overline{R}_{lin,c}$	**S1**	$\overline{s}_{lin,c}$
R2	$\overline{R}_{q,c}$		
EU	E_c^{up}	**ED**	E_c^{down}

```
[Mat,2,151/   ED,     EU,     0,      0,        LBK,     1/
              R0,     R1,     R2,     S0,       S1,      0.0] LIST
```

Option 3. Fröhner's parameterization (**LBK** = 3)

Notion (See Eqs. (48 and 49) Sect. D.1.7.7 for meanings of these quantities):

R0	$\overline{R}_c$	**S0**	$\overline{s}$
GA	Γ_γ		
EU	E_c^{up}	**ED**	E_c^{down}

```
[Mat,2,151/   ED,     EU,     0,      0,        LBK,     1/
              R0,     SO      GA,     0.0,      0.0,     0.0] LIST
```

2.2.1.7.2.3 Tabulated phase shifts (KPS = 1)

When phase shifts are calculated externally (from optical model potentials, for example), rather than generated from the usual hard-sphere phase shift formulae, then the phase shifts must be presented in tabular form.

If parameter KPS is equal to 0, all phase shifts are calculated from the hard-sphere phase shift formulae (see Table D.1.7.1 for non-Coulomb, Sect. D.1.7.2 for Coulomb hard-sphere phase shifts).

For KPS >0, one LIST record (and two TAB1 records, for tabulated values) is included for each channel of the current spin group, a total of NCH records. The particular option to be used for the channel is identified by parameter **LPS**. The formats for the two options are as follows:

*Option 0. Hard-sphere phase shifts (***LPS** = 0)

No additional information is conveyed in this record, other than LPS = 0.

```
[Mat,2,151/   0.0,     0.0,     0,       0,          LPS,      1/
              0.0,     0.0,     0.0,     0.0,        0.0,      0.0] LIST
```

*Option 1. Phase shift is a tabulated complex function of energy (***LPS** = 1)

Notation:

PSR Value of real part of tabulated phase shift

PSI Value of imaginary part of tabulated phase shift

```
[Mat,2,151/ 0.0,   0.0,   0,     0,     LPS,   1/
            0.0,   0.0,   0.0,   0.0,   0.0,   0.0] LIST
[Mat,2,151/ 0.0,   0.0,   0,     0,     NR,    NP/ Eint / PSR (E) / TAB1
            0.0,   0.0,   0,     0,     NR,    NP/ Eint / PSR (E) / TAB1
```

(Recall that NR and NP are parameters, which define the interpolation scheme for TAB1 records, as defined in Sect. 0.7.7. Energy values given by E_{int} are in units of eV.)

2.3. Unresolved Resonance Parameters (LRU=2)

2.3.1. Formats

Only the SLBW formalism for unresolved resonance parameters is allowed (see Appendix D for pertinent formulae). However, several options are available for specifying the energy-dependence of the parameters, designated by the flag LRF. Since unresolved resonance parameters are averages of resolved resonance parameters over energy, they are constant with respect to energy throughout the energy-averaging interval. However, they are allowed to vary from interval to interval, and it is ***this*** energy-dependence, which is referred to above and in the following paragraphs.

The parameters depend on both *l* (neutron orbital angular momentum) and J (total angular momentum). Each width is distributed according to a chi-squared distribution with a certain number of degrees of freedom. This number may be different for neutron and fission widths and for different (*l*,J) channels.

The following quantities are defined for use in specifying unresolved resonance parameters (LRU=2):

SPI Spin of the target nucleus, I.

AP Scattering radius in units of 10^{-12} cm. No channel quantum number dependence is permitted by the format.

LSSF Flag governing the interpretation of the File 3 cross sections.

LSSF=0, File 3 contains partial "background" cross sections, to be added to the average unresolved cross sections calculated from the parameters in File 2.

LSSF=1, File 3 contains the entire dilute cross section for the unresolved resonance region. File 2 is to be used solely for the calculation of the self-shielding factors, as discussed in Section 2.4.21.

NE	Number of energy points at which energy-dependent widths are tabulated. (NE≤250).
NLS	Number of *l*-values (NLS≤3).
ES_i	Energy of the i^{th} point used to tabulate energy-dependent widths.
L	Value of *l*.
AWRI	Ratio of the mass of a particular isotope to that of the neutron.
NJS	Number of J-states for a particular *l*-state. (NJS≤6).
AJ	Floating-point value of J (the spin, or total angular momentum of the set of parameters).
D	Average level spacing for resonances with spin J. (D may be energy dependent if LRF=2).
AMUX	Number of degrees of freedom used in the competitive width distribution. (Assuming it is inelastic, 1.0≤AMUX≤2.0, determined by whether the spin of the first excited state is zero or not.)[5]
AMUN	Number of degrees of freedom in the neutron width distribution. (1.0≤AMUN≤2.0)
AMUG	Number of degrees of freedom in the radiation width distribution. (At present AMUG = 0.0. This implies a constant value of Γ_γ.)
AMUF	Number of degrees of freedom in the fission width distribution. (1.0≤AMUF≤4.0)
MUF	Integer value of the number of degrees of freedom for fission widths. (1≤MUF≤4)
INT	Interpolation scheme to be used for interpolating between the ***cross sections*** obtained from average resonance parameters. ***Parameter interpolation*** is discussed in the Procedures Section 2.4.2.
GN0	Average reduced neutron width. It may be energy-dependent if LRF=2.
GG	Average radiation width. It may be energy-dependent if LRF=2.
GF	Average fission width. It may be energy-dependent if LRF=1 or 2.
GX	Average competitive reaction width, given only when LRF=2, in which case it may be energy-dependent.

The structure of a ***subsection***[6] depends on whether LRF=1 or LRF=2. If LRF=1, only the fission width is given as a function of energy. If LRF=1 and the fission width is not given (indicated by LFW=0), then the simplest form of a subsection results. If LRF=2, energy-dependent values may be given for the level density, competitive width, reduced neutron width, radiation width, and fission width. Three sample formats are shown below (all LRU=2).

A. LFW=0 (fission widths not given),
LRF=1 (all parameters are energy-independent).
The structure of a subsection is:

```
[MAT, 2,151/ SPI,     AP,  LSSF,     0,    NLS,    0] CONT
[MAT, 2,151/ AWRI,  0.0,      L,     0, 6*NJS, NJS/
                 D1,    AJ1, AMUN1,  GN01,    GG1, 0.0,
```

[5] See Appendix D. Section D.2.2.6.

[6] The structure of a **section** was defined previously, and covers both resolved resonance and unresolved resonance subsections.

```
                    D2,   AJ2, AMUN2,  GN02,   GG2, 0.0,
                  ------------------------------------
                    DNJS, AJNJS, AMUNNJS, GN0NJS, GGNJS, 0.0] LIST
```

The LIST record is repeated until data for all *l*-values have been specified. In this example, AMUG is assumed to be zero, and there is no competitive width.

B. LFW=1 (fission widths given),
LRF=1 (only fission widths are energy-dependent; the rest are energy-independent).
The structure of a subsection is:

```
[MAT, 2,151/  SPI,  AP, LSSF,   0,   NE, NLS]  CONT
              ES1, ES2,   ES3, ------------
             --------------------------   ESNE] LIST
[MAT, 2,151/ AWRI, 0.0,    L,   0,  NJS,   0] CONT
[MAT, 2,151/  0.0, 0.0,    L, MUF, NE+6,   0/
                D,  AJ, AMUN, GN0,  GG, 0.0,
               GF1,  GF2,  GF3,--------------
             ---------------------------- GFNE] LIST
```

The last LIST record is repeated for each J-value (there will be NJS such LIST records). A new CONT(*l*) record will then be given which will be followed by its NJS LIST records until data for all *l*-values have been specified (there will be NLS sets of data).

In the above section, no provision was made for INT, and interpolation is assumed to be lin-lin. AMUG is assumed to be zero, AMUF equals MUF, and there is no competitive width.

C. LFW=0 or 1 (does not depend on LFW).
LRF=2 (all energy-dependent parameters).
The structure of a subsection is:

```
[MAT, 2,151/  SPI,  AP, LSSF,     0,      NLS,     0] CONT
[MAT, 2,151/ AWRI, 0.0,    L,     0,      NJS,     0] CONT
[MAT, 2,151/   AJ, 0.0,  INT,     0,(6*NE)+6,    NE/
              0.0, 0.0, AMUX, AMUN,     AMUG, AMUF,
              ES1,   D1,  GX1, GN01,      GG1,  GF1,
              ES2,   D2,  GX2, GN02,      GG2,  GF2,
              ----------------------------
             ESNE,  DNE,  GXNE, GN0NE,     GGNE,  GFNE] LIST
```

The LIST record is repeated until all the NJS J-values have been specified for a given *l*-value. A new CONT(*l*) record is then given, and all data for each J-value for that *l*-value are given. The structure is repeated until all *l*-values have been specified. This example permits the specification of all four degrees of freedom.

2.4. Procedures for the Resolved and Unresolved Resonance Regions

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2.4.23 Completeness and Convergence of Channel Sums
2.4.24 Channel Spin and Other Considerations

2.4.1. Abbreviations

UR(R)	unresolved resonance (region)
RR(R)	resolved resonance (region)
RRP	resolved resonance parameter(s)
URP	unresolved resonance parameter(s)
SLBW	single-level Breit-Wigner
MLBW	multi-level Breit-Wigner
MLAG	multi-level Adler-Gauss
UCS	unresolved cross section(s)

2.4.2. Interpolation in the Unresolved Resonance Region (URR)

For energy-dependent formats (LRF=2, or LRF=1 with LFW=1), the recommended procedure is to interpolate on the ***cross sections*** derived from the unresolved resonance parameters (URP). This is a change from the ENDF/B-III and IV procedure, which was to interpolate on the parameters. The energy grid should be fine enough so that the cross sections at intermediate energy values can be computed with sufficient accuracy using this procedure. Normally, three to ten points per decade will be required to obtain reasonable accuracy. Some evaluations prepared for earlier versions of ENDF/B do not meet these standards. In such cases, if two adjacent grid points differ by more than a factor of three, the processing code should add additional intermediate energy points at a spacing of approximately ten-per-decade and compute the cross sections at the intermediate points using parameter interpolation. Additional cross sections can then be obtained by cross section interpolation in the normal way.

For many isotopes, there is not sufficient information for a full energy-dependent evaluation. In these cases, the evaluator may provide a single set of unresolved resonance parameters based on systematics or extrapolation from the resolved range (see LRF=1, LFW=0). Such a set implies a definite energy-dependence of the unresolved cross sections due to the slowly-varying wave number, penetrability, and phase shift factors in the SLBW formulas. It is not correct to calculate cross sections at the ends of the URR, and then to compute intermediate cross sections by cross section interpolation. Instead, the processing code should generate a set of intermediate energies using a spacing of approximately ten-per-decade and then compute the cross sections on this grid using the single set of parameters given in the file. Additional intermediate values are then obtained by linear cross section interpolation as in the energy-dependent case.

It is recommended that evaluators provide the URP's on a mesh dense enough that the difference in results of interpolating on either the parameters or the cross sections be small. A 1% maximum difference would be ideal, but 5% is probably quite acceptable.

Finally, even if the evaluator provides a dense mesh, the user may end up with different numbers than the evaluator "intended". This is particularly true when genuine structure exists in the cross section and the user chooses different multigroup breakpoints than those in the evaluation. There is no solution to this problem, but the dense mesh procedure minimizes the importance of the discrepancy.

In order to permit the user to determine what "error" he is incurring, it is recommended that evaluators state in the documentation what dilute, unbroadened average cross sections they intended to represent by the parameters in File 2. Note that the self-shielding factor option specified by the flag LSSF (Sections 2.3.1 and 2.4.21) greatly reduces the impact of this interpolation ambiguity.

2.4.3. Unresolved Resonances in the Resolved Resonance Range

As discussed in section 2.4.4, the boundary between the resolved and unresolved resonance regions should be chosen to make the statistical assumptions used in the URR valid. This creates problems in evaluating the resonance parameters for the RRR.

Problem l: At the upper end of the resolved range, the smaller resonances will begin to be missed. An equivalent contribution could be added to the background in File 3. This contribution will not be self-shielded by the processing codes, so it cannot be allowed to become "significant". A better procedure is to supply fictitious resolved parameters, based on the statistics of the measured ones, checking that the average cross section agrees with whatever poor-resolution data are available.

If both procedures are employed, care should be taken not to distort the statistics of the underlying parameter distributions.

Problem 2: Because d-wave resonances are narrower than p-waves, which are narrower than s-waves, everything else being equal, the point at which p-waves will be instrumentally unresolved can be expected to be lower in energy than for s-waves, and lower still for d-waves. Thus the unresolved region for p-waves will usually overlap the resolved region for s-waves, and similarly for d-waves. Current procedure does not permit representing this effect explicitly - one cutoff-point must serve for all *l*-values.

The remedies are the same as above, either putting known or estimated resonances into the background in the URR, or putting fictitious estimated resonances into the RRR. The latter is preferred because narrow resonances tend to self-shield more than broad ones, hence the error incurred by treating them as unshielded File 3 background contributions is potentially significant.

2.4.4. Energy Range Boundary Problems

There may be as many as four different kinds of boundaries under current procedures which permit multiple RRR's:

1. between a low-energy File 3 representation (range 1) and EL for the RRR (range 2),
2. between successive RR ranges,
3. between the highest RRR and the URR,
4. between EH for the URR and the high-energy File 3 representation.

Discontinuities can be expected at each boundary. At 1, a discontinuity will occur if range 1 and range 2 are not consistently Doppler-broadened. In general, only an identical kernel-broadening treatment will produce continuity, *i.e.*, only if the range-1 cross sections are broadened from the temperature at which they were measured, and range-2 is broadened from absolute zero. A kernel treatment of range 1, or no broadening at all, will be discontinuous with a Ψ-χ treatment of range 2. This effect is not expected to be serious at normal reactor temperatures and presumably, the CTR and weapons communities are cognizant of the Doppler problem. In view of these problems, a double energy point will not usually produce exact continuity in the complete cross section, (file 2 + file 3), unless evaluator and user employ identical methods throughout.

Discontinuities will occur between successive RRR's, unless the evaluator takes pains to adjust the "outside" resonances for each RRR to produce continuity at absolute zero. If the unbroadened cross sections in two successive RRR's are broadened separately, the discontinuity will be preserved, and possibly enhanced. These discontinuities are not believed to be technologically significant.

A discontinuity at #3 is unavoidable, because the basic representation has changed. However if the RRR cross sections are group-averaged or otherwise smoothed, the discontinuity[7] should be reasonably small. A discontinuity greater than 10 or 15% obtained with a suitable averaging interval indicates that the evaluator might want to reconsider his parameterization of the poor-resolution data. Some materials have large genuine fluctuations in the URR, and for these the 10-15% figure is not applicable. A double energy point will normally occur at this boundary, but will not eliminate the discontinuity.

[7] This refers to the discontinuity between the ***average*** cross section in the RRR, and the dilute (unshielded) pointwise cross section in the URR, which has been generated from the URR parameters. If the self-shielding factor option has been chosen (LSSF=1, Section 2.3.1), File 3 will contain the entire dilute cross section and no File 2 unresolved region calculation will be needed to ascertain the discontinuity.

Discontinuity at #4 should be small, since both the URR and the high-energy range represent rather smooth cross sections, and the opportunity for error ought to be small. Anything over 5% or so should be viewed with suspicion.

The upper and lower energy limits of any energy range indicate the energy range of validity of the given parameters for calculating cross sections. Outside this energy range the cross sections must be obtained from the parameters given in another energy range and/or from data in file 3.

The lower energy limit of the URR should be chosen to make the statistical assumptions used in this range valid. The basic requirement is that there be "many" resonances in an energy-averaging interval, and that the energy-averaging interval be narrow with respect to slowly-varying functions of E such as wave number and penetrability. As an example, assume that the energy-averaging interval can extend 10% above and below the energy point, that the average resonance spacing is 1 eV, and that "many" is 100. Then the lowest reasonable energy for the URR would be about 500 eV, as given by 0.2 E=100×1. Some implications of this choice for the RRR-URR boundary were discussed in Section 2.4.3.

It is sometimes necessary to give parameters whose energies lie ***outside*** a specified energy range in order to compute the cross section for neutron energies that are ***within*** the energy range. For example, the inclusion of bound levels may be required to match the cross sections at low energies, and resonances will often be needed above EH to compensate the opposite, positive, bias at the high energy end.

For materials that contain more than one isotope, it is recommended that the lower energy limit of the resolved resonance region be the same for all isotopes. If resolved and/or unresolved resonance parameters are given for only ***some*** of the naturally occurring isotopes, then AP should be given for the others.

If more than one energy range is used, the ranges must be contiguous and not overlap.

Overlapping of the resolved and unresolved ranges is not allowed for any one isotope, but it can occur in an evaluation for an element or other mixture of different isotopes. In fact, it is difficult to avoid since the average resonance spacing varies widely between even-even and even-odd isotopes. Such evaluations are difficult to correctly self-shield. A kernel broadening code must first subtract the infinitely-dilute unresolved cross section, broaden the pointwise remainder, then add back the unresolved component. A multigroup averaging code that uses pointwise cross sections must first subtract the infinitely-dilute unresolved cross section to find the pointwise remainder, and then add back a self-shielded unresolved cross section computed for a background cross section which includes a contribution from the pointwise remainder.

2.4.5. Numerical Integration Procedures in the URR

The evaluation of effective cross sections in the URR can involve Doppler effects, flux-depression, and resonance-overlap as well as the statistical distributions of the underlying resonance parameters for a mixture of materials.

The previous ENDF/B recommendation for doing the complicated multi-dimensional integrations was the Greebler-Hutchins scheme, Reference 1, basically a trapezoidal integration. For essentially the same computing effort, a more sophisticated weighted-ordinate method can be used and it has been shown that the scheme in MC^2-II, Reference 2, produces results differing by up to several percent from G-H. The MC^2-II subroutine[8], is the recommended procedure.

[8] This subroutine was provided by H. Henryson, II (ANL).

The M. Beer [Ref.3], analytical method has also been suggested, and is quite elegant, but unfortunately will not treat the general heterogeneous case.

2.4.6. Doppler-Broadening of File 3 Background Cross Sections

1. In principle, the contribution to each cross section from File 3 should be Doppler-broadened, but in practice, many codes ignore it. It is therefore recommended that the evaluator keep file 3 contributions in the RRR and URR small enough and/or smooth enough so that omission of Doppler-broadening does not "significantly" alter combined File 2 plus File 3 results up to 3000 K. Unfortunately, the diversity of applications of the data in ENDF/B makes the word "significantly" impossible to define.

2. A possible source of structured File 3 data is the representation of multilevel or MLBW cross sections in the SLBW format, the difference being put into File 3. This difference is a series of residual interference blips and dips, which may affect the between-resonance valleys and possibly the transmission in thick regions or absorption rates in lumped poisons, shields, blankets, *etc*. Users of the SLBW formalism should consider estimating these effects for significant regions. A possible remedy is available in the Multilevel Adler-Gauss form of MLBW. (See Section 2.4.14). If the resonance-resonance interference term in MLBW is expanded in partial fractions, it becomes a single sum of symmetric and asymmetric SLBW-type terms. Two coefficients occur which require a single sum over all resonances for each resonance, but these sums are weakly energy dependent and lend themselves to approximations that could greatly facilitate the use of ψ- and χ-functions with MLBW.

3. An "in-principle" correct method for constructing resonance cross sections is:

   a.) Use a Solbrig kernel [Ref.12] to broaden File 2 to the temperature of File 3, since the latter may be based on room-temperature or other non-zero ^{0}K data.

   b.) Add File 2 and File 3.

   c.) Sollbrig-broaden the result to operating temperature.

   Using a Gaussian kernel instead of Sollbrig incurs a small error at low energies, unless it is misused, in which case the error can be large. Using Ψ- and χ-functions introduces further errors. In fact, the Sollbrig kernel already approximates the true motion of the target molecules by a free-gas law, but anything more accurate is quite difficult to handle.

4. Some heavy element evaluations use a File 3 representation below the resolved resonance region. Often these cross sections are room-temperature values, so that if they are later broadened assuming they are zero-degrees Kelvin, they get broadened twice.

   A simple way to reduce the impact of this procedure without altering the representation of the data is to calculate the cross sections from the resonance parameters, ***broadened to room temperature***, and carry the calculation down through the low-energy region. Subtract these broadened values from the file 3 values and leave only the ***difference*** in file 3. Then extend the lower boundary of the resonance region to the bottom of the file. Now the "double-broadening" problem affects only the (small) residual file 3 and not the entire cross section.

   Note that subtracting off a ***zero degree*** resonance contribution would accomplish nothing.

2.4.7. Assignment of Unknown J-values

In all multilevel resonance formalisms except Adler-Adler, the J-value determines which resonances interfere with each other. Usually, J is known only for a few resonances, and measurers report $2g\Gamma_n$ for the others. If this number is assumed to be Γ_n, one incurs an error of uncertain magnitude, depending on how different

$$g = \frac{2J+1}{2(2I+1)}$$

is from l/2, how large Γ_n is relative to the other partial widths, and how important resonance-resonance interference is.

It is recommended that evaluators assign J-values to each resonance, in proportion to the level density factor 2J+l. To reduce the amount of interference, the J-values of strong neighboring resonances, which would produce the largest interference effects, can be chosen from different families.

In the past, some evaluations have put J=I, the target nucleus spin, for resonances with unknown J-values. This corresponds to putting g=1/2, rather than its true value. Mixing of the J=I resonances with the physically correct I±1/2 families can result in negative scattering cross sections, or distortions of the potential scattering term, depending on what formalism is used and how it is evaluated. For this reason, such J=I resonances must not be used.

In the amplitude-squared form of the MLBW scattering cross section,

$$\sigma_{nn} = \sum_{lsJ} g_J \left| A^{lsJ}_{pot} + A^{lsJ}_{resonance} \right|^2 \qquad (2.1)$$

the use of J=I resonances will destroy the equivalence between this form and the "squared" form of MLBW in Appendix D since the sum on *l*sJ does not go over physically-correct values.

An exception to the prohibition against J=I is the case where no J-values are known, since if ***all*** resonances are assigned J=I, the MLBW scattering cross section will be non-negative.

2.4.8. Equivalent Single-Level Representations

The single-level Breit-Wigner formalism is incorporated into the basic structure of many engineering codes used for reactor design. Its use is so widespread, that despite any shortcomings in the calculational procedures, such codes must be supplied with SLBW parameters. For ENDF/B evaluations employing other representations, one requires an "equivalent" set of SLBW parameters. This is not to minimize the importance of using improved methods, but such improved methods ***do not eliminate*** the need for SLBW parameters in reactor design. For example, the Adler formalism provides a multilevel, multichannel fission cross section in pseudo-SLBW format, permitting ψ,χ-broadening. This is very useful, but not to a code that does not recognize asymmetric fission or capture.

The following equivalences are recommended:

1. MLBW. Use the parameters "as is".
2. Reich-Moore. Use the parameters "as is", except that the absolute values of the partial fission widths are added together to form Γ_f. (Alternatively, convert Reich-Moore to Adler-Adler, and use the equivalence for that formalism).
3. Adler-Adler. Reasonable success in converting A-A parameters for ^{241}Pu and ^{233}U was obtained using a method described in Reference 4.

2.4.9. Use of the Reich-Moore Formalism

If the evaluation of fissionable, low energy, s-wave-only, materials is carried out with a Reich-Moore formalism, then the parameters may be transformed to the Adler-Adler representation. R-M has some advantages in evaluating data, mainly that it uses resonance spins, is more closely tied to familiar resonance parameters, and is more "physical", but the Adler format is more convenient for the user since it permits ψ- and χ-functions for Doppler broadening.

The computer code POLLA [Ref.5], as well as some others, will convert a set of Reich-Moore multilevel s-wave resonance parameters to Adler format. If the conversion causes differences between the Adler and R-M cross sections which exceed 0.l%, these should be put into File 3, since it is not the intent of the procedure to in any way alter the original cross sections. Such differences can possibly be reduced by feeding the POLLA output parameters to a least-squares search code based on the Adler formalism, and "fitting" the original R-M values.

According to the discussion in BNL-50296[9], the Reich-Moore code RAMPl, incorporated in RESEND, sets the shift factor equal to zero. This is correct for s-waves, and should pose no problem for p- and d-waves, provided that the evaluator has included this shift factor when the calculation was performed.

2.4.10. Competitive Width in the Resonance Region

2.4.10.1. Resolved Region

Procedures for the Resolved Resonance Region are contained in Section D.3.l of Appendix D.

2.4.10.2. Unresolved Region

Procedures for the Unresolved Resonance Region are contained in Section D.3.2 of Appendix D. Users are directed to the discussion of the total cross section in Appendix D, Section D.3.3, since, as pointed out by H. Henryson, II, in connection with MC^2 procedures, a possibility for erroneous calculations exists.

2.4.11. Negative Cross Sections in the Resolved Resonance Region

2.4.11.1. In the SLBW Formalism

Capture and fission use the positive symmetric Breit-Wigner shape and are never negative. Scattering involves an asymmetric term which goes negative for $E < ER$ and can cause negative cross sections. A single resonance, or a series of well-separated resonances, will usually not produce negative cross sections, but when two or more resonances "cooperate", their negative tails can combine to produce negative values. In nature, the negative tails are compensated by either the positive tails of lower-lying resonances or multilevel interference effects. However, in evaluated data files the resonances are usually given only down to "E=0", a quite arbitrary point from the standpoint of the compound nucleus, so that "negative-energy" resonances are needed to compensate the negativity bias.

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[9] M.R. Bhat, **BNL-50296** (ENDF l48) *ENDF/B Processing Codes for the Resonance Region*, June, l97l,

Although the negative ***scattering*** cross sections themselves can usually be classed as an inconvenience, their effect in distorting the ***total*** cross section, which governs neutron penetration, can be more serious. Perhaps more important is the fact that even when the cross section remains positive, it is still often too low due to the same effect and this bias again affects the total cross section and calculated absorption rates. To compensate this bias, the evaluator should put in either a series of negative energy resonances with reasonable size and spacing ("picket fence", or reflect the positive-energy ones around E=0) or a few large fictitious ones ("barber poles"), or a compensating background in File 3 (*e.g.*, see Reference 6).

To compensate interior-region negativity requires a multilevel treatment of which MLBW is the simplest. Although there is no ***guarantee*** that MLBW cross sections will be more accurate than SLBW, they ***are*** guaranteed to be non-negative (but see next section) and are generally to be preferred over SLBW.

A similar bias occurs at the upper end of the resolved resonance range, where it is less noticeable because it is a positive bias, and most calculations are not as sensitive to this region as they are to the low-energy end. The remedy is the same - extra resonances above the RRR, or compensation in file 3. The latter remedy requires a negative file 3 contribution, which is physically acceptable, but produces undesirable side-effects in some processing codes, hence the extra-resonance remedy is preferred. It is probably safe to say that there is rarely a compelling reason to use the SLBW formula for the calculation of pointwise scattering cross sections. If one is doing a calculation that is sophisticated enough to warrant the use of pointwise cross sections, then a multilevel formalism is certainly justifiable. If one is merely deriving multigroup cross sections, then the other approximations involved justify the use of any reasonable "fix" for the negative scattering, such as simply setting $\sigma_S = 0$ when it goes negative. Such a procedure should usually be accompanied by a corresponding increase in the ***total*** cross section.

2.4.11.2. In the MLBW Formalism

Capture and ***fission*** use the SLBW formulas and are positive. Scattering uses a formula, which can be written as an absolute square and as such is non-negative. The use of J=I resonances (Section 2.4.7) can destroy the correspondence between the absolute-square form and the expanded form given in Appendix D and result in negative scattering cross sections. Despite its non-negativity, MLBW still produces biased cross sections at both ends of the RRR unless compensating extra resonances or File 3 contributions are included above and below. The evaluator should generally correct for this effect.

2.4.11.3. In the R-matrix, Reich-Moore, and R-function Formalisms

These are again based on an absolute square and cannot be negative. However, they can be biased and extra resonances, background R-values, or File 3 contributions should be provided. If conversion of Reich-Moore to Adler format produces negative cross sections, dummy parameters should be provided to eliminate them.

2.4.11.4. In the Adler Formalism

Although the formulae are derived from an absolute square and are in principle non-negative, in practice the parameters are chosen to fit measured data, so that the physical and mathematical constraints among the parameters, which prevent negative cross sections, are lost, and any of the cross sections can be negative. If the Adler formalism is used for evaluations, negativity should be checked for. The end-effect bias exists in this formalism also and should be checked for in the scattering and total cross sections by comparing with experiment.

2.4.12. Negative Cross Sections in the Unresolved Resonance Region

R. Prael, while at ANL, reported a difficulty with SLBW resonance ladders created by VIM from the unresolved resonance parameters in Mo (MAT l287), namely that the negative File 3 ***capture*** background sometimes caused negative capture cross sections in the resonance valleys. The evaluator intended the background to compensate for an excess of capture in the average unresolved capture cross section, but did not anticipate the problem that would arise when the parameters were used in a different context. One remedy is to drop out the negative File 3 background and adjust $<\Gamma_\gamma>$ on whatever energy mesh is needed to produce agreement with the dilute poor-resolution data.

The creation of SLBW ladders from average parameters can be expected to produce the same kind of end-effect bias and frequent negative scattering cross sections found in the resolved resonance region. Again, the scattering cross section per se may not be important, but the biased total cross section may adversely affect calculated reaction rates.

2.4.l3. Use of Two Nuclear Radii

The current ENDF formats defines two different nuclear radii:

a) the scattering radius, AP, and

b) the channel radius, *a*.

The scattering radius is also referred to as "the effective scattering radius" and "the potential scattering radius". The channel radius is also referred to as "the hard-sphere radius", or "the nuclear radius". The former is the quantity defined as AP (for a_+ or â) in File 2, which must be given even if no resonance parameters are given. The nuclear radius is defined in Appendix D, Equation (D.0).

The channel radius is a basic quantity in R-matrix theory, where the internal and external wave-functions are joined and leads to the appearance of hard-sphere phase shifts defined in terms of it. The necessity to relax the definition and permit two radii can be thought of as a "distant-level effect", sometimes not explicit in R-matrix discussions.

The original ENDF/B formats made provision for an AM, or "A-minus", although it was always required that evaluators put AM=0, to signify that it was equal in value to AP. In the current formats, AM is eliminated, but one can anticipate that more sophisticated evaluation techniques may eventually force the reinstatement of not only AM, but a more general dependence of the scattering radius on the channel quantum numbers, especially as higher energies become important.

In theory, the scattering radius depends on all the channel quantum numbers, and in practice it is common to find that different optical model parameters are required for different *l*-values (s, p, d,...) and for different J-values ($p^{1/2}$, $p^{3/2}$, ,,,). This implies that one would require a different scattering radius for each of these states.

For the special case of s-waves, only two J-values are possible, namely I±1/2, commonly denoted J_+ and J_-. This is the origin of the terminology a_+ and a_-.

Up through ENDF/B-V, the recommended ENDF/B procedure was to use the above equation for the channel radius in the penetrabilities $P_l(ka)$ and the shift factors $S_l(ka)$, but to use the scattering radius to calculate the hard-sphere phase shifts $\varphi_l(ka)$.

Since the phase-shifts define the potential scattering cross section, the evaluator had the freedom to fit AP to a measured cross section while still leaving undisturbed those codes that use the $A^{1/3}$ formula to calculate the channel radius.

For ENDF/B-VI, new parameters NRO and NAPS are available to give the evaluator more flexibility for the SLBW, MLBW, and RM formalisms, by allowing the evaluator to use AP everywhere and to make AP energy-dependent (Section 2.1).

The full flexibility of channel-dependent radii is provided for the RML format.

2.4.14. The Multilevel Adler-Gauss Formula for MLBW

Appendix D gives (implicitly) for the MLBW formalism the equations:

$$\begin{aligned}
\sigma_{n,\gamma}^{MLBW}(E) &\equiv \sigma_{n,\gamma}^{SLBW}(E)\,, \\
\sigma_{n,f}^{MLBW}(E) &\equiv \sigma_{n,f}^{SLBW}(E)\,, \\
\sigma_{n,n}^{MLBW}(E) &\equiv \sigma_{n,n}^{SLBW}(E) + \sum_{l=0}^{NLS-1} \sigma_{n,n,RRI}^{l}(E)\,,
\end{aligned} \tag{2.2}$$

where RRI labels the resonance-resonance-interference term for a given *l*-value:

$$\frac{\pi}{k^2}\sum_J g_J \sum_{r=2}^{NR_J}\sum_{s=1}^{r-1} \frac{2\Gamma_{nr}\Gamma_{ns}\left[(E-E'_r)(E-E'_s)+\Gamma_r\Gamma_s/4\right]}{\left[(E-E'_r)^2+(\Gamma_r/2)^2\right]\left[(E-E'_s)^2+(\Gamma_s/2)^2\right]} \tag{2.3}$$

As most users are aware, this double sum over resonances can eat prodigious amounts of computer time unless handled very tactfully. Thus, for a 200-resonance material, there are ~40,000 cross terms, of which only 20,000 need to be evaluated because the expression is symmetric in r and s.

It has been noted many times in the past that partial fractions can reduce Equation (2.3) to a form with only a single Breit-Wigner denominator. Most recently, DeSaussure, Olsen, and Perez (Reference 6) have written it compactly as

$$\begin{aligned}
&\frac{\pi}{k^2}\sum_J g_J \sum_{r=1}^{NR_J} \frac{G_r\Gamma_r + 2H_r(E-E'_r)}{(E-E'_r)^2+(\Gamma_r/2)^2}\,, \quad \text{where} \\
G_r &= \frac{1}{2}\sum_{s=1}^{NR_J} \frac{\Gamma_{nr}\Gamma_{ns}(\Gamma_r+\Gamma_s)}{(E'_r-E'_s)^2+\frac{1}{4}(\Gamma_r+\Gamma_s)^2}\,, \quad s \neq r \\
H_r &= \sum_{s=1}^{NR_J} \frac{\Gamma_{nr}\Gamma_{ns}(E'_r-E'_s)}{(E'_r-E'_s)^2+\frac{1}{4}(\Gamma_r+\Gamma_s)^2}\,, \quad s \neq r
\end{aligned} \tag{2.4}$$

The authors give the special case for I=*l*=0, but it is valid for any set of quantum numbers. Thus an existing SLBW code can be converted to MLBW by adding $G_r\Gamma_r$ to the symmetric part of the SLBW formula, $\Gamma_{nr}^2 \cos 2\phi_l - 2\Gamma_{nr}(\Gamma_r - \Gamma_{nr})\sin^2 \phi_l$, and $2H_r$ to the coefficient of $(E\text{-}E'_r)$ in the asymmetric part, $2\Gamma_{nr} \sin 2\phi_l$.

Since G_r and H_r are weakly energy-dependent, via the penetrabilities and shift factors, they lend themselves to approximations that can sharply reduce computing time compared to the form with the "double" Breit-Wigner denominator. In fact, if the resonances are all treated as s-wave (shifts of zero, penetrabilities of $\sqrt{E}$), and the total widths are taken as constant, then G_r/k^2 and H_r/k^2 become independent of the neutron energy and consume a negligible amount of computing time so that MLBW and SLBW become equivalent in that respect.

The amplitude-squared form of MLBW, Section 2.4.19, also reduces computing time.

2.4.l5. Notes on the Adler Formalism

Questions concerning the ENDF/B treatment of the Adler formalism are enumerated below[10], together with recommended procedures for handling them:

1. The resonance energy μ and total half-width v are the same for each reaction for a given resonance in the Adler formalism, but, for the October l970 version of ENDF-l02, the formulae on page D-7, and the format descriptions of pages 7.9 and N-l2 permit different values for the total, fission, and capture cross sections.

   This is a misreading of the formalism; the remedy is to constrain the equalities $DET_N = DEF_N = DEC_N$ and $DWT_N = DWF_N = DWC_N$. The formulas for capture and fission should also have the phases eliminated in Appendix D.

2. The Adler formalism, as applied by the Adlers, breaks the resolved resonance region up into sub-regions, and each is analyzed separately. This avoids problems with contributions from distant resonances, but requires that the polynomial background be tailored to each sub-region. However, the ENDF/B formats allow only one resolved resonance energy region, so this procedure cannot be used.

   If a single set of polynomial background constants is insufficient, additional background can be put into File 3, point-by-point.

3. The ENDF/B formats formerly permitted incomplete specification of the cross sections. The allowed values of LI were 5 (total and capture widths); 6 (fission and capture); and 7 (total, fission, and capture). LI=6 leaves the scattering (and total) undefined and LI=5 is deficient for fissile elements. LI=6 is now restricted to ENDF/A, and LI=5 should be used only for non-fissile elements.

4. The nomenclature for the G's and H's is not entirely consistent among different authors. The Adlers use for the total cross section the definitions:

   $G_t = \alpha \cos(2ka) + \beta \sin(2ka)$;
   $H_t = \beta \cos(2ka) - \alpha \sin(2ka)$;

[10] The following is a condensation and updating of the Appendix in the June, l974, Minutes of the Resonance Region Subcommittee.

and then the combination:

$$\nu G_t + (\mu - E)\, H_t \, .$$

For the reaction cross sections there are no phases, and they write

$$\nu G_c + (\mu - E)\, H_c \quad \text{(capture)};$$
$$\nu G_f + (\mu - E)\, H_f \quad \text{(fission)};$$

G and H are properly designated as "symmetrical" and "asymmetrical" parameters. This manual changes α to G_t and to H_t, viz:

$$\nu\,[G_t \cos(2ka) + H_t \sin(2ka)] + (\mu - E)\,[H_t \cos(2ka) - G_t \sin(2ka)]$$

These G_t's and H_t's are no longer symmetrical and asymmetrical, but are referred to that way. The precedent for this nomenclature is probably Reference 7.

DeSaussure and Perez, in their published tables of G and H, incorporate the Adler's constant c into their definition, but otherwise leave the formalism unchanged.

Users and evaluators should adhere to the definitions in this manual.

5. The flag NX, which tells what reactions have polynomial background coefficients given, should be tied to LI, so that the widths and backgrounds are given for the same reactions, *i.e.*, use NX=2 with LI=5 (total and capture), and NX=3 with LI=7 (total, capture, and fission). Since no NX is defined for LI=6 (fission and capture), one is forced to use NX=3 with the background total coefficients set equal to zero, but this now occurs only in ENDF/A, if at all.

2.4.16. Multilevel Versus Single-Level Formalisms in the Resolved and Unresolved Resonance Regions

2.4.16.1. In the Resolved Resonance Region

The SLBW formalism is adequate for resonance treatments that do not require actual pointwise scattering cross sections, as, *e.g.*, multigroup slowing-down codes. Because of the frequent occurrence of negative scattering cross sections, when two or more resonance-potential interference terms overlap, SLBW should not be used to compute pointwise scattering cross sections. Instead, the MLBW formalism should be used, although MLBW is not a true multilevel formalism, but a limit, which is valid if Γ/D is small.

The Reich-Moore reduced R-matrix formalism is a true multilevel formalism, and is recommended for low-energy fissionable s-wave evaluations. All of its cross sections are non-negative, and its only significant drawbacks, apart from the effort required for its application, are the difficulty of determining a suitable R^{∞} to represent distant-level effects, and of determining the parameters of negative-energy resonances.

The Adler form of the Kapur-Peierls formalism is also a true multilevel treatment, but in actual applications the parameters are determined by fitting data and the theoretical constraints among them are lost, so that any Adler cross section can be negative.

The simplest true multilevel formalism is the reduced R-function, in which all channels except elastic scattering have been eliminated. It makes a very adequate evaluation tool for non-fissile elements up to the threshold for inelastic scattering, since below that the eliminated channels are (usually) simply radiative capture. It can be corrected for distant-level effects by substituting optical-model phase shifts for the hard-sphere ones which occur in the formalism, and by

introducing an appropriate R^{∞}. It can be carried above the inelastic threshold by augmenting it with the use of SLBW formulas for the reactions other than elastic scattering, since such reactions often show negligible multilevel effects. For structural and coolant materials, either Reich-Moore or R-Matrix Limited can be used. The latter provides more detail in describing competitive reactions, plus angular distributions, and allows treating resonances with both l>0 and I>0.

Multi-channel multilevel fitting is also feasible for light elements, and permits the simultaneous use of non-neutron data leading to the same compound nucleus. Due to the complexity of such calculations, they may be presented in ENDF/B as file 3 pointwise cross sections, although the R-Matrix Limited format can handle this case.

2.4.16.2. In the Unresolved Resonance Region

In principle, if the statistical distributions of the resolved resonance parameters are known, any formalism can be used to construct fictitious cross sections in the unresolved region. At the present time, only the SLBW formalism is allowed in ENDF/B, for the reason that no significant multilevel effect can be demonstrated, when SLBW is properly handled.

If resolved region statistics are used without adjustment to poor resolution data, then large multilevel/single-level differences can result, but there is no simple way to determine which is better. If both are adjusted to yield the same average cross sections, and for fissile materials, the same capture-to-fission ratio, then the remaining differences are within the statistical and measurement errors inherent in the method. The above comments on multilevel effects in the unresolved resonance region are based on the work of DeSaussure and Perez [Ref.8].

As noted in Section 2.4.l2, the use of SLBW to construct resonance profiles in the unresolved region will result in the defects associated with this formalism elsewhere, and is not recommended. This application calls for MLBW or better, and the SLBW scheme should be used only for constructing average cross sections where the negative scattering effects will combine with the other approximations and presumably be "normalized out" somewhere along the line.

2.4.17. Preferred Formalisms for Evaluating Data

Unless there is strong reason to do otherwise, the R-Matrix Limited format (LRF=7) should be used for reporting results of new evaluations, as it is the most comprehensive of the current formats.

1. Light nuclei: Use multilevel, multichannel R-matrix. Present either as pointwise cross sections in file 3, or as R-matrix parameters using LRF=7.
2. Materials with negligible or moderate multilevel effects, and no multichannel interference: Reich-Moore or MLBW. These are equivalent in computing time and all require kernel broadening, although MLBW lends itself to the ψ,χ-approximation discussed in Section 2.4.14. However, RM and RML provide the angular distribution of elastically-scattered neutrons, which MLBW does not.
3. Materials with strong multilevel effects, but no multichannel interference: Reich-Moore or R-Matrix Limited. The structural materials do not exhibit channel-channel interference, but have level-level interference that is too strong for an MLBW treatment.
4. Materials with observable channel-channel interference: Reich-Moore or R-Matrix Limited. In the past, only low-energy fissionable materials have shown channel-channel interference, and this is unlikely to change. Reich-Moore evaluations can be converted to Adler format for presentation in ENDF/B. The reason why Reich-Moore is preferred to Adler-Adler as the basic

evaluation tool is that it has less flexibility and is therefore better able to distinguish between various grades of experimental data. However, it requires kernel broadening whereas Adler-Adler uses ψ and χ, making the latter more convenient to broaden. Unfortunately some of this convenience is lost in practice because there is no simple equivalence between Adler-Adler and SLBW (see Section 2.4.8). With modern computers and modern computer codes, the slight advantage offered by kernel broadening is no longer an important issue.

5. Materials with channel-channel interference and one or more competitive reactions: R-matrix, using the format LRF=7 to present the parameters.

2.4.18. Computer Time for Generating MLBW Cross Sections

Previous solutions to the problem of evaluating the double-sum form of the MLBW resonance-resonance interference term in a reasonable amount of time have been to use the amplitude-squared form from which it was derived, and kernel-broaden it, or to optimize the calculation of inner and outer loop quantities.

A third solution is to use the Multilevel Adler-Gauss formulas discussed in Section 2.4.14 and possibly approximate the energy-dependence of the G_r- and H_r-coefficients.

The amplitude-squared form of MLBW is discussed in Section 2.4.l9.

2.4.19. Amplitude-Squared Form of the MLBW Formulas

The form of the MLBW scattering cross section given in Appendix D and in Section 2.4.l4, is mathematically identical to the more fundamental "amplitude-squared" form given in Appendix D, as Equations (5) - (7) of Section D.l.2.

Those equations can be coded in complex Fortran, or broken up into their real and imaginary parts before coding. The essential point is that they sum the resonances before squaring. This avoids turning two "linear" sums into one "quadratic" one. If an isotope has 200 resonances, the above formulas have two sums with 200 terms each, whereas the ENDF form has a sum with 40000 cross terms. A discussion of points to consider in coding the above equations is given in Sections 2.4.23 and 2.4.24.

The main drawback to the above equations is that they do not admit Doppler-broadening with ψ- and χ-functions, but require kernel methods instead.

2.4.20. Degrees of Freedom for Unresolved Resonance Parameters

A resonance in the system (neutron plus a target of mass A) corresponds to a quasi-stationary state in the compound nucleus A + 1. Such a resonance can decay in one or more ways, each described as a channel. These are labeled by the identity of the emitted particle (two-body decay), the spins I and i of the residual nucleus and the emitted particle, and the orbital angular momentum *l* of the pair. To uniquely specify the channel, two more quantum numbers are needed, since the magnetic quantum numbers can be eliminated for unpolarized particles.

It is common to give the channel spin, s, which is the vector sum of I and i, plus $\vec{J} = \vec{s} + \vec{l}$, since this facilitates the isolation of the *l*-dependence of all channel quantities. The important point is that the same set of three ingredient angular momenta, I, i, and *l*, will give rise to a number of different channels, according to the rules for coupling angular momenta. The resonance will decay into each of these channels, with a probability that is governed by a real number $\gamma_{\alpha IiJls}$, the reduced width amplitude, where α gives the identity of the emitted particle, the state of excitation of the daughter nucleus, *etc*. The partial width for the channel is:

$$\Gamma_{\alpha IiJls} = 2P_{\alpha IiJls}\,\gamma^2_{\alpha IiJls}\,.$$

The penentrabilities depend only on *l*, and are given in Appendix D for uncharged particles. For charged particles, their Coulomb analogs can be found in texts on the subject, and for gamma rays one uses $\sqrt{\Gamma_\gamma}$ rather than γ and P.

If the collection of channel quantum numbers (αIiJ*l*s) is denoted by c, then the total width for the level is $\Gamma = \Sigma_c\Gamma_c$. [$\Sigma_c$ means a sum over all channels]. The argument from statistical compound nucleus theory is that the γ_c's are random variables, normally distributed with zero mean and equal variance. The population referred to is the set of γ_c's for a given channel and all the levels (or resonances). It follows that the total width is distributed as a chi-squared distribution with N degrees of freedom, since this is the statistical consequence of squaring and adding N normal variates. For N=l, this is the Porter-Thomas distribution. In determining the behavior of any quantity that is going to be averaged over resonances, it is necessary to know the way in which the widths are distributed, hence the inclusion of these degrees of freedom in ENDF/B.

1. The neutron width is governed by AMUN, which is specified for a particular *l*-value. Usually, only the lowest allowed *l*-value will be significant in any decay, although the formats would allow giving both s- and d-wave widths for the same resonance. Since there is only one J-value for a given resonance, and we label the widths by one *l*-value, there can be at most two channels for neutrons (i = 1/2), labeled by the channel spin values s = I±1/2. If I = 0, there is only one channel, s = i = ½; hence the restriction, 1.0≤AMUN≤ 2.0. AMUN is the quantity $\mu_{l,J}$, discussed in Section D.2.2.2.

   Although there is no supporting evidence, it is assumed that the average partial widths for each channel spin are equal, and that $\langle\Gamma_n\rangle$ is the sum of two equal average partial widths. In Appendix D this factor of two is absorbed into the definition of $\langle\Gamma_n\rangle$, through the use of a multiplicity, which is the number of channel spins, 1 or 2.

2. The competitive width is currently restricted to inelastic scattering, which has the same behavior as elastic scattering, measured from a different "zero channel energy," hence

   $$1.0 \le \text{AMUX} \le 2.0$$

   Note that one should not set AMUX = 0 out of ignorance of its true value, as suggested in previous versions of ENDF-l02. This implies a constant from resonance to resonance, since the chi-squared distribution approaches a delta function as $N\to\infty$. An inelastic reaction can be expected to proceed through a small number of channels and hence to fluctuate strongly from level to level.

Specifically, AMUX = $\mu_{i,J}$, where J is the spin of the resonance, and is $\vec{l}$ the orbital angular momentum of the inelastically scattered neutron. Since the daughter nucleus may have a spin $\vec{I}$ different from the target spin I, $\vec{l}$ may be different from *l*, and the number of channel spin values $\mu_{i,J}$ may be different from $\mu_{i,J}$.

3. For the radiative capture process, AMUG should be set equal to zero. Radiative capture proceeds through many channels and it is not worthwhile deciding if AMUG is 30 or 40. (If some nucleus has selection rules that restrict radiative decay to a few channels, then a different value of AMUG might be appropriate.)

4. The fission value should be given as 1.0≤AMUF≤4.0 and the value zero would be incorrect. These small values violate the previous discussion of (Wigner-type) channels and obey instead statistics governed by fission barrier tunneling (Bohr-channels). The actual value of AMUF is determined by comparison between calculated and measured cross sections.

The degrees of freedom are constant throughout the unresolved resonance region.

2.4.21. Procedures for the Unresolved Resonance Region

Up to 250 energy points are permitted for specifying energy-dependent average parameters. This number is presumed to be sufficient to reproduce the gross structure in the unresolved cross sections. Within a given isotope the same energy grid must be used for all J- and *l*-values. The grids may be different for different isotopes. Unresolved resonance parameters should be provided for neutron energy regions where temperature-broadening or self-shielding effects are important. It is recommended that the unresolved resonance region extend up to at least 20 keV.

If the flag LSSF (Section 2.3.1) is set equal to one, the evaluator can specify the gross structure in the unresolved range on as fine an energy grid as he desires, subject only to the overall 10000-point limitation. Under this option, File 3 represents the entire dilute unresolved cross section, and no File 2 contribution is to be added to it. Instead, File 2 is to be used to compute a "slowly-varying" self-shielding factor that may be applied to the "rapidly-varying" File 3 values. The self-shielding factor is defined as the ratio of File 2 average shielded cross section to the average unshielded value computed from the same parameters. This ratio is to be applied as a multiplicative factor to the values in File 3.

If LSSF is set equal to zero, File 3 will be interpreted in the same way as a resolved-region File 3, *i.e.*, it will represent a partial background cross section to be added to the average cross section, dilute or shielded that is computed from File 2.

The self-shielding-factor procedure has certain advantages over the "additive" procedure:

1. The energy-variation of the dilute cross section in the unresolved region can be more accurately specified, without the 250-point limitation imposed in File 2.
2. The energy grids in File 2 and File 3 are basically uncoupled, so that the File 2 grid can be made coarser and easier to process.
3. In principle, the results can be more accurate, since File 2 can be devoted entirely to representing changes in the average parameters that are significant for shielding. The burden of representing fluctuations in the size of the dilute cross section is taken over entirely by File 3.

4. The same representation can be used by codes requiring probability tables. For this application, the average parameters in File 2 can be used to generate random ladders of resonances, and the resulting cross sections can be used to calculate probability tables in the usual way. However, instead of using the tables directly, they are normalized by dividing the various cross section bands by the average cross section in the interval. These normalized probabilities are then converted back to cross sections by multiplying them into the File 3 values. The rationale is the same as for the shielding-factors - the dilute cross section is represented in "poor-resolution" format in File 3, while the real fine-structure is established in File 2.

   The following caution should be noted by evaluators in choosing this option:
   Because File 3 is energy varying, it inherently has the possibility to energy-self-shield itself. If File 2 also shields it, one may actually "double-shield". The problem will probably be most acute just above the boundary between the resolved and unresolved regions, since the experimental resolution may still be good enough to see clumps of only a few resonances.

   One might consider "correcting" for this in the choice of File 2 parameters, but this would be difficult because the degree of shielding is application dependent. A better procedure would be to insure that each significant structure in File 3 actually represents a statistically meaningful number of resonances, say ten or more. If the raw data do not satisfy this criterion, then additional smoothing should be applied by the evaluator to make it a correct condition on the data. A careful treatment will require the use of statistical level theory to determine the true widths and spacings underlying the File 3 structures.

2.4.22 Procedures for Computing Angular Distributions in the Resolved Resonance Range

2.4.22.1. Background

Quantum mechanical scattering theory, which underlies all of the resonance formalisms in this chapter, describes the angular distribution of exit particles as well as the magnitudes of the various reactions. When the R-matrix formalism is used to parameterize the collision matrix, as in the Reich-Moore format (Section D.1.3) or the RML format (Section D.1.7), then the angular distributions exhibit a resonant behavior, in the sense that they may change substantially in passing through a resonance. An explicit tabulation of this detailed resonance behavior will usually imply a very large data file.

Blatt and Biedenharn [Ref. 7] simplified the general expression for the angular distribution, which is an absolute square of an angle-dependent amplitude, so that it became a single sum over Legendre polynomials. Their expression, particularized to the RML format, is given in Sections D.1.7. In the past, Reich-Moore has been a vehicle for low-energy fissionable isotope evaluations, usually s-waves only, so that the angular distribution is isotropic. If it were used for higher energies and higher angular momenta, then the angular distributions would become anisotropic. Of course, since the formulas define a center-of-mass distribution, even the isotropic case generally defines an anisotropic laboratory distribution.

In principle, similar angular distribution formulas underlie the SLBW, MLBW, and Adler-Adler formalisms, but since these are not formulated in terms of collision matrix elements (U_{lsJ}), the Blatt and Biedenharn formulas are not immediately applicable to them.

Although the Blatt and Biedenharn formulas have been around for thirty-five years, and have been much used in the physics literature of scattering theory, they have not been widely employed in neutron cross section evaluation. ENDF/B files most often contain either experimental data or calculated data derived from an optical model. Both of these types represent a "smoothing" or "thinning" of the underlying resonant angular distributions. In the case of experiment, the smoothing is done by the resolution-broadening of the measuring apparatus, combined with the necessarily limited number of energies at which data can be taken. In the optical model case, the smoothing is done in an obscure, highly implicit manner. It seems quite clear that an explicit energy-average over resonant Blatt and Biedenharn Legendre coefficients will differ from both of the above representations.

This raises the question of whether the Blatt and Biedenharn average will be better or worse than the others. That question is dealt with in the following paragraphs, which are somewhat "theoretical", since there is not much hard experience in this area.

2.4.22.2 Further Considerations

Firstly, if in some ideal case, all the resonance spins and parities were precisely known, then the Blatt and Biedenharn values would be exact, and clearly superior to any other representation. The next step down the accuracy ladder would be a case where the major resonances, or anti-resonances ("windows") were known, but some minor, narrower ones were uncertain. For this case, one might find that errors in the "minor" resonances canceled each other, again producing a superior result, or one might find an erroneous cooperation, resulting in spurious-values.

Finally, there are evaluations that use compiled resonance parameters, with many guessed J and *l*-values, in which case the cancellations and/or cooperations dominate the angular distributions. In both of the two latter cases, the evaluator either will or will not have compared with experiment and made a decision on the accuracy of the Blatt and Biedenharn representation. The flag LAD allows him to inform the processing code whether or not it is "safe" to calculate from the Blatt and Biedenharn formulas. Such a flag is necessary because File 4 is limited to 1200 angular distributions, which is usually not enough to represent a fully-detailed Blatt and Biedenharn representation. The recommended ENDF/B procedure is for the evaluator to provide an under-1200-energy-point representation in File 4, and to signal the user with LAD whether he can independently generate $\sigma(\theta)$ on a finer energy mesh.

For the File 4 representation, the evaluation should smooth the data so as to preserve significant structure in the first Legendre coefficient, or μ. As always, the word ***significant*** is difficult to define exactly but the File 4 representation should be adequate for most ordinary reactor engineering applications.

In any case, a user who wishes to examine the implications for his own work of a finer mesh is free to use the Blatt and Biedenharn formulas. The flag LAD tells him either that the evaluator has approved this procedure (LAD=1), or that it is either of unknown quality or known to be poor (LAD=0). In the case of LAD=0, the evaluator should tell which of these is the case by putting comments into File 1 and the associated documentation.

2.4.22.3. Summary of Recommendations for Evaluation

1. Supply an under-1200-point representation of the elastic scattering angular distribution in File 4. Preserve significant structure in μ.
2. If the Blatt and Biedenharn angular distributions were not examined, or if they were examined and found to be inaccurate, supply LAD=0 in File 2. Tell which of these is the case in File 1 and in the associated documentation.
3. If the Blatt and Biedenharn angular distributions were found, or are believed, to be accurate, supply LAD=1, and describe the evaluation procedures in the documentation.

2.4.23. Completeness and Convergence of Channel Sums

Two possible errors in the calculation of cross sections from a sum over individual channels are:

1.) omission of channels because they contain no resonances (such "non-resonant" or "phase-shift-only" channels must still be included because they contribute to the potential scattering cross section), and

2.) failure to include enough non-resonant channels to insure convergence of the potential-scattering cross section with respect to *l* at high energy.

Avoiding the first is the responsibility of the processing codes for the SLBW, MLBW, A-A, and R-M formalisms, since the formats do not allow the evaluator to specify empty channels explicitly. For the RML formalism, where such specification ***is*** explicit, the responsibility is the evaluator's. Avoiding the second is always the evaluator's responsibility, since it would be awkward for a processing code to decide whether the omission was intentional or not.

In the channel spin representation, the incident spin, i, is coupled to the target spin, I, to form the channel spin, s, which takes on the values:

$$|I-i| \leq s \leq I+i.$$

The channel spin couples to the orbital angular momentum to form the total angular momentum J, with the values:

$$|l-s| \leq J \leq l+s.$$

If $I > 0$ and $l > 0$, the same *J*-value may occur for each of the two channel spins, $s = I \pm 1/2$, and ***each*** of these *J*-values must be ***separately*** included. A width Γ_{lJ} is a sum of the two components, $\Gamma_{l s_1 J}$ and $\Gamma_{l s_2 J}$; and in the SLBW, MLBW, and A-A formalisms, only the sum is used. In the Reich-Moore format, the specification of *J* implicit (via the use of a signed AJ value). For the RML format, the evaluator should specify two separate channels (for the two values of *s*) within the same spin group in this situation.

There is rarely enough information on channel-spin widths to guide the evaluator in apportioning the total width between the two sub-channels, but fortunately, most neutron reactions are insensitive to the split, so that putting it all in one and none in the other, or splitting it 50/50 works equally well. Angular distributions are in principle more sensitive, but it is similarly unusual to find measured data of sufficiently high precision to show an effect.

The channel sums are infinite,

$$\sum_{l=0}^{\infty} \sum_{s=\left|I-\frac{1}{2}\right|}^{I+\frac{1}{2}} \sum_{J=|l-s|}^{l+s} \chi_{lsJ}$$

so the question of convergence arises. The simplest case is where the summand is an SLBW ***reaction*** term, as in Section D.1.6.2, in which case one sums only over channels in which there are resonances. There are then no convergence considerations.

If one is summing ***scattering*** cross section terms, as in Section D.1.6.1, there is a potential-scattering amplitude in ***every*** channel, independent of whether there are resonances or not. The l=0, or s-wave amplitudes, are finite at zero energy, but the higher l-waves only come in at higher energies. The convergence criterion is therefore that the addition of the next higher l-wave produces a negligible change in the cross section at the highest energy covered by the resonance region. In a conventional R-matrix treatment, the non-resonant channels contain hard-sphere phase shifts whose behavior has to be compared with experiment.

For the R-Moore format, NLS is defined as that value which converges the cross section calculation. This is different from the SLBW/MLBW definition, which is the number of l-channels with resonances. The latter is more liable to cause neglect of higher-l non-resonant channels. Such neglect would show up as incorrect between-resonance scattering at high energies, admittedly not the easiest defect to see.

If ***angular distributions*** are to be calculated, as in Sections D.1.5.9 and D.1.6.5, besides having more complicated sums, the range of l-values is much greater, the requirement being that the angular distributions converge at the highest energies. Because the high l-amplitudes interfere with the low ones, non-negligible cross terms occur which are absent from the cross section sums. The different convergence criteria, NLS and NLSC, are compatible because only the B_0 moment contributes to the cross sections. All the higher moments integrate to zero. Computer codes which reconstruct such moments should have recursive algorithms for l-dependent quantities up to l=20.

For the R-Matrix Limited format, all terms and only those terms specified by the evaluator (i.e., included in the File 2 information) are to be included in every calculation.

2.4.24. Channel Spin and Other Considerations

For the R-Matrix Limited format, channel spin is explicit and the evaluator must in general provide partial widths that depend on s as well as l and J.

For the Adler-Adler formalism, the usual area of application is to low-energy fissile nuclides, with l = 0, so that channel spin is not mentioned in the formulae of Appendix D.

For the Reich-Moore formalism, in those cases where two channel spins are possible, the channel spin is specified by the sign of the AJ parameter. In older evaluations where the channel spin is not specified (*i.e.*, where all AJ are positive), all resonances are assumed to have the same channel spin and the hard-sphere contribution from the second channel spin must be added separately.

For MLBW the absolute square has been expanded out and all imaginary quantities eliminated. This has several consequences.

1. Channel spin is effectively eliminated, because the partial widths occur in "summed" form.

$$\Gamma_{lJ} = \Gamma_{ls_1J} + \Gamma_{ls_2J}$$

   Since only the sum is required, the evaluator is spared the necessity of specifying the separate s-values. This converts an (l,s,J) formalism into an (l,J) formalism. The same effect can be achieved by assuming that I=0, a popular assumption often made independently of the truth, as in many optical model calculations.

2. The convergence criterion is more transparent, because the potential-scattering cross section splits off from the resonance and interference terms, as

$$\frac{4\pi}{k^2}(2l+1)\sin^2\phi_l .$$

   Despite the simpler nature of this term than its parent amplitudes, one must still carry enough terms to make the results physically correct, and if this cannot be done, then File 3 must be invoked to achieve that goal.

3. The resonance profiles are expressible in terms of symmetric and asymmetric Breit-Wigner shapes, and thus admit ψ,χ Doppler broadening. The price one pays for these three advantages is increased computing time, when the number of resonances is large.

Similar remarks apply to the SLBW formalism, which is MLBW without the resonance-resonance interference terms. The computing time goes way down, but the scattering cross section is very poor. SLBW has useful applications in certain analytical and semi-analytical procedures, but should never be used for the calculation of explicit pointwise scattering cross sections.

The omission of an explicit channel-spin quantum number in the SLBW formalism, while convenient in the resolved resonance region, has occasioned some difficulty in the unresolved region. Sections D.2.2 through D.2.4 attempt to clarify the situation with respect to level densities, strength functions, and spin statistics.

2.5. References for Chapter 2

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