Notes and a few figures for discussion of μ-bar *vs. E* for neutron elastic scattering on actinides *at low energies*

D. Roubtsov, K. Kozier
CRL, AECL, Canada
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See presentations of T. Kawano, CSEWG-2010 (in Santa Fe, NM)
http://www.nndc.bnl.gov/proceedings/2010csewgusndp/Thursday/AFCIP/modscat-Kawano.pdf

and at WINS-2010 (Strasbourg).

In a typical ENDF/B file, for MT=2 (*i.e.*, for the elastic scattering channel of $n + A$), there are two data blocks: MF=3, MT=2 for the scattering cross sections, $\sigma_s(E)$, and MF=4, MT=2 for the scattering angular distributions, $P_s(E, \mu)$, usually given in the CM-frame and normalized to one, $\int_{-1}^{1} P_s(E, \mu)\, d\mu = 1$.

For heavy elements, CM- and LAB-frames of $n + A \rightarrow n + A$ are almost indistinguishable, *i.e.*,

$$P_s^{(CM)}(E, \mu_{CM}) \approx P_s^{(LAB)}(E, \mu_{LAB}).$$

Then, the elastic scattering differential cross section, $d\sigma_s(E, \mu)/d\Omega$, can be written as

$$d\sigma_s(E, \mu)/d\Omega = \sigma_s(E)\times P_s(E, \mu)/2\pi, \text{ in [b/sr]}.$$

There is **no** MF=6, MT=2 data block for $d^2\sigma_s(E \rightarrow E', \mu)/dE'd\Omega$ in ENDF/B files because

$$d^2\sigma_s(E \rightarrow E', \mu)/dE'd\Omega = \sigma_s(E)\times P_s(E, E', \mu)/2\pi = \sigma_s(E)\times P_s(E, \mu)\times P_s(E \rightarrow E')/2\pi,$$

i.e., $P_s(E, E', \mu) = P_s(E, \mu)\, P_s(E \rightarrow E')$. It is assumed that the energy distribution of elastic scattering $P_s(E \rightarrow E')$ is independent of μ and it follows from the kinematics (in the limit $T \rightarrow 0$ K). As $P_s(E, \mu)$ is normalized to unity, the average scattering cosine of neutron elastic scattering, μ-bar, can be calculated as follows:

$$\mu\text{-bar} = \iint \mu\times d^2\sigma_s(E \rightarrow E', \mu)/dE'd\Omega \,/\, \iint d^2\sigma_s(E \rightarrow E', \mu)/dE'd\Omega = \int_{-1}^{1} \mu\times P_s(E, \mu)\, d\mu.$$

Assume that a given ENDF/B file was processed by NJOY99 into a **fast** ACE file corresponding to a given temperature $\boldsymbol{T}$ ($\neq 0$ K). Then, $\sigma_s(E)$ is Doppler broadened, $\sigma_s(E) \rightarrow \sigma_s(E; T)$, using the resonance parameters from MF = 2 (if any).

What happens with $P_s(E, \mu)$?

In other words, how does **NJOY99** process **MF=4, MT=2** data for **MCNP(X)** ?

If $P_s(E, \mu)$ is given in the form of tables, *i.e.*, for each E_j, there is a table of k entities,

$$(\mu_{jk}, P_{s,\,jk}), \quad -1.0 \le \mu_{jk} \le 1.0,$$

then these data points are transferred to the fast ACE file *as they are* in the original ENDF/B file. Thus, NJOY99 does the following transformation:

$$\text{ENDF/B MF=4, MT=2 } (E_j, \mu_{jk}, P_{s,\,jk}) \;\rightarrow\; \textbf{ACE } (E_j, \mu_{jk}, P_{s,\,jk}, P^c_{s,\,jk}). \qquad (1)$$

Here, $P^c_{s,jk}$ is the cumulative angular distribution, $P^c_s(E, \mu) = \int_{-1}^{\mu} P_s(E, \mu')\, d\mu'$.

Note that there are **no changes**: the same grids for E_j and for μ_{jk} are in both ENDF/B MF=4, MT=2 and in the corresponding ACE part, and $P_{s,\,jk}$ and $P^c_{s,jk}$ are independent on temperature T.

If $P_s(E, \mu)$ is given in the form of Legendre polynomial expansion, *i.e.*, for each E_j, there is a 'vector' of coefficients,

$$a_{s,\,jl},\quad l = 1, \cdots, l_{max,\,j},$$

then **acer** module of NJOY99 [ptleg2] converts vectors $a_{s,\,jl}$ into tables (μ_{jk}, $P_{s,\,jk}$) by choosing an **optimal grid** of the scattering cosines μ_{jk} (for each E_j) and applying

$$P_{s,\,jk} = 1/2 + \Sigma_{l=1}\left((2l+1)/2\right) \times a_{s,\,jl} \times P_l(\mu_{jk}).$$

Therefore, NJOY99 does the following transformation:

$$\text{ENDF/B MF=4, MT=2}\ \ (E_j, a_{s,\,jl}, l_{max,\,j}) \ \rightarrow\ \textbf{ACE}\ \ (E_j, \mu_{jk}, P_{s,\,jk}, P^c_{s,jk}). \qquad (2)$$

Note that the same grid E_j is in both ENDF/B MF=4, MT=2 and in the corresponding ACE part, and $P_{s,\,jk}$ and $P^c_{s,jk}$ are independent on T.

As $P_1(\mu) = \mu$, the coefficient $a_{s,\,j1}$ (l = 1) is the μ-bar for neutron elastic scattering at E_j,

$$\mu\text{-bar}(E_j) = a_{s,\,j1}.$$

$P^c_s(E, \mu)$ data given in ACE files are useful to estimate the integral backward-to-forward scattering ratio (B2FR) *vs.* E (in the CM frame, strictly speaking):

$$\text{B2FR} = \int_{-1}^{0} P_s(E, \mu)\, d\mu \,/\, \int_0^1 P_s(E, \mu)\, d\mu = P^c_s(E, \mu = 0) \,/\, \left(1 - P^c_s(E, \mu = 0)\right).$$

One can check Figures given at https://t2.lanl.gov/nis/data/endf/endfvii-n.html under "*view PDF plots*". These plots are visualization of the typical results obtained by processing of a given ENDF/B file of ENDF/B-VII.0 into a fast ACE file (at room temperature) with NJOY99.
For ^{238}U, check Figure **36** (page 36), subtitle "*angular distribution for elastic*": this is $P_s(E, \mu)$ plotted from the data block (E_j, μ_{jk}, $P_{s,\,jk}$) calculated/processed by **NJOY99** (**acer**) from the original MF=4, MT=2 of ^{238}U.
Below, we show a similar figure for $P_s(E, \mu)$ of ^{238}U obtained from an ACER output in the energy region 1eV < E < 1.0 MeV. We used JENDL 4.0 ^{238}U because MF=4, MT=2 of this file has a better (denser) E_j grid for visualization of $P_s(E, \mu)$ at low energies.

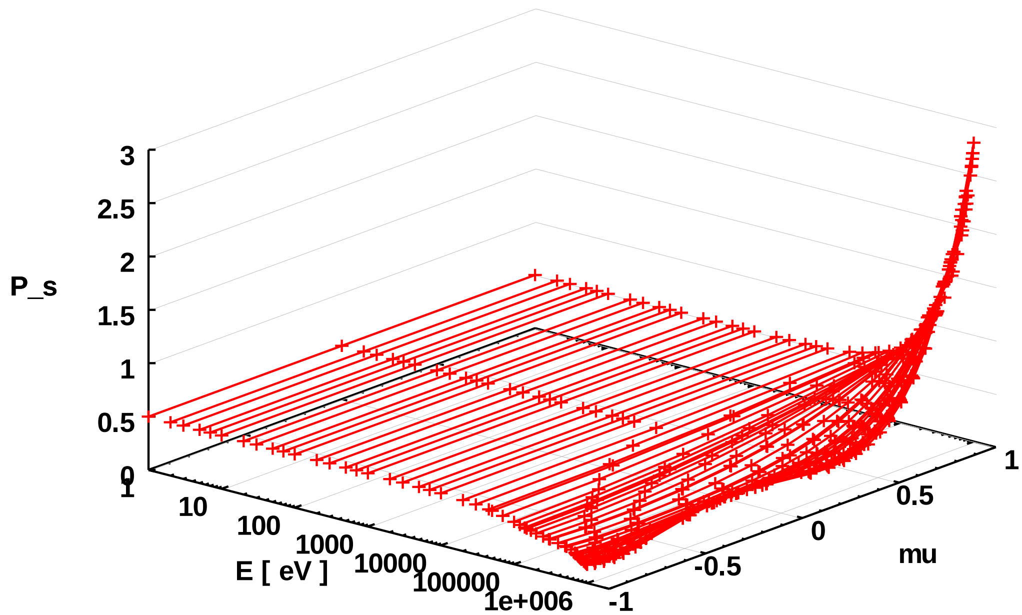

Fig. 1: $P_s(E, \mu)$ of ^{238}**U** (JENDL 4.0), 1.0 eV < E < 1.0 MeV.
Conversion from (E_j, $a_{s,\,jl}$) to (E_j, μ_{jk}, $P_{s,\,jk}$) and selection of optimal μ_{jk} are done by **acer** module of NJOY99. For example, $dim_k(\mu_{jk}) = 3$ for $E_j \leq 20.0$ keV.

As follows from Fig. 1, in the Resolved Resonance Energy Region, E < 20 keV (ENDF/B-VII.0), one can use **P1** approximation for $P_s(E, \mu)$ of ^{238}U:

$$P_s(E, \mu) \approx 1/2 + (3/2)\times\mu\text{-bar}(E)\times\mu.$$

μ-bar(E) for ^{238}U is given in Fig. 2 for low neutron energies, 1 eV < E < 0.3 MeV.

We did not find experimental data for $d\sigma_s(E, \mu)/d\Omega$ or $P_s(E, \mu)$ of ^{238}U at the incident energies E lying in the ^{238}U **RRR** in EXFOR database. The lowest energy data sets that we noticed are
E = 55 keV by Murzin-1987 and E = 75 keV by Barnard-1966, then $E \approx$ 150 keV, *etc.*, *i.e.*, the lowest energies are lying in the ^{238}U **URR**.
(EXFOR search: U-238; n,*; DA.)
Note that, at E > 50-100 keV, the **inelastic** scattering channels with excitation of the lowest levels of ^{238}U open up.

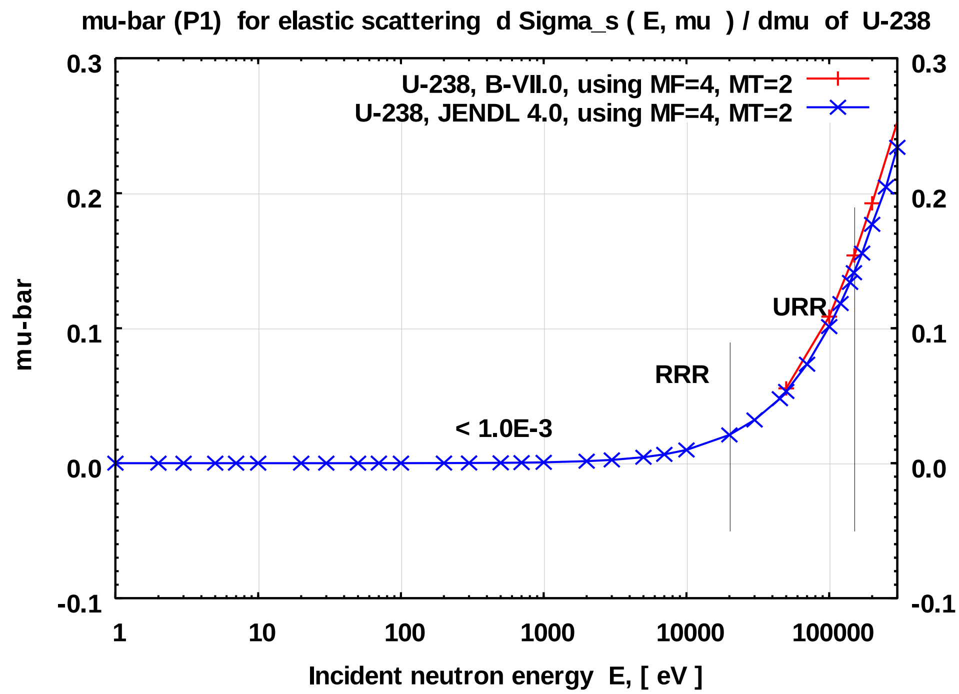

Fig. 2: μ-bar(E) for ^{238}**U**; μ-bar(E) < 10^{-3} at E < 1–2 keV;
RRR boundary: 20 keV, URR boundary: 149 keV (ENDF/B-VII.0).
(In ENDF/B-VII.0, the grid starts as $E_1 = 10^{-5}$ eV, E_2 = 50 keV, … in MF=4, MT=2 of ^{238}U.)

Similar results can be obtained for ^{232}Th.
As follows from Fig. 3, in the Resolved Resonance Energy Region, E < 4 keV (ENDF/B-VII.0), one can use P1 approximation for $P_s(E, \mu)$ of ^{232}Th:

$$P_s(E, \mu) \approx 1/2 + (3/2) \times \mu\text{-bar}(E) \times \mu.$$

μ-bar(E) for ^{232}Th is given in Fig. 4 for low neutron energies, 1 eV < E < 0.3 MeV.
Similarly, we did not find experimental data for $d\sigma_s(E, \mu)/d\Omega$ or $P_s(E, \mu)$ of ^{232}Th at the incident energies E in the ^{232}Th **RRR** in EXFOR database.
The angular distribution data in EXFOR are at E > 100 keV, *i.e*., they are even outside ^{232}Th URR (and at the incident neutron energies at which the inelastic scattering channels open up).
EXFOR search: `Th-232; n,*; DA`.
There is a paper by Samosvat-1970, "ANGULAR DISTRIBUTIONS OF SCATTERING OF 1-40 KEV NEUTRONS" with Legendre coefficients ($a_{s,\,j1}$ **?**) and E_{min} = 1.6 keV.

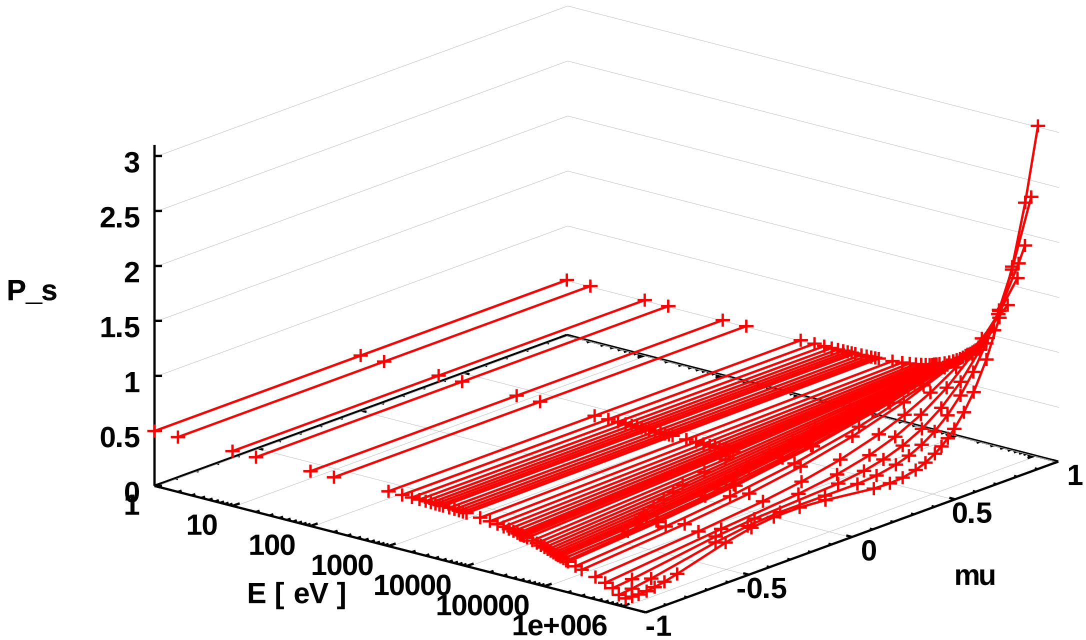

Fig. 3: $P_s(E, \mu)$ of **^{232}Th** (ENDF/B-VII.0), 1eV < E < 1.0 MeV.
Conversion from (E_j, $a_{s,\,jl}$) to (E_j, μ_{jk}, $P_{s,\,jk}$) and selection of optimal μ_{jk} are done by **acer** module of NJOY99. For example, $dim_k(\mu_{jk}) = 3$ for $E_j \leq 60$ keV.
(We added a few E_j between the original grid points, $E_1 = 10^{-5}$ eV and $E_2 = 1.0$ keV of MF=4, MT=2 of ^{232}Th to improve visual perception).

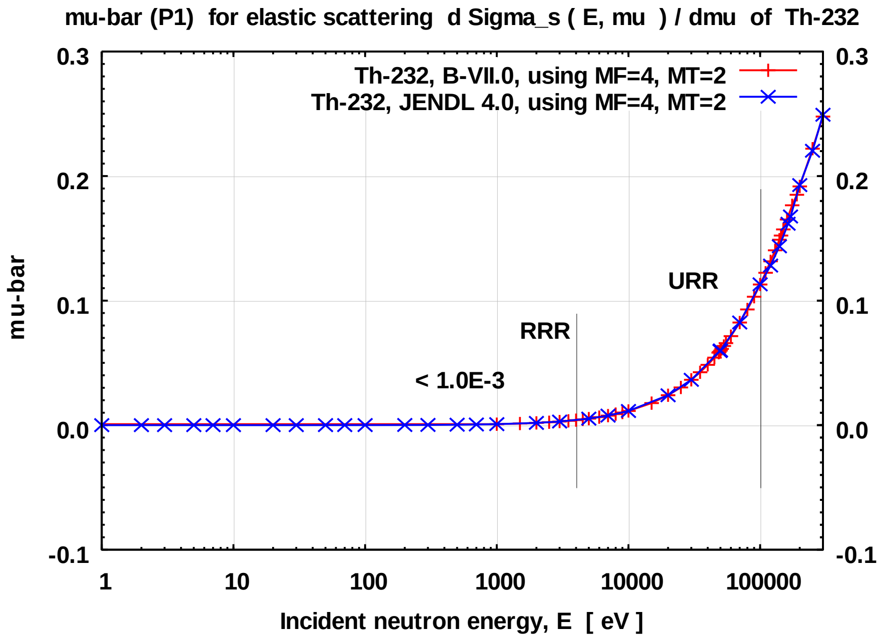

Fig. 4: μ-bar(E) for ^{232}Th; μ-bar(E) < 10^{-3} at E < 1.0-1.5 keV.
RRR boundary: 4 keV, URR boundary: 100 keV (ENDF/B-VII.0).
(In ENDF/B-VII.0, the grid starts as $E_1 = 10^{-5}$ eV, E_2 = 1.0 keV in MF=4, MT=2 of ^{232}Th.)

In Fig. 5, we show the resonance behavior of $\sigma_s(E)$ and $\sigma_{n,\gamma}(E)$ for ^{238}U and ^{232}Th at low energies, 1 eV< E < 1 keV. As σ_s *vs.* E has a pronounced ***s*-wave** resonance character at low energies, we have, roughly,

$$P_s(E, \mu) \approx 1/2,$$

i.e., nearly isotropic angular scattering distributions at low energies E < 1 keV for n + ^{238}U and n + ^{232}Th.
(**p-wave** resonances contribute to $\sigma_s(E)$ at E > 1 keV, roughly.)

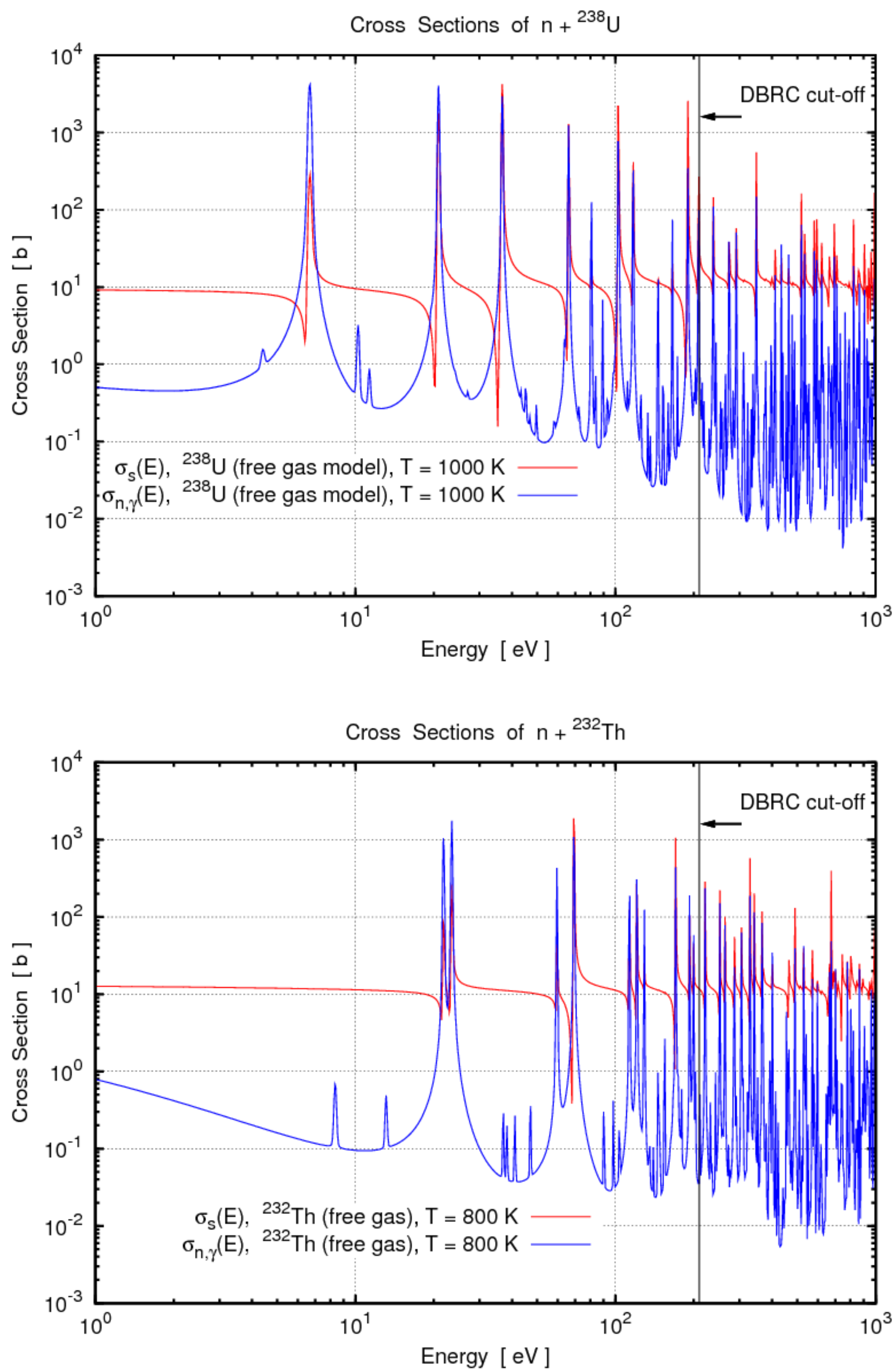

Fig. 5: low-lying neutron resonances of ^{238}U and ^{232}Th (ENDF/B-VII.0, NJOY99) at 1 eV< E < 1 keV. Almost all the low-lying **scattering** resonances of $\sigma_s(E)$ are *s*-wave type and μ-bar(E) < 10^{-3} at E < 1.0 keV. (DBRC cut-off = 210.0 eV, R. Dagan).