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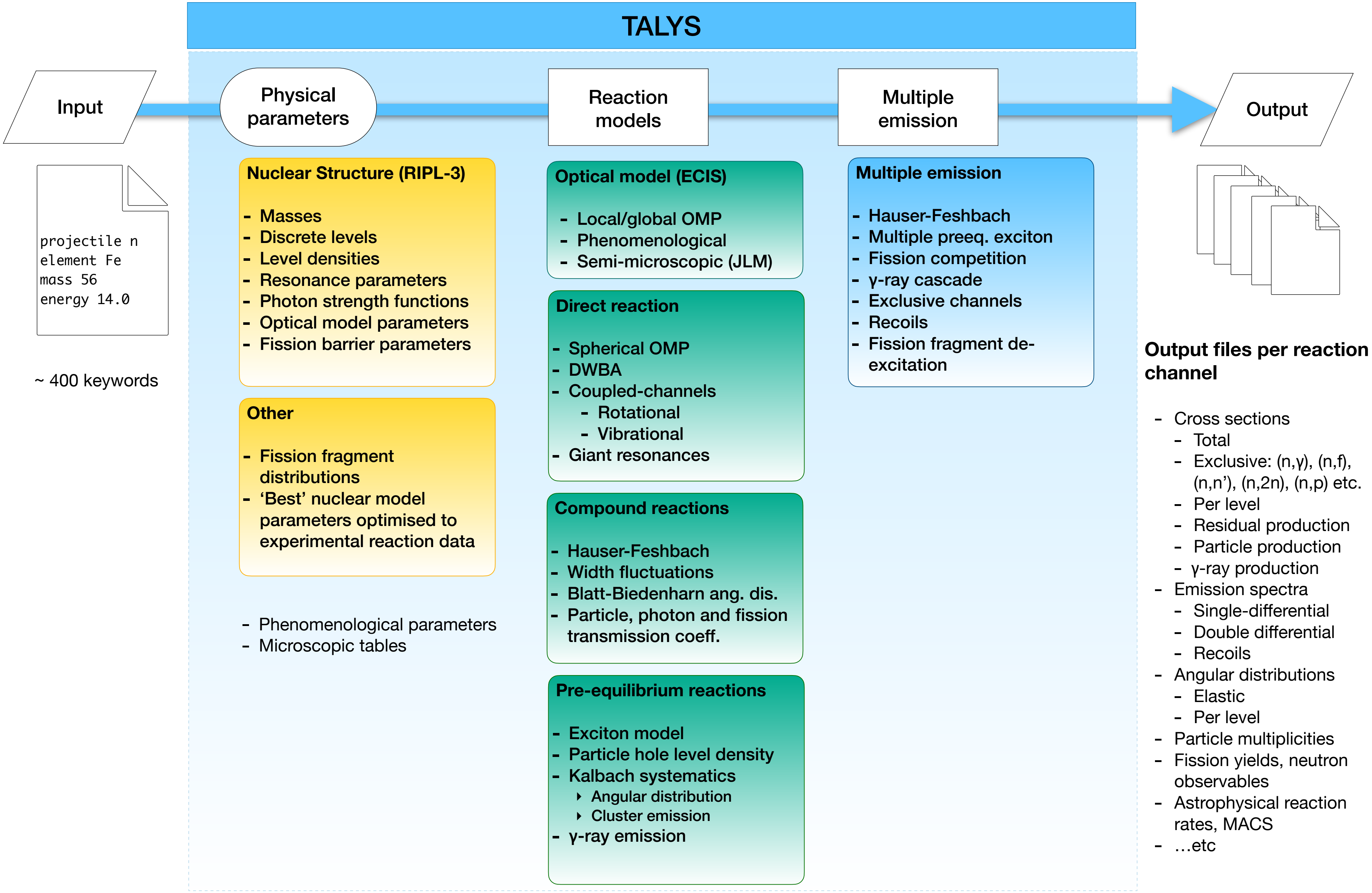
Some views of a level density end user

Arjan Koning, IAEA

IAEA, Consultancy meeting on Level densities, June 26-28 2023

Introduction

- TALYS
- Global level density API
- Adjustment possibilities for cross section calculations
- Discrete level scheme connection and generation
- Spin distribution and its validation
- Format
- Some suggestions for CRP



TALYS

Input

```
projectile n
element Fe
mass 56
energy 14.0
```

~ 400 keywords

Physical parameters

Nuclear Structure (RIPL-3)

- Masses
- Discrete levels
- Level densities
- Resonance parameters
- Photon strength functions
- Optical model parameters
- Fission barrier parameters

Other

- Fission fragment distributions
- 'Best' nuclear model parameters optimised to experimental reaction data

- Phenomenological parameters
- Microscopic tables

Reaction models

Optical model (ECIS)

- Local/global OMP
- Phenomenological
- Semi-microscopic (JLM)

Direct reaction

- Spherical OMP
- DWBA
- Coupled-channels
  - Rotational
  - Vibrational
- Giant resonances

Compound reactions

- Hauser-Feshbach
- Width fluctuations
- Blatt-Biedenharn ang. dis.
- Particle, photon and fission transmission coeff.

Pre-equilibrium reactions

- Exciton model
- Particle hole level density
- Kalbach systematics
  - Angular distribution
  - Cluster emission
- γ-ray emission

Multiple emission

Multiple emission

- Hauser-Feshbach
- Multiple preeq. exciton
- Fission competition
- γ-ray cascade
- Exclusive channels
- Recoils
- Fission fragment de-excitation

Output

Output files per reaction channel

- Cross sections
  - Total
  - Exclusive: (n,γ), (n,f), (n,n'), (n,2n), (n,p) etc.
  - Per level
  - Residual production
  - Particle production
  - γ-ray production
- Emission spectra
  - Single-differential
  - Double differential
  - Recoils
- Angular distributions
  - Elastic
  - Per level
- Particle multiplicities
- Fission yields, neutron observables
- Astrophysical reaction rates, MACS
- …etc

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THE EUROPEAN
PHYSICAL JOURNAL A

Review

TALYS: modeling of nuclear reactions

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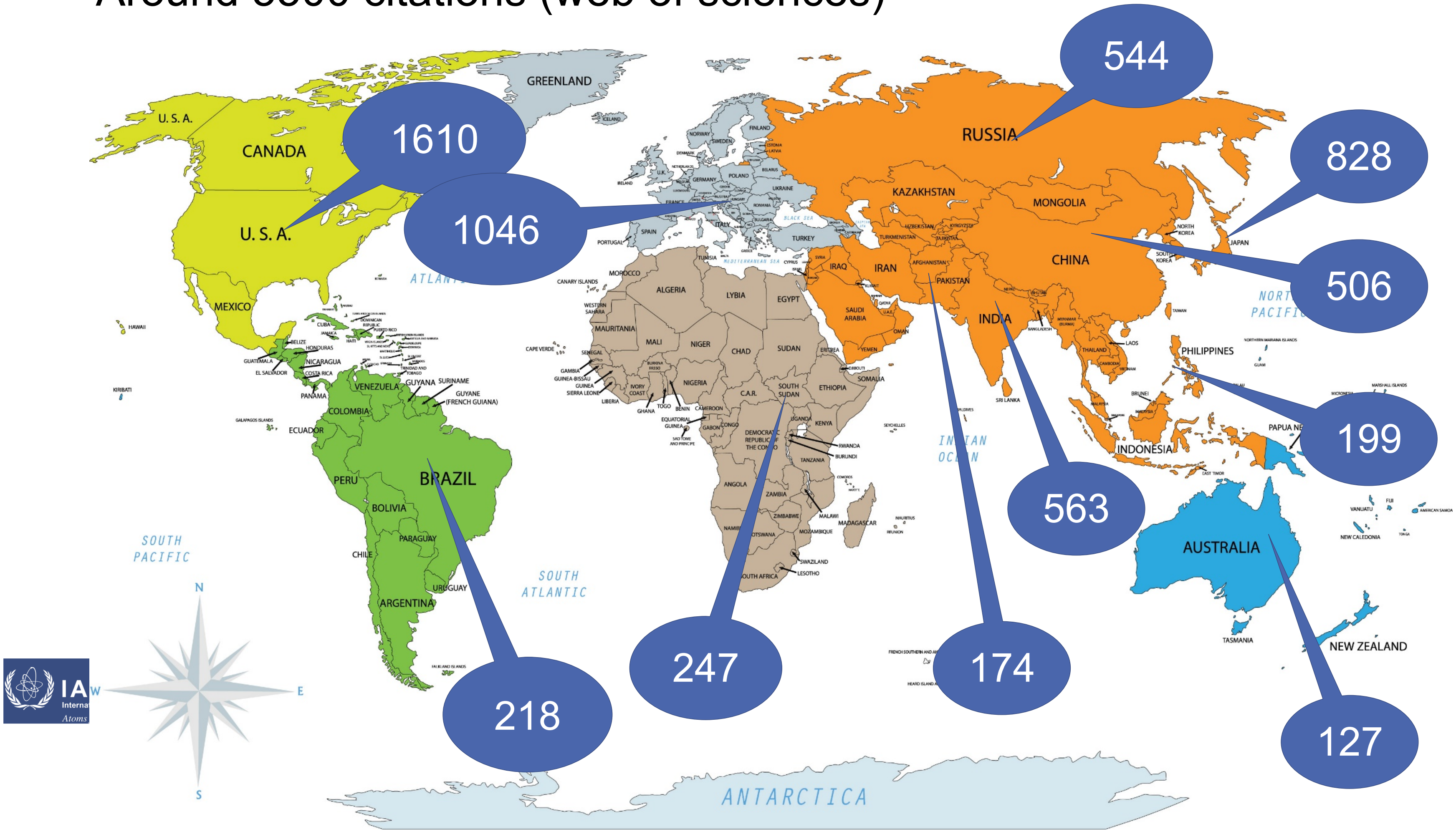
Communicated by Nicolas Alamanos

Abstract TALYS is a software package for the simulation of nuclear reactions below 200 MeV. It is used worldwide for the analysis and prediction of nuclear reactions and is based on state-of-art nuclear structure and nuclear reaction models. A general overview of the implemented physics and capabilities of TALYS is given. The general nuclear reaction mechanisms described are the optical model, direct reactions, compound nucleus model, pre-equilibrium reactions and fission. The most important nuclear structure models are those for masses, discrete levels, level densities, photon strength functions and fission barriers. A wide variety of nuclear reactions simulated with TALYS will be demonstrated, ranging from low-energy neutron cross sections, astrophysics, high-energy charged particle reactions and other reactions. TALYS is a nuclear reaction software which aims to give a complete description of nuclear reaction observables, and to be an important link between fundamental nuclear physics and applications.

TALYS around the World (status 2022)

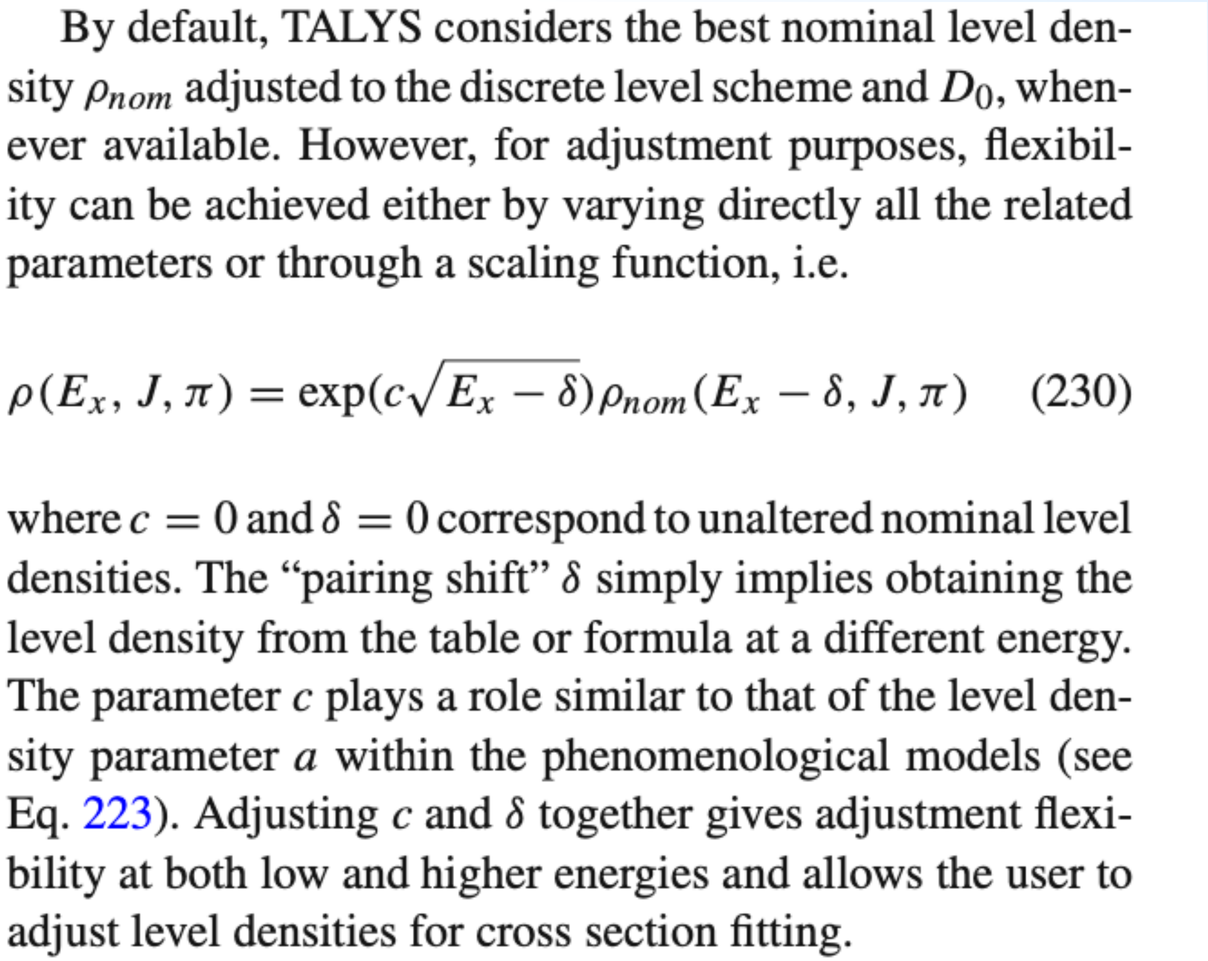
- Around 5500 citations (web of sciences)



Could this be the future?

- More harmonisation between nuclear model codes:
  - Only tabulated level densities are provided, even if they come from analytical models
  - Easy API, e.g. get_level_density(Z=21, A=45, Emin=0., Emax=200., model=‘CTM’, number_of_energies=500, etc.)
    - …possibly in different languages (Python, C++, Fortran etc.)
  - Well-established tweaking (parameter adjustment) possibilities

Parameter adjustment



By default, TALYS considers the best nominal level density ρ_{nom} adjusted to the discrete level scheme and D_0, whenever available. However, for adjustment purposes, flexibility can be achieved either by varying directly all the related parameters or through a scaling function, i.e.

$$\rho(E_x, J, \pi) = \exp(c\sqrt{E_x - \delta})\rho_{nom}(E_x - \delta, J, \pi) \tag{230}$$

where $c = 0$ and $\delta = 0$ correspond to unaltered nominal level densities. The "pairing shift" δ simply implies obtaining the level density from the table or formula at a different energy. The parameter c plays a role similar to that of the level density parameter a within the phenomenological models (see Eq. 223). Adjusting c and δ together gives adjustment flexibility at both low and higher energies and allows the user to adjust level densities for cross section fitting.

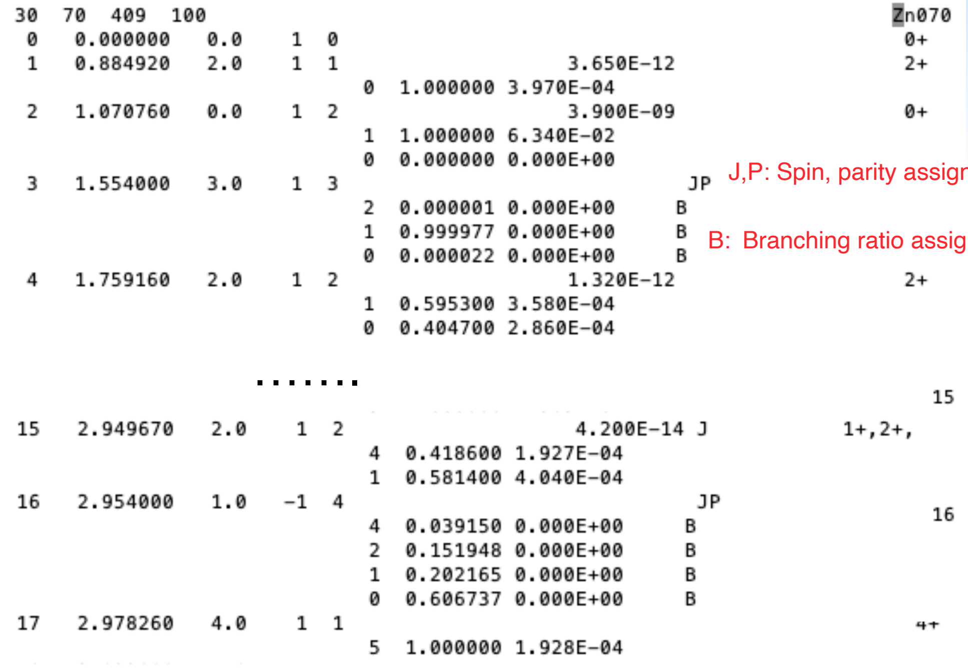
Eq. (230) appropriate for Fermi gas range but not for constant T range

Should be extended by adjustment of the spin distribution (is already in latest version of TALYS)

Is applicable to both microscopic and analytic LD's

TALYS discrete levels for Zn070 (RIPL-based)

Experimental

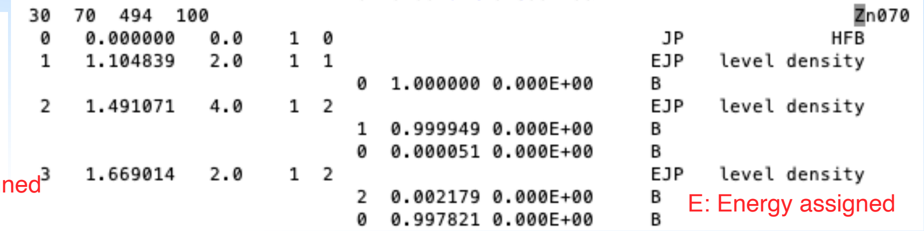


```
30   70   409   100                                                    Zn070
 0    0.000000    0.0     1  0                                          0+
 1    0.884920    2.0     1  1                     3.650E-12            2+
                              0  1.000000 3.970E-04
 2    1.070760    0.0     1  2                     3.900E-09            0+
                              1  1.000000 6.340E-02
                              0  0.000000 0.000E+00
 3    1.554000    3.0     1  3                            JP
                              2  0.000001 0.000E+00      B
                              1  0.999977 0.000E+00      B
                              0  0.000022 0.000E+00      B
 4    1.759160    2.0     1  2                     1.320E-12            2+
                              1  0.595300 3.580E-04
                              0  0.404700 2.860E-04

                     .......

15   2.949670   2.0     1  2                     4.200E-14 J          1+,2+,
                              4  0.418600 1.927E-04
                              1  0.581400 4.040E-04
16   2.954000   1.0    -1  4                            JP
                              4  0.039150 0.000E+00      B
                              2  0.151948 0.000E+00      B
                              1  0.202165 0.000E+00      B
                              0  0.606737 0.000E+00      B
17   2.978260   4.0     1  1                                            4+
                              5  1.000000 1.928E-04
```

J,P: Spin, parity assigned

B: Branching ratio assigned

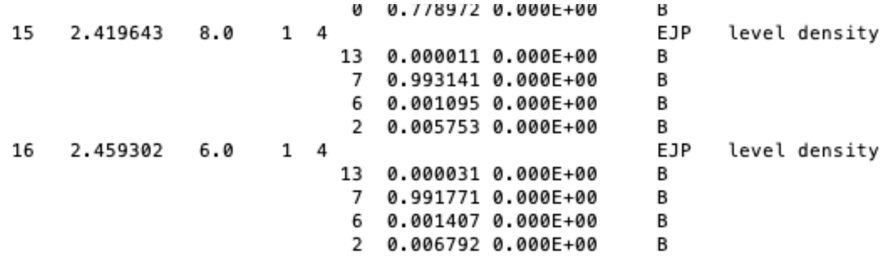
Theoretical



```
30   70   494   100                                                    Zn070
 0    0.000000    0.0     1  0                            JP          HFB
 1    1.104839    2.0     1  1                            EJP   level density
                              0  1.000000 0.000E+00      B
 2    1.491071    4.0     1  2                            EJP   level density
                              1  0.999949 0.000E+00      B
                              0  0.000051 0.000E+00      B
 3    1.669014    2.0     1  2                            EJP   level density
                              2  0.002179 0.000E+00      B
                              0  0.997821 0.000E+00      B
```

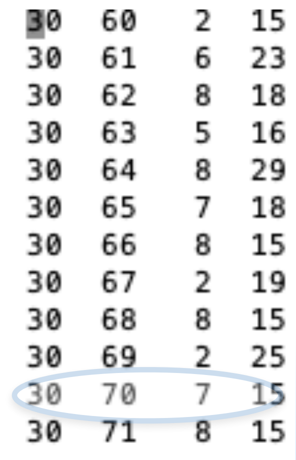
E: Energy assigned

....



```
                              0  0.778972 0.000E+00      B
15   2.419643   8.0     1  4                            EJP   level density
                             13  0.000011 0.000E+00      B
                              7  0.993141 0.000E+00      B
                              6  0.001095 0.000E+00      B
                              2  0.005753 0.000E+00      B
16   2.459302   6.0     1  4                            EJP   level density
                             13  0.000031 0.000E+00      B
                              7  0.991771 0.000E+00      B
                              6  0.001407 0.000E+00      B
                              2  0.006792 0.000E+00      B
```

Nlow Ntop



```
30   60    2   15
30   61    6   23
30   62    8   18
30   63    5   16
30   64    8   29
30   65    7   18
30   66    8   15
30   67    2   19
30   68    8   15
30   69    2   25
30   70    7   15
30   71    8   15
```

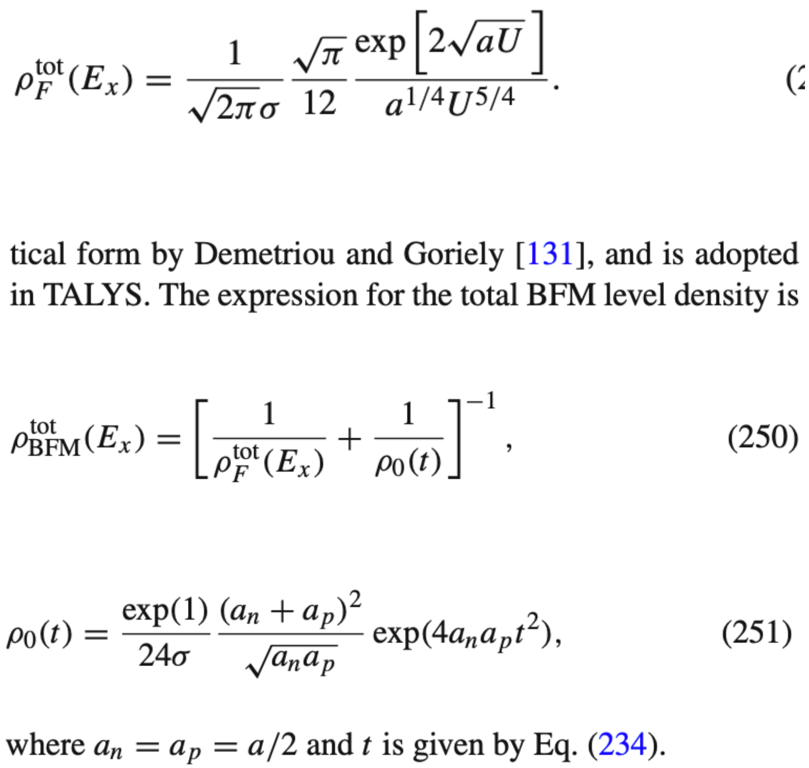
Above Ntop, cumulative discrete levels start to underestimate LD's

Experimental levels above Ntop are not taken into account in Hauser-Feshbach calculations, while their E, J, P, B are valuable.

Origin of theoretical levels: As soon as integral dEx.rho(Ex,J,P) crosses an integer number, assign a level at that energy

Possibility: merge and mix experimental and theoretical levels for each nuclide from Ntop - N=200? Which LD model?

Room for a phenomenological model intermediate between CTM (4 parameters) and BSFM (2 parameters)?



$$\rho_F^{\mathrm{tot}}(E_x) = \frac{1}{\sqrt{2\pi}\sigma}\frac{\sqrt{\pi}}{12}\frac{\exp\left[2\sqrt{aU}\right]}{a^{1/4}U^{5/4}}. \qquad (2$$

tical form by Demetriou and Goriely [131], and is adopted in TALYS. The expression for the total BFM level density is

$$\rho_{\mathrm{BFM}}^{\mathrm{tot}}(E_x) = \left[\frac{1}{\rho_F^{\mathrm{tot}}(E_x)} + \frac{1}{\rho_0(t)}\right]^{-1}, \qquad (250)$$

$$\rho_0(t) = \frac{\exp(1)}{24\sigma}\frac{(a_n+a_p)^2}{\sqrt{a_n a_p}}\exp(4a_n a_p t^2), \qquad (251)$$

where $a_n = a_p = a/2$ and t is given by Eq. (234).

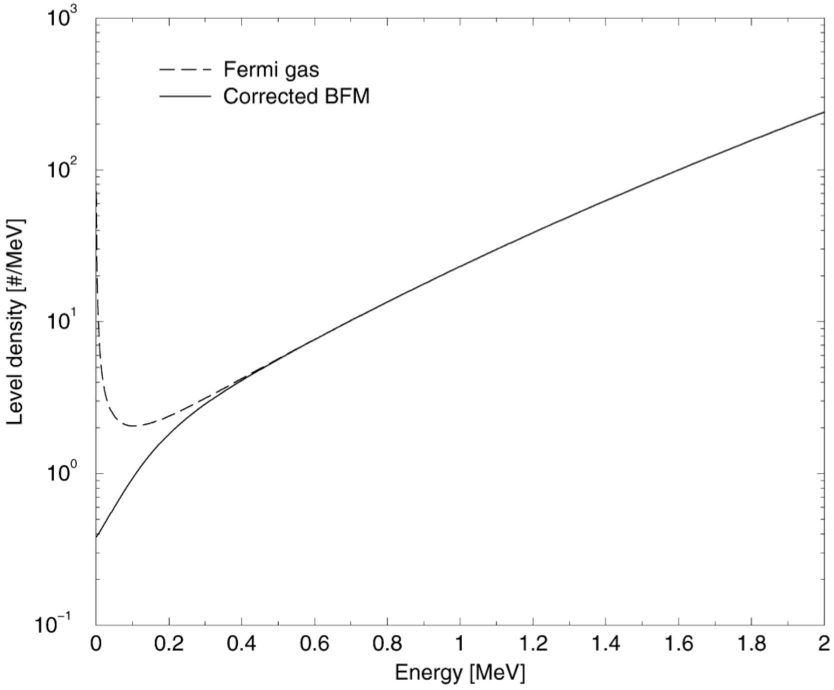


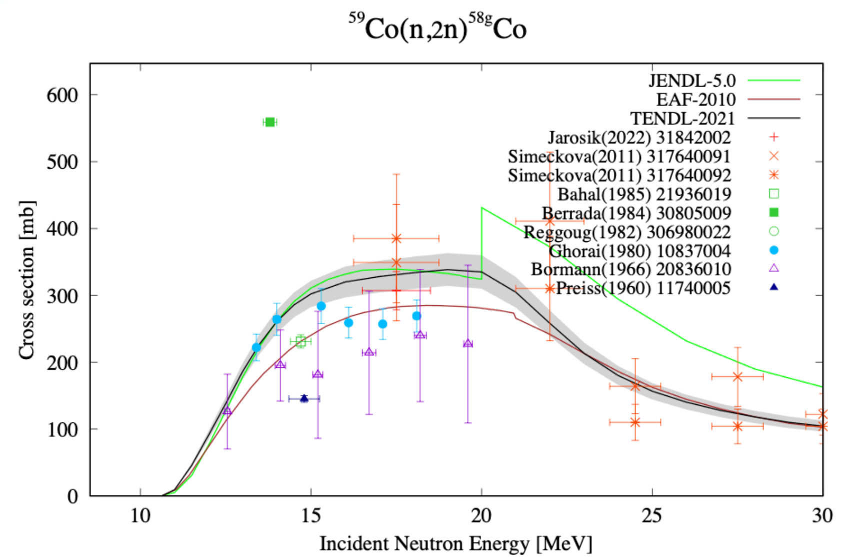
Fig. 1. Grossjean–Feldmeier correction of the Fermi gas formula at low energies for a medium mass nuclide with $a = 15\ \mathrm{MeV}^{-1}$.

Can one make e.g. ’t’ in Eq. (251) adjustable to mimic a constant temperature effect?

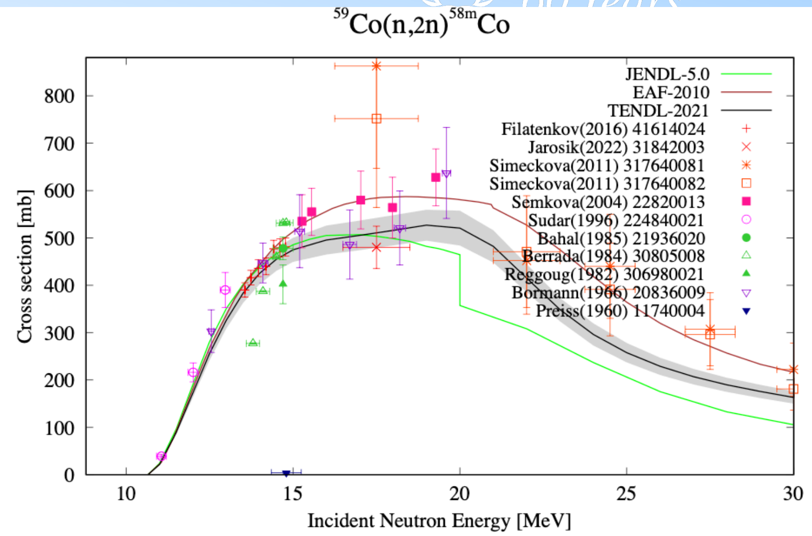
Validation of level density spin distribution

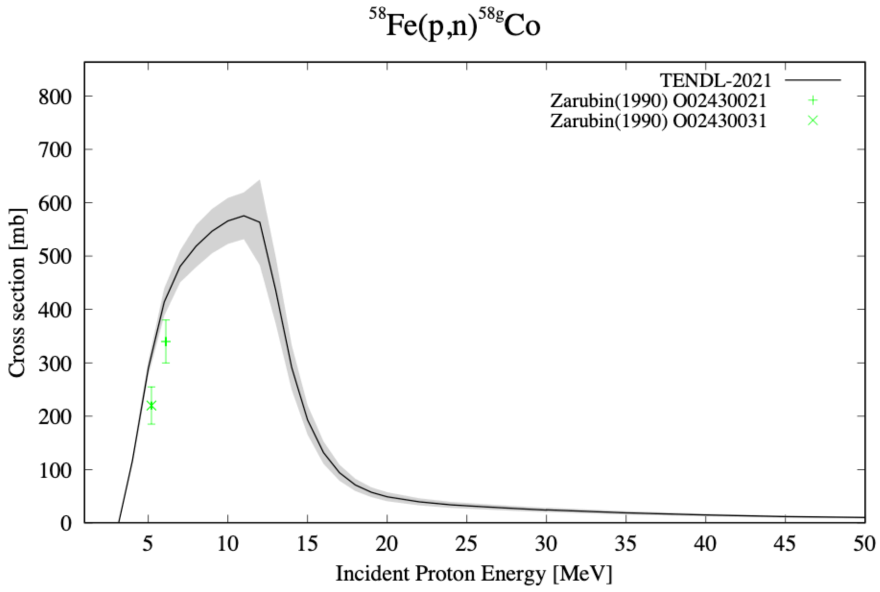
- Isomeric ratios of cross sections
- Gamma-ray production cross sections

Isomeric cross section ratios

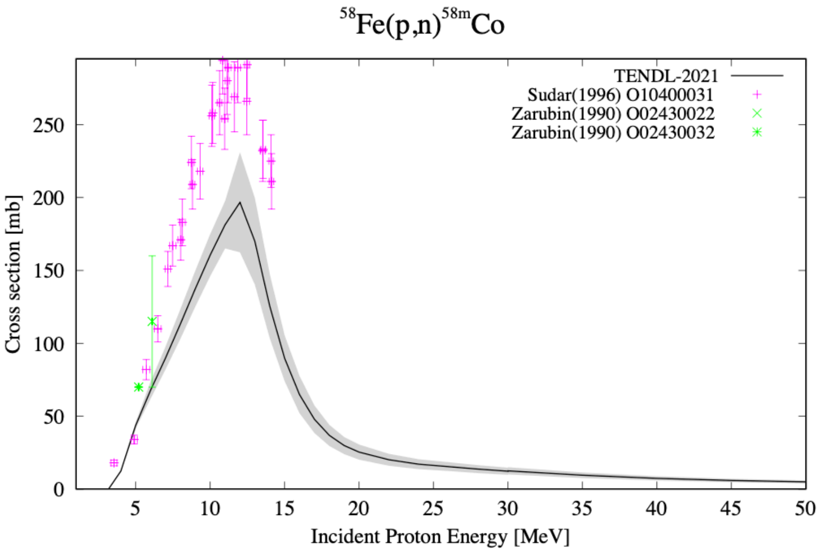


Good



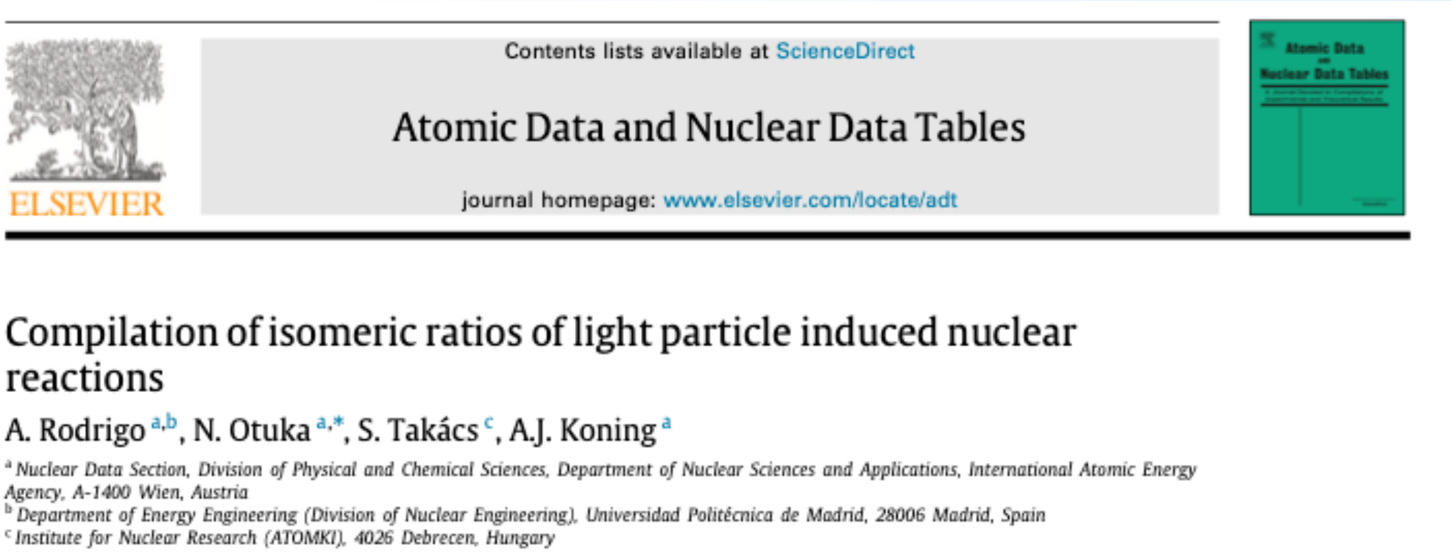


Bad



Two sensitive inputs: 1. (Missing) spins and branching ratios of discrete level scheme
2. Width of the level density spin distribution

Isomeric cross section ratios



Contents lists available at ScienceDirect

Atomic Data and Nuclear Data Tables

journal homepage: www.elsevier.com/locate/adt

Compilation of isomeric ratios of light particle induced nuclear reactions

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[b] Department of Energy Engineering (Division of Nuclear Engineering), Universidad Politécnica de Madrid, 28006 Madrid, Spain
[c] Institute for Nuclear Research (ATOMKI), 4026 Debrecen, Hungary

Averaged over all nuclides and reactions:

Spin cutoff factor could be multiplied by 0.4 - 0.6 to get global best result

Similar required reduction observed for fission yields, and other work, Sudar 2018, Uppsala, to be published, etc.)

A new level density model should have the best result automatically!

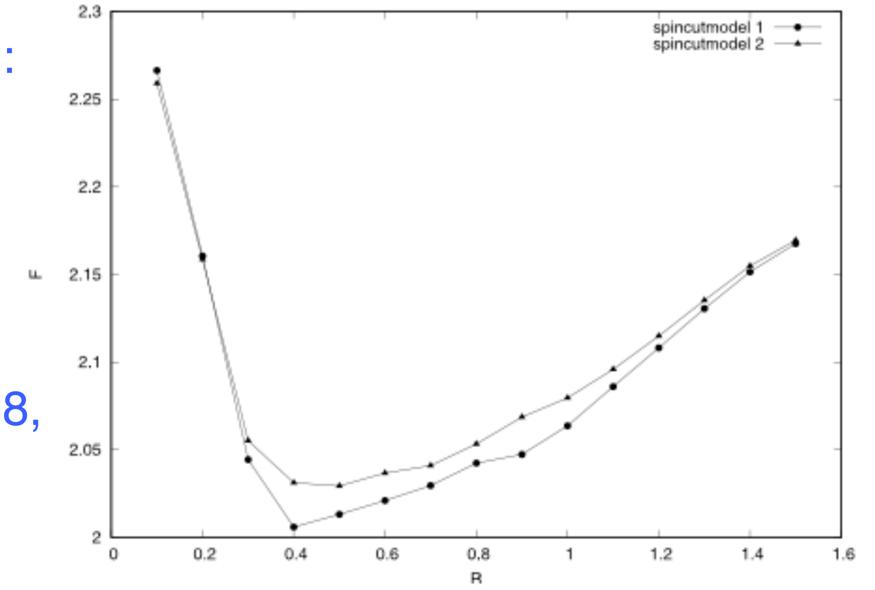

Fig. 3. *R* dependence of the *F*-value for the isomeric ratios predicted by TALYS-1.96 with two spin cut-off models.

Gamma-ray production cross sections

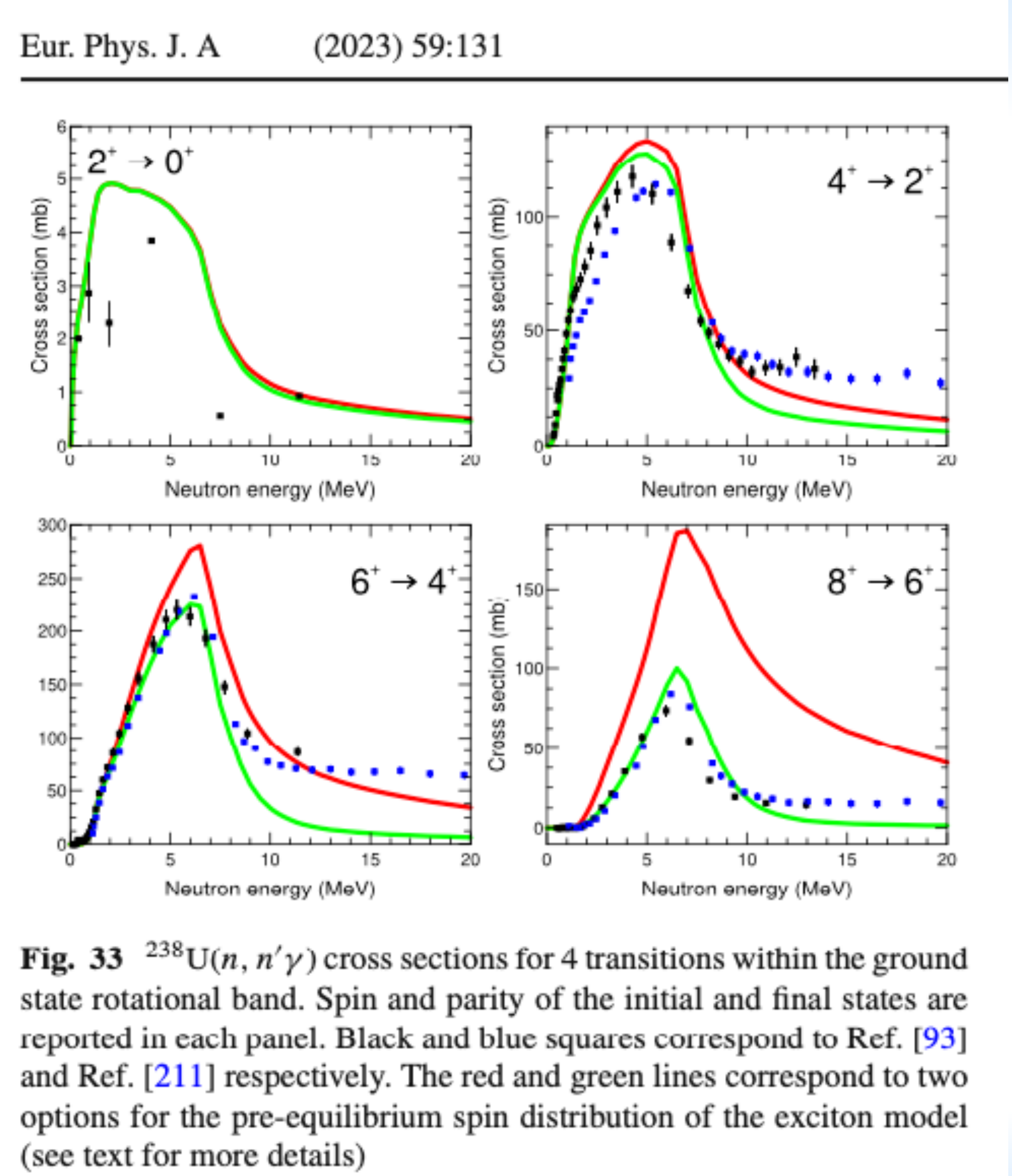

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Fig. 33 ^{238}U$(n, n'\gamma)$ cross sections for 4 transitions within the ground state rotational band. Spin and parity of the initial and final states are reported in each panel. Black and blue squares correspond to Ref. [93] and Ref. [211] respectively. The red and green lines correspond to two options for the pre-equilibrium spin distribution of the exciton model (see text for more details)

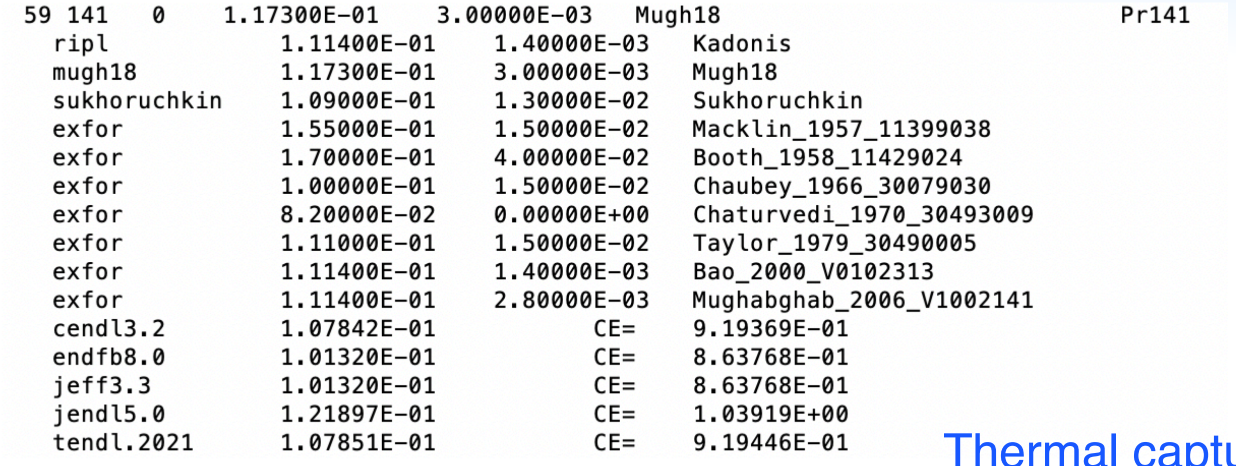
Two effects:

Particle-hole state density spin distribution (this example)

Total level density spin distribution

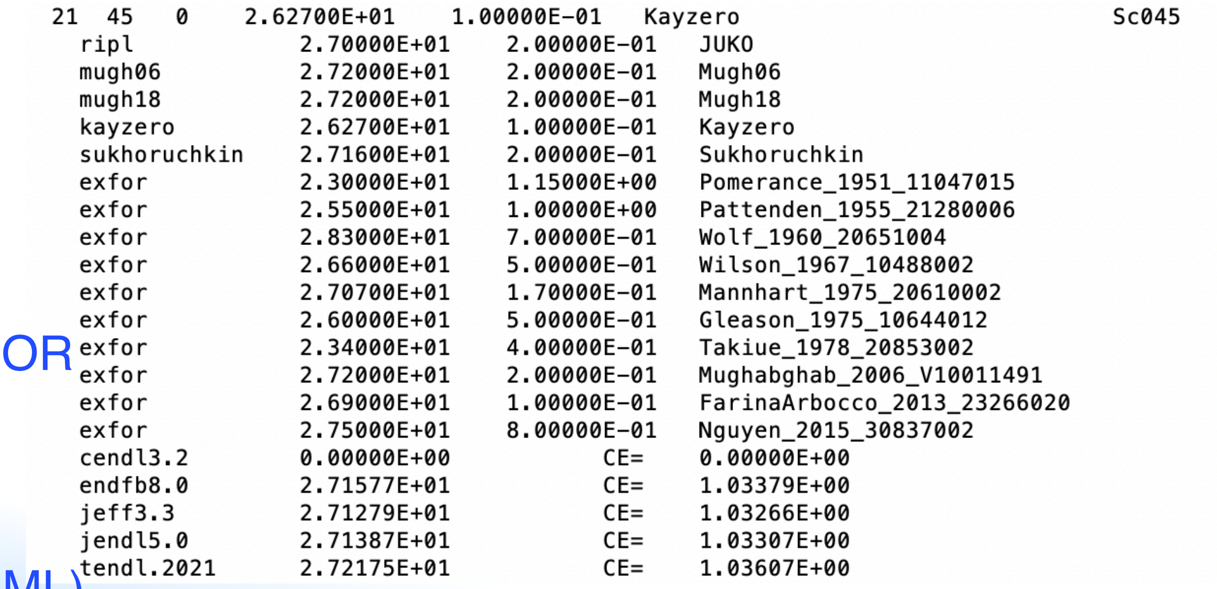
Completeness of compilations/evaluations

MACS



```
59 141    0     1.17300E-01     3.00000E-03    Mugh18                            Pr141
   ripl              1.11400E-01     1.40000E-03    Kadonis
   mugh18            1.17300E-01     3.00000E-03    Mugh18
   sukhoruchkin      1.09000E-01     1.30000E-02    Sukhoruchkin
   exfor             1.55000E-01     1.50000E-02    Macklin_1957_11399038
   exfor             1.70000E-01     4.00000E-02    Booth_1958_11429024
   exfor             1.00000E-01     1.50000E-02    Chaubey_1966_30079030
   exfor             8.20000E-02     0.00000E+00    Chaturvedi_1970_30493009
   exfor             1.11000E-01     1.50000E-02    Taylor_1979_30490005
   exfor             1.11400E-01     1.40000E-03    Bao_2000_V0102313
   exfor             1.11400E-01     2.80000E-03    Mughabghab_2006_V1002141
   cendl3.2          1.07842E-01            CE=     9.19369E-01
   endfb8.0          1.01320E-01            CE=     8.63768E-01
   jeff3.3           1.01320E-01            CE=     8.63768E-01
   jendl5.0          1.21897E-01            CE=     1.03919E+00
   tendl.2021        1.07851E-01            CE=     9.19446E-01
```

Thermal capture cross section

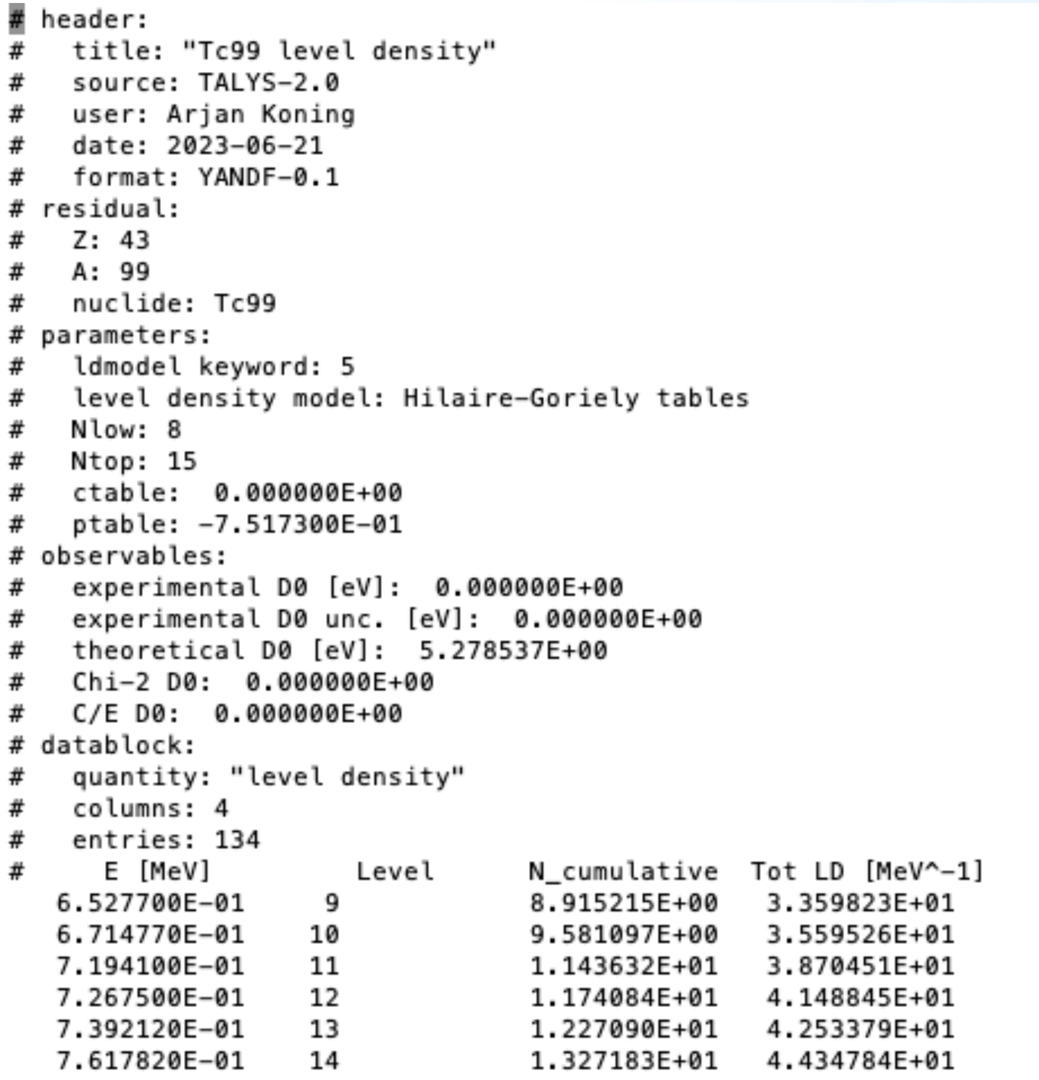


```
21  45    0      2.62700E+01     1.00000E-01    Kayzero                           Sc045
   ripl              2.70000E+01     2.00000E-01    JUKO
   mugh06            2.72000E+01     2.00000E-01    Mugh06
   mugh18            2.72000E+01     2.00000E-01    Mugh18
   kayzero           2.62700E+01     1.00000E-01    Kayzero
   sukhoruchkin      2.71600E+01     2.00000E-01    Sukhoruchkin
   exfor             2.30000E+01     1.15000E+00    Pomerance_1951_11047015
   exfor             2.55000E+01     1.00000E+00    Pattenden_1955_21280006
   exfor             2.83000E+01     7.00000E-01    Wolf_1960_20651004
   exfor             2.66000E+01     5.00000E-01    Wilson_1967_10488002
   exfor             2.70700E+01     1.70000E-01    Mannhart_1975_20610002
   exfor             2.60000E+01     5.00000E-01    Gleason_1975_10644012
   exfor             2.34000E+01     4.00000E-01    Takiue_1978_20853002
   exfor             2.72000E+01     2.00000E-01    Mughabghab_2006_V10011491
   exfor             2.69000E+01     1.00000E-01    FarinaArbocco_2013_23266020
   exfor             2.75000E+01     8.00000E-01    Nguyen_2015_30837002
   cendl3.2          0.00000E+00            CE=     0.00000E+00
   endfb8.0          2.71577E+01            CE=     1.03379E+00
   jeff3.3           2.71279E+01            CE=     1.03266E+00
   jendl5.0          2.71387E+01            CE=     1.03307E+00
   tendl.2021        2.72175E+01            CE=     1.03607E+00
```

We may need this for D0 too:

- All available values from compilations (RIPL2-3, Mugh18 and EXFOR), including the rejected values
- requires data mining from EXFOR
- show the “confidence” of the evaluation (was there only 1 choice, or 10?)
- In key-value format (JSON, YAML)

Unified level density table format?



```
# header:
#   title: "Tc99 level density"
#   source: TALYS-2.0
#   user: Arjan Koning
#   date: 2023-06-21
#   format: YANDF-0.1
# residual:
#   Z: 43
#   A: 99
#   nuclide: Tc99
# parameters:
#   ldmodel keyword: 5
#   level density model: Hilaire-Goriely tables
#   Nlow: 8
#   Ntop: 15
#   ctable:  0.000000E+00
#   ptable: -7.517300E-01
# observables:
#   experimental D0 [eV]:   0.000000E+00
#   experimental D0 unc. [eV]:   0.000000E+00
#   theoretical D0 [eV]:   5.278537E+00
#   Chi-2 D0:   0.000000E+00
#   C/E D0:   0.000000E+00
# datablock:
#   quantity: "level density"
#   columns: 4
#   entries: 134
#     E [MeV]          Level      N_cumulative   Tot LD [MeV^-1]
   6.527700E-01     9           8.915215E+00    3.359823E+01
   6.714770E-01    10           9.581097E+00    3.559526E+01
   7.194100E-01    11           1.143632E+01    3.870451E+01
   7.267500E-01    12           1.174084E+01    4.148845E+01
   7.392120E-01    13           1.227090E+01    4.253379E+01
   7.617820E-01    14           1.327183E+01    4.434784E+01
```

Just an example:

YANDF (Yet Another Nuclear Data Format), used to unify all output of TALYS and related Software

CRP on Level densities

- New D0, D1 database
- Include ‘nuclear reaction validators’:
  - Isomeric cross sections ratios
  - Gamma-ray production cross sections
  - Disentangle PSF and LD effects on e.g. MACS predictions
- Level densities for fission barriers
- Think about the best retrieval method and website.

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Thank you!