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Title: Some Notes on Neutron Up-Scattering and the Doppler-Broadening of High-Z Scattering Resonances

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Some Notes on Neutron Up-Scattering and the Doppler-Broadening of High-Z Scattering Resonances

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Introduction

When neutrons are scattered by target nuclei at elevated temperatures, it is entirely possible that the neutron will actually gain energy (i.e., up-scatter) from the interaction. This phenomenon is in addition to the more usual case of the neutron losing energy (i.e., down-scatter). Furthermore, the motion of the target nuclei can also cause extended neutron down-scattering, i.e., the neutrons can and do scatter to energies lower than predicted by the simple asymptotic models.

In recent years, more attention has been given to temperature-dependent scattering cross sections for materials in neutron multiplying systems. This has led to the inclusion of neutron up-scatter in deterministic codes like Partisn and to free gas scattering models for material temperature effects in Monte Carlo codes like MCNP and cross section processing codes like NJOY. The free gas scattering models have the effect of Doppler Broadening the scattering cross section output spectra in energy and angle.

The current state of Doppler-Broadening numerical techniques used at Los Alamos for scattering resonances will be reviewed, and suggestions will be made for further developments. The focus will be on the free gas scattering models currently in use and the development of new models to include high-Z resonance scattering effects. These models change the neutron up-scattering behavior.

The Asymptotic Approach to Neutron Scattering

As a backdrop to the free gas scattering models being discussed, the essential elements of the elementary asymptotic approach to neutron elastic scattering include:

(1) The target nucleus is assumed to be at rest
(2) The neutron scattering off of the target nucleus is assumed to be isotropic in the center of mass system
(3) The scattering cross section is assumed to be a constant with respect to incident neutron energy (or at least very slowly varying).

With these assumptions, no neutron up-scattering is possible and neutron down-scattering is limited to a set fraction of the incident neutron energy, $(A-1)^2/(A+1)^2$ where A is the atomic weight ratio of the target nucleus and the neutron. Furthermore, the angle of scattering has a one to one correspondence with the energy loss. The maximum energy loss for the neutron occurs for backscattering reactions and the minimum energy loss occurs with forward scattering.

Neutron Up-Scattering in Monte Carlo Calculations

The effect of the free gas scattering model is to Doppler Broaden the scattering cross sections, (specifically, the scattered neutron output spectra in energy and angle). MCNP[J1,J2] handles neutron up-scattering as an inherent part of the free gas scattering model used to model material temperature effects. The free gas model also allows neutron down-scattering beyond the $(A-1)^2/(A+1)^2$ limit of the asymptotic theory.

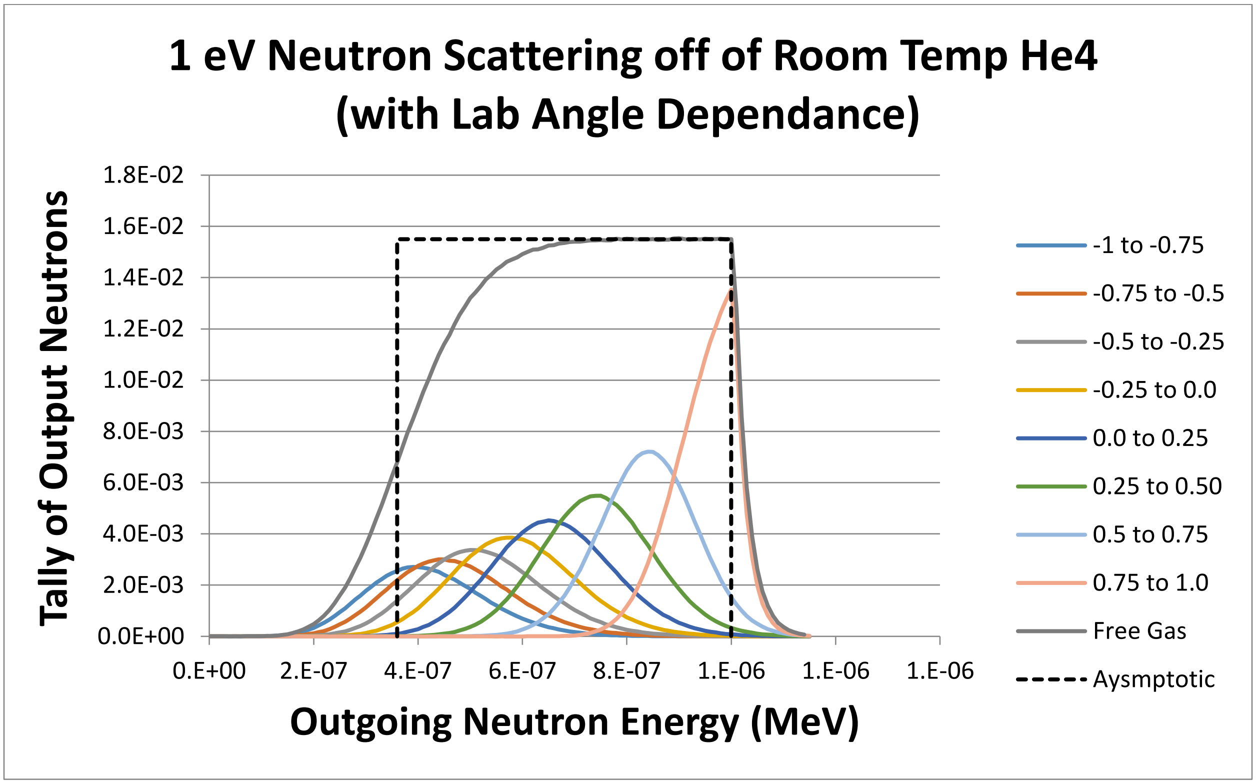

Figure 1: Neutron Scattering off of He-4 at Room Temperature

This is seen in Figure 1, where the up-scattering is seen on the high energy side of the asymptotic result and the extended down-scattering is seen on the low energy side. These results for the scattered neutron energy distributions were calculated with MCNP6 by using a pencil beam problem geometry with a given neutron energy source and tallying the once-scattered neutrons.

The broadening of the output neutron energies with respect to the angle of scattering is also seen in Figure 1. Also notice that the Asymptotic and Free Gas curves have the same integral area under their curves.

The method used in MCNP is called “Sampling the Velocity of the Target Nucleus” and it is described in the older MCNP5 manual’s chapter 2, “Geometry, Data, Physics and Mathematics” [J1]. This theoretical description is not currently in any of the MCNP6 documentation.

This MCNP up-scattering method includes more physics (e.g., the velocity of the target nucleus) than the asymptotic models (i.e., the target nucleus is assumed to be at rest) taught in introductory nuclear engineering or nuclear physics classes. The MCNP model also limits back to the simple asymptotic model when the neutron energy is much, much larger than the energy of the target nucleus. If 10 eV incident neutrons had been used in Figure 1, the free gas spectral shapes would have been much more rectangular, i.e., much more like the asymptotic shape.

In actual code practice, MCNP uses analytic formulas for neutron scattering off of Hydrogen, and the "Sampling the Velocity of the Target Nucleus" for all other materials at all temperatures as long as the incident neutron energy is less than 400 kT, where kT is the material of the target nucleus temperature in the same energy units as the neutron. When the neutron energy is 400x more than the target neutron energy, then the simpler asymptotic approach is used.

Similar to the Doppler Broadening of resonance capture cross sections, the "Sampling the Velocity of the Target Nucleus" method modifies the scattering cross section to find an effective scattering cross section which includes the effect of target nucleus motion. This is shown in equation (2.1) of the MCNP5 documentation[J1]. (Note that the MCNP5 manual equation has an incorrect *dv;* it should be a *dV* instead)

$$v(E)\sigma(E) = \iiint v_r \sigma_0(E_r) V \, dV d\Omega d\Phi \tag{1}$$

where the LHS has the lab quantities for the neutron velocity, v, and the cross section, σ,
the RHS has the quantities for the relative velocity, v_r the zero-temperature scattering cross section, σ_0, and the nucleus velocity, V.

The levels of integration are for every target nuclei velocity, V, every angle between the incident neutron velocity and the target nucleus velocity, Ω, and every center of mass scattering angle, Φ, for the collision between the neutron and the target nucleus.

The idea of equation (1) is to calculate an effective scattering cross section (dependent only on the lab energy of the neutron) by averaging over the zero-temperature scattering cross section (as a function of relative velocity), the relative velocity between the neutron and the target nucleus, and the Maxwellian distribution of target nuclei velocities at the given temperature.

In the implementation of the "Sampling the Velocity of the Target Nucleus" method, one key simplifying assumption is made; namely, the zero-temperature scattering cross section as a function of the relative velocity is assumed to be a constant. This assumption is valid in the case of down-scattering off of low-Z nuclei (e.g., hydrogen with its 20 barn cross section), but is much less valid for high-Z nuclei and their scattering resonances.

In the calculation of the effective scattering cross section, the relative velocity between the neutron and the target nucleus becomes very important. The distribution of the target nuclei velocity directions is assumed to be isotropic, hence the relative velocity can be described as in the equation just below 2.1 of the MCNP5 manual. (Note that the MCNP5 manual equation misses the subscripting of the μ_t term, it has μt.)

$$v_r = (v^2 + V^2 - 2vV\mu_t)^{1/2} \tag{2}$$

where μ_t = the cosine of the angle between the original neutron velocity, v, and the target nucleus velocity, V.

Following the development in the MCNP5 documentation, this leads to a probability distribution function of (and note that the MCNP5 documentation omits the "+" sign and uses an infinity sign for the proportionality)

$$P(V,\mu_t) \propto (v^2 + V^2 - 2vV\mu_t)^{1/2} (V^2 \exp(-\beta^2 V^2)) \qquad (3)$$

where β is defined as $((Am_n)/(2kT))^{1/2}$,
A is the atomic weight ratio,
m_n is the neutron mass,
T is the material temperature, and
$1.0/\beta$ is the most likely scalar velocity of the target nuclei in the Maxwellian distribution.

This leads to a sampling method when a rejection scheme is added to account for the impossibility or improbability of collision events for arbitrary combinations of the target nucleus velocity, the original neutron velocity, and the scattering cosine between the 2 velocities. For example, if the original neutron velocity is the same as the target velocity, and if the directions of travel are identical, then no collision can or will happen. This is a relatively rare combination, though, and the minimum efficiency for this rejection scheme is 2/3. (Note that the MCNP5 manual incorrectly gives 68% for this number.)

The minimum efficiency (lowest probability of collision) occurs when the neutron and the target nucleus have the same velocity. The 2/3 number can be calculated from the following integral, obtained from the rejection formula by assuming that the incident neutron and the target nucleus have the same velocity and integrating over all angles.

$$\text{Min. Eff.} = 1.0 / (2.0)^{1/2} * \int (1 - \mu_t)^{1/2}\, d\mu_t = 2/3 \qquad (4)$$

where the integral goes from -1.0 to 1.0.

This "Sampling the Velocity of the Target Nucleus" methodology in MCNP calculates the correct normalized magnitude for the scattering cross section and is thus approximate only in the scattering output spectra with respect to energy and angle. This approximation is due to the assumption of constant scattering cross sections.

Extension of the Monte Carlo Neutron Up-Scattering Methodology to Include Non-Constant Scattering Cross Sections

Over the years, a large number of papers have been published which document the development of techniques to extend the Doppler Broadening methodology to include the effects of non-constant scattering cross sections[A1-A10]. One method which was developed and explored for a while was to generate S(α,β) tables for the high Z target nuclei[E1-E6]. This method was shown to work correctly, but the extra effort required to calculate problem specific tables was found to be burdensome.

In more recent years, the DBRC (Doppler Broadening Rejection Correction) technique[D1-D13] has been developed for Monte Carlo codes to include the effects of non-constant scattering cross sections. Though DBRC is not currently in the production version of MCNP, it has been tested in both a branch version[D9] of MCNP5 and a branch version[D1] of MCNP6. One requirement for the implementation of the DBRC method into a Monte Carlo transport code is that the zero degree scattering cross sections for the target nucleus must be available. In MCNP, the simple expedient of including the zero degree cross sections in a material card and in a tally satisfies this requirement.

The DBRC adds another rejection criterion to the MCNP "Sampling the Velocity of the Target Nucleus" methodology. The zero-temperature scattering cross section is not assumed to be a constant in equation 1 and an additional rejection scheme is employed to account for the non-constant cross sections. Because of the spiky nature of cross section shapes near resonance energies, this rejection scheme can become quite inefficient. There are methods available[D3] to ameliorate this inefficiency, but at present, they are not available in MCNP.

With the DBRC scheme, MCNP calculates not only the correct normalized magnitude for the scattering cross sections but also the correct scattering output spectra of energy and angle. Furthermore, in the absence of neutron scattering resonances, the DBRC limits back to the free gas scattering model.

The general effect of the resonance scattering is to enhance the scattering of neutrons towards the scattering resonance energies – where at least for the large low-lying resonances of U-238 and Pu-240 – the peak energies of the scattering and capture resonances coincide. Thus, the parasitic neutron capture is enhanced. This effect is well-known in the LEU reactor world and is sometimes known as the Doppler Defect. For a typical LWR, this reactivity effect is in the 10's or a few 100's of PCM, where 1 PCM is 0.00001 in k_{eff}.

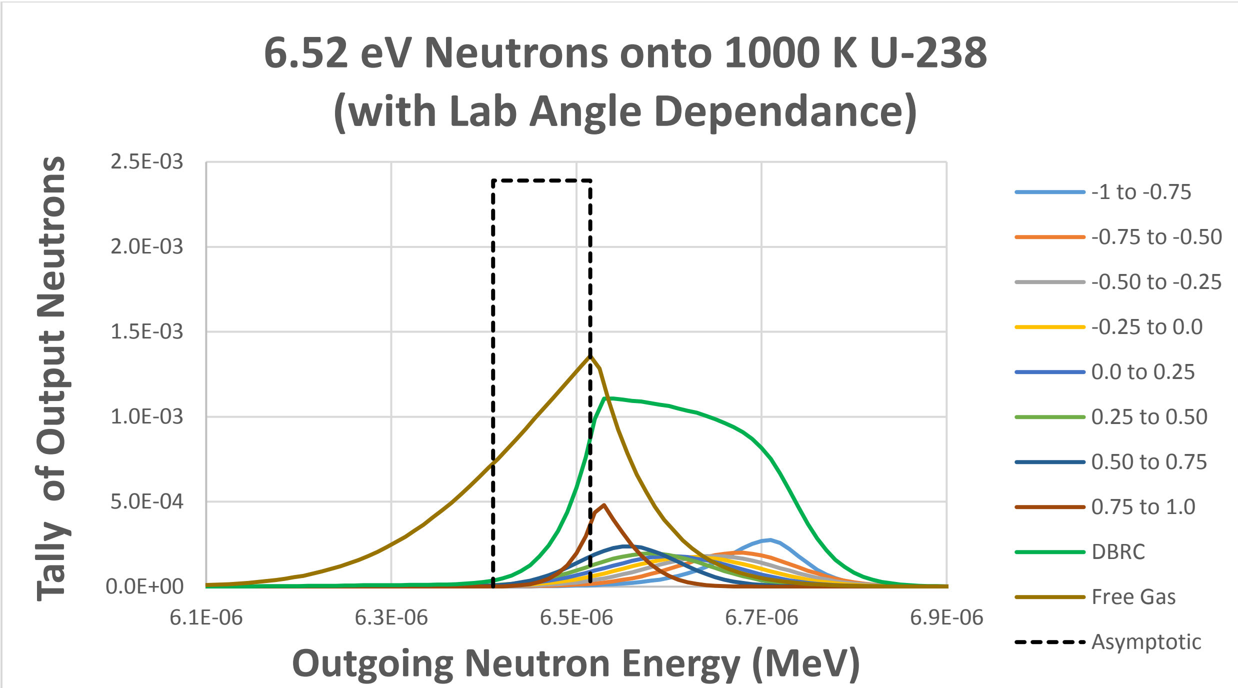

Figure 2: Neutron Scattering off of 1000 K U-238

A sample DBRC result is shown in Figure 2.

There is a big U-238 scattering resonance at 6.67 eV, and the DBRC result clearly shows its influence on the scattering output distribution in energy. Up-scatter is actually the most likely result for the collisional event, despite the relatively low material temperature.

This up-scatter effect is generally seen for neutron incident energies just **below** any big scattering resonance. Also notice that the directionality of the lab scattering angle is reversed with respect to the normal (non-resonance) situation. Back-scattered ($\mu < 0$) neutrons come out at higher energies than do the forward-scattered ($\mu > 0$) neutrons for this specific case of the incident neutron energy being just **below** a big scattering resonance.

When the neutron incident energy is just **above** a big scattering resonance, then the down-scattering is enhanced, but the directionality is the same as the normal (non-resonance) situation. Back-scattered neutrons come out at lower energies than do the forward-scattered neutrons.

Angular Distribution of Scattered Neutrons in Monte Carlo Calculations

In the asymptotic approach to neutron scattering, scattering events are assumed to be isotropic in the center of mass system. For low Z targets, the resultant lab scattering is not isotropic. However, for high Z target nuclei, the resultant lab scattering is still nearly isotropic. Even though this lab scattering is nearly isotropic in an integral sense, it is not isotropic with respect to the detailed outgoing neutron energy.

In the free gas scattering and DBRC models, some differences in angular dependence are seen.

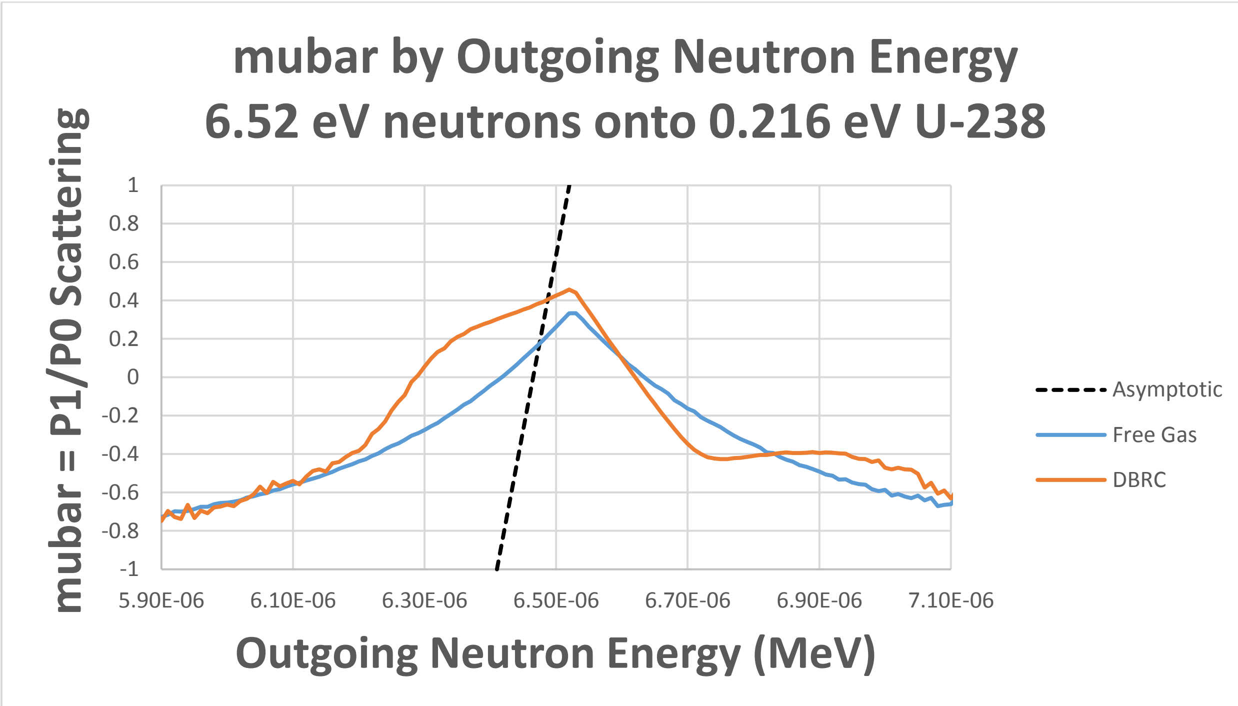

Figure 3: mubar as a Function of Outgoing Neutron Energy

mubar is the ratio of the P1 component of scattering to the P0 component. In Figure 3, the dependence of the average lab scattering angle with respect to the outgoing neutron energy is seen for all 3 models. The effects of the scattering resonance at 6.67 eV in U-238 can be seen on mubar for the case of DBRC. Thus, the scattering resonance affects the angular distribution of the scattered neutrons.

It is also noted that the most forward scattering (maximum mubar) always occurs for neutron self-scatter (i.e., no energy change).

Neutron Up-Scattering in the Cross Section Processing for Deterministic Calculations

In contrast to Monte Carlo methods where the up-scattering physics is carried out in the transport calculation, the up-scattering physics in deterministic methods is carried out in the neutron cross section processing codes (e.g., in NJOY[J4]) and the results are then included in the multi-group cross sections used by the transport codes (e.g., Partisn[J3]). However, the two basic approaches of free gas scattering (with and without resonance scattering effects) are still present in deterministic methods.

For neutron up-scattering without high-Z resonance effects, NJOY uses a free gas scattering approach taken from the inelastic incoherent scattering methodology in THERMR. Like MCNP's methodology, this includes the velocity of the target nuclei and it also limits back to the asymptotic approach when the incident neutron energy is much, much greater than the target nucleus energy.

In actual code practice, NJOY uses free gas scattering (with up-scattering) for incident neutron energies up to 10 eV for all materials at temperatures less than 3000 K. For materials at temperatures higher than 3000 K, NJOY uses free gas scattering for incident neutron energies up to 38.68 * the material temperature. Otherwise, the asymptotic approach is used in NJOY, except that NJOY does not require the neutron scattering in the center of mass to be isotropic. It uses the actual non-isotropic center of mass ENDF scattering data if such data is available for the target nucleus.

When the material temperature is greater than 3000 K, the 10 eV maximum energy for free gas scattering is scaled upward by the following quantity:

$$\text{Matl Temp}(eV) * 11604.5(K/eV) \,/\, 3000(K) \tag{5}$$

where the units are given in parentheses.

There is a minor typo in the NJOY documentation (including the most recent manual[J4]) in regards to the energy grid scaling performed by THERMR. The energy grid is used to calculate the free gas scattering quantities of interest. The top of the new scaled energy grid is:

$$\text{OLD EGRID(NGRID)} * \text{Matl Temp} \,/\, 293.6 \tag{6}$$

where NGRID is the number of points (117) in the energy grid,
EGRID(NGRID) is the highest energy point on the grid,
OLD EGRID(NGRID) = 10 eV, and
the material temperature is in degrees K.

The NJOY documentation gives an incorrect value of 300 K in equation (6) and also states that EMAX is scaled in the same way. The maximum value, EMAX, for free gas scattering (including up-scattering) is actually scaled upward by the quantity shown in Equation (5).

This energy grid scaling number will be approximately 10x larger that the transition energy, EMAX, between the asymptotic and the free gas scattering models. Thus, THERMR calculates scattering for one more decade of incident neutron energies than are actually needed by GROUPR. However, the user can extend the up-scattering range in GROUPR by increasing the user input EMAX to values higher than 10 eV. A value of 100 eV would establish a criterion very much like MCNP's 400x (actually 386.82x) the material temperature and would still be within the range of values calculated by THERMR.

Values for the user input of EMAX less than 10 eV are appropriate for thermal scattering situations when $S(\alpha,\beta)$ tables are used. However, such low values in an elevated temperature up-scattering context limit the energy grid scaling performed in THERMR. This is done by truncating the EGRID at the value corresponding to the user supplied EMAX and also thus limiting the free gas scattering model application in GROUPR to lower multiples (< 38.68) of the material temperature. The effective OLD EGRID(NGRID) becomes OLD EGRID(some value < NGRID) and thus the 10 eV implicit in Equation 5 becomes the user-supplied EMAX < 10 eV. The EMAX input in the THERMR module of NJOY is thus overloaded and should probably be replaced by 2 variables; one for thermal scattering at very low neutron energies and one for neutron up-scattering at elevated material temperatures.

In NJOY, the effective scattering cross section is calculated using an $S(\alpha,\beta)$ approach, where α and β are dimensionless quantities related to the change in momentum and the change in energy, respectively, of the scattered neutron.

$$\alpha = (E' - E + 2\,\mu_t\,(E'E)^{1/2}) / AkT \qquad (7)$$

$$\beta = (E' - E) / kT \qquad (8)$$

where E is the incident neutron energy
E' is the outgoing neutron energy
A is the atomic weight ratio of the scattered nucleus mass to the neutron mass
kT is the material temperature expressed in the same energy units as E and E'.

β is thus negative for neutron down-scattering and positive for neutron up-scattering. Also note that for high Z (i.e., large A) targets, β will generally be larger than α.

As coded in the THERMR routine of NJOY, the free gas $S(\alpha,\beta)$ kernel used to calculate cross sections is

$$S(\alpha,\beta) = \exp(\,-\,(\alpha+\beta)^2/(4\alpha)\,) / (4\pi\alpha)^{1/2} \qquad (9)$$

However, the symmetric form in which the free gas thermal scattering kernel data is stored in ENDF is

$$SS(\alpha,\beta) = \exp(\,-\,(\alpha^2+\beta^2)/(4\alpha)\,) / (4\pi\alpha)^{1/2} \qquad (10)$$

where

$$S(\alpha,\beta) = SS(\alpha,\beta) * \exp(-\beta/2) = SS(\alpha,\beta) * \exp(-2\alpha\beta/4\alpha) \qquad (11)$$

For large values of β, the $S(\alpha,\beta)$ form used to calculate cross sections in Equation (10) has potential numerical precision problems with the $\exp(-\beta/2)$ term in Equation (11). Large values of $|\beta|$ also generally correspond with the conditions of the asymptotic approach, i.e., a large neutron energy relative to the nucleus energy.

An un-normalized shape of the scattered neutron energy distribution can be determined by the integrating the following partial equation over all angles for a given incident neutron energy of E:

$$f(E') \propto \int ((E'/E)^{1/2} * S(\alpha,\beta))\, d\mu_t \qquad (12)$$

As for the angular distribution of scattered neutrons from the NJOY free gas scattering, the shape is determined for given values of E and E' (since the μ_t dependence is buried in the α term):

$$f(\mu_t) \propto \; S(\alpha,\beta) \qquad (13)$$

Since μ_t is already in the lab coordinate system, calculations of Legendre coefficients appropriate for multi-group scattering cross sections are fairly straightforward.

A sample NJOY result for free gas scattering is shown in Figure 4:

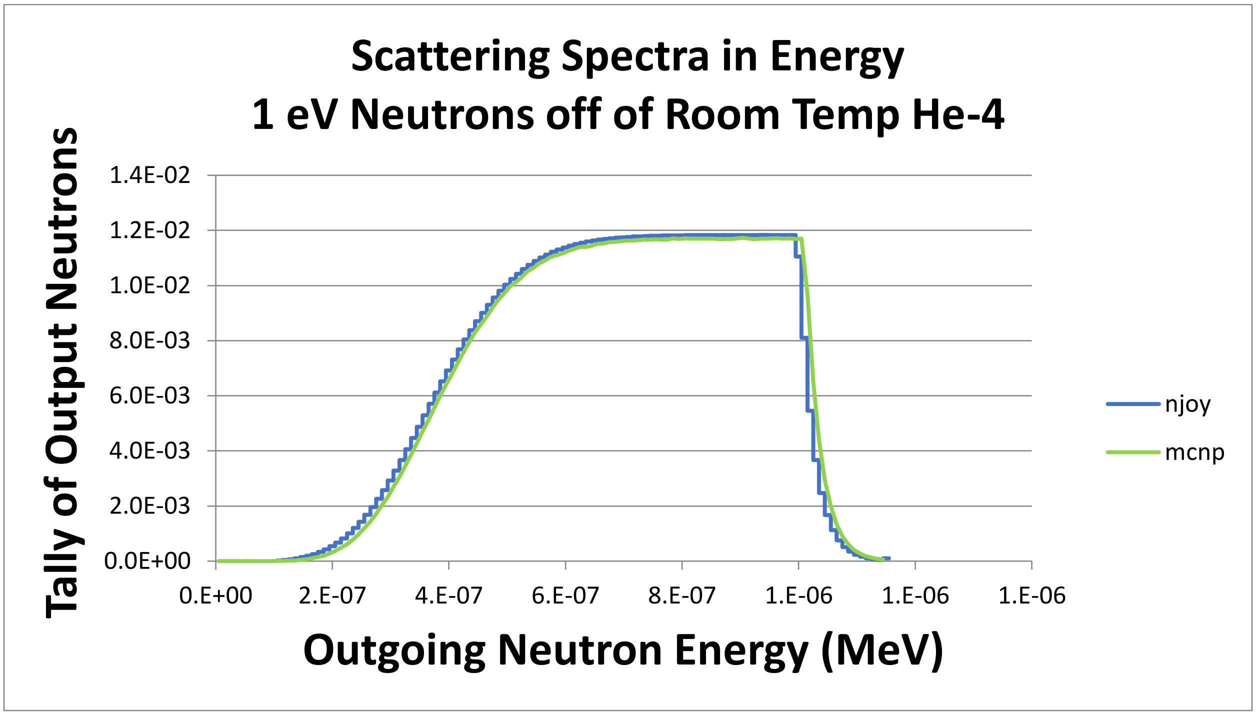

Figure 4: Comparison of MCNP and NJOY Scattering Spectra for He-4

The NJOY scattering results were generated with a very fine group mesh in GROUPR. The source neutron energy was modelled as one of the very fine energy groups.

Figure 5 is an additional NJOY sample result.

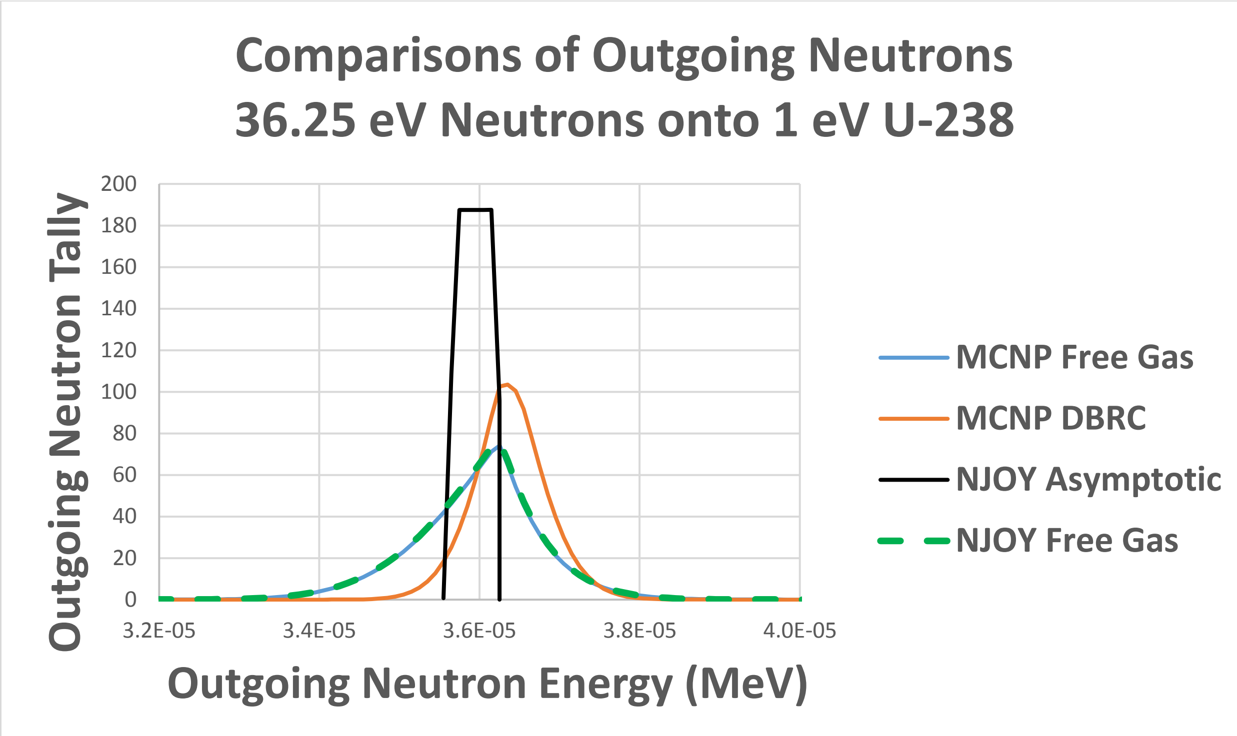

Figure 5: Comparison of MCNP and NJOY Scattering Spectra for U-238

The big scattering resonance for Figure 5 is at 36.67 eV. The consistency between the MCNP and NJOY free gas scattering approaches is again seen in Figure 5. Also notice the slightly non-rectangular asymptotic result from NJOY. The outward bowing of the asymptotic curve is due to the fact that the scattering range determined by $(A-1)^2/(A+1)^2$ does not exactly coincide with the energy group boundaries used in GROUPR. So the outward bowing represents groups on the edges which only partially contain the asymptotic scattering range.

Yet another important NJOY result is apparent from Figure 5. If the neutron energy had been only a little bit higher (say > 38.682 eV), then NJOY would have switched from the free gas model to the asymptotic model and missed a lot of physics. At 36x the material temperature, Figure 5 shows that the free gas scattering model has not yet begun to approach the asymptotic model. This is why the 38.68x the material temperature in NJOY should be extended to something more like MCNP's 400x criterion.

Though it is not shown here, the angular dependence of the scattered neutrons from the NJOY free gas scattering model is just like the angular dependence of the scattered neutrons from the MCNP free gas model shown in Figure 3.

The Los Alamos version of NJOY does not currently include the capability to include resonance scattering effects into the Doppler Broadening of scattering cross sections, though two such deterministic capabilities[B1-B3, C1-C8] exist elsewhere. One of the methods[B1-B3] decomposes the energy variation into Legendre polynomials and uses integration by parts and the other[C1-C8] uses analytic integration with ultra-fine energy groups.

Development of a Hybrid Scheme to Calculate Resonance Effects on Free Gas Scattering

A hybrid approach to free gas neutron scattering in the vicinity of high Z scattering resonances is being developed at Los Alamos for future inclusion into the THERMR module of NJOY. It is based on a direct numerical integration of the equations used in MCNP's "Sampling the Velocity of the Target Nucleus" methodology. It includes the resonance scattering effects by a weighting scheme analogous to implicit capture weights used in Monte Carlo transport. It also includes the milder weights from the rejection scheme used to account for the impossibility or implausibility of certain combinations of neutron and target nucleus velocities and directions.

This new scheme is not necessarily efficient in a figure of merit sense, but it is conceptually simple. (There are some techniques under investigation which should improve its efficiency.) In either MATLAB or FORTRAN, the actual coding is less than 300 lines. As each phase space element of the numerical integrals is evaluated, the results are accumulated into finely meshed output energy and angular bins. These integrals must be carried out in the relative velocity phase space (to pick up the Doppler Broadening effects) and only then can the results be mapped onto the lab system for usage in deterministic codes. This is quite different from the free gas scattering approach, where the calculational results are obtained directly in the lab system.

Provision is also made for a distribution of starting energies for the incident neutron in order to model a multi-group bin. Of course, specific single incident energies can also be used. The output neutron energy distributions can then integrated into neutron energy groups, while the angular distribution within an output energy group can be decomposed into Legendre components.

For the energy dependence of the scattered neutrons, three levels of nested integration are required. The three levels are the velocity of the target nucleus, the angle between the incident neutron velocity and the target nucleus velocity, and the center of mass scattering angle (once a collision has occurred) between the incident neutron and the target nucleus.

For the angular dependence of the scattered neutrons, a fourth level of integration is also required. It has to do with the rotation from the center of mass back to the lab coordinates. An integration around the center of mass azimuthal angle (or at least around a symmetric ½ of the azimuth) – is required. Azimuthal symmetry is present in the center of mass system, but the angular dependence does not rotate back unchanged to the lab system, and the final multi-group cross sections for deterministic transport must be in the lab system.

This scheme may be considered a form of "stratified sampling", where the sampled quantities of the target nucleus velocity, the cosine of the angle between the incident neutron and the target nucleus directions, and the center of mass scattering angle (once the scattering collision has occurred) are uniformly distributed. If the fourth level of integration is needed, the azimuthal angles in the center of mass are also uniformly sampled.

Figure 6 compares the outgoing neutron energy spectrum from the DBRC result in Figure 2 with the hybrid result.

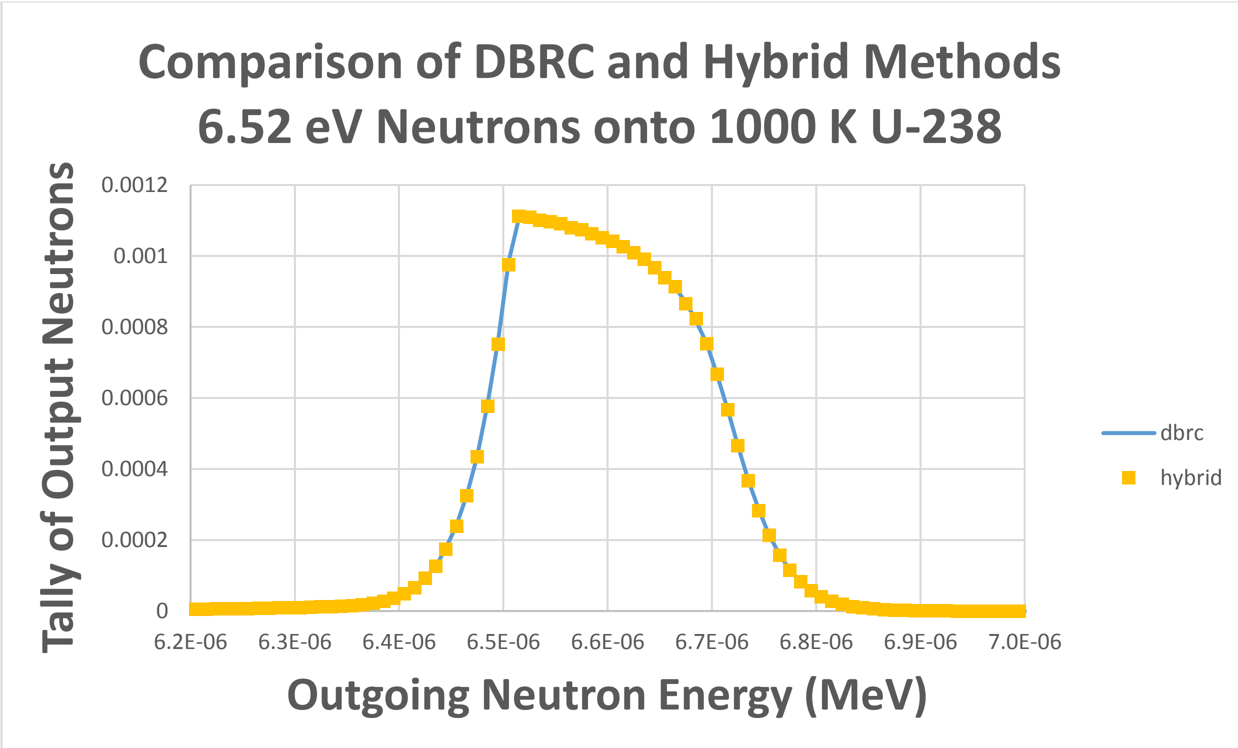

Figure 6: Comparison of DBRC and the hybrid method on the Outgoing Neutron Energy

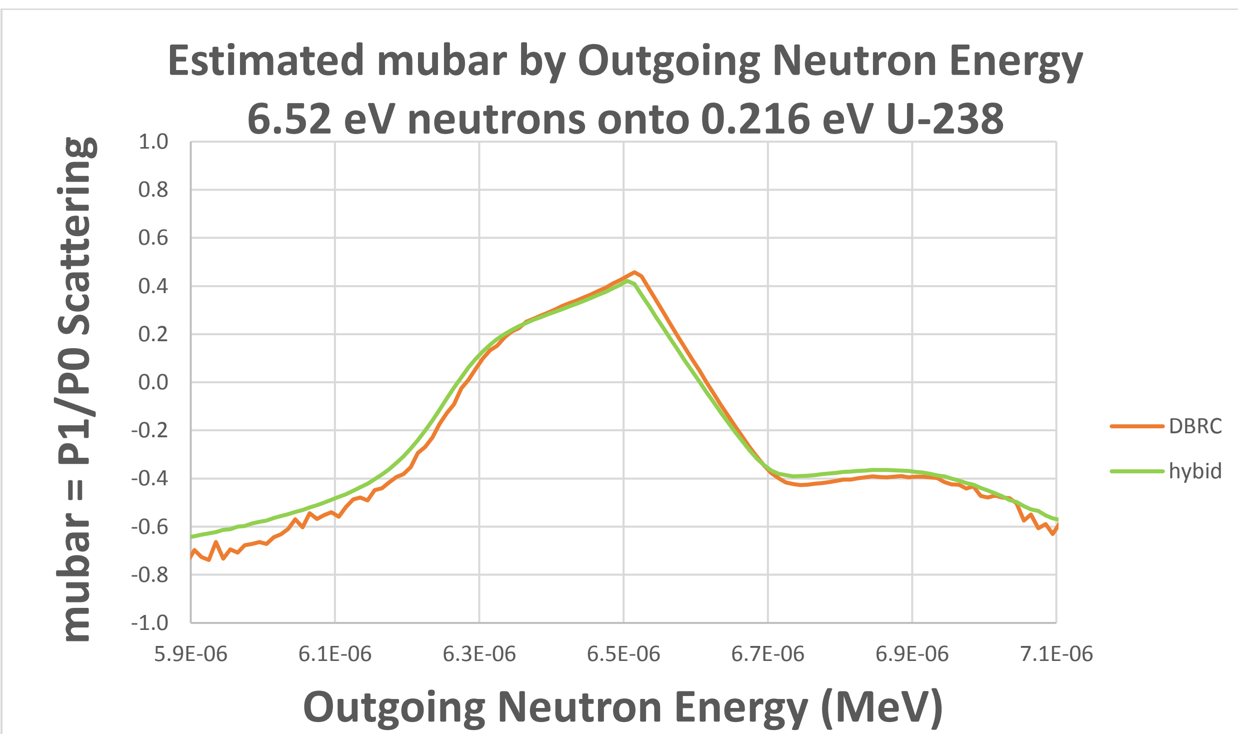

Figure 7: Comparison of mubar from DBRC and from the hybrid method as a function of the Outgoing Neutron Energy

Figure 7 gives a sample angular result when comparing DBRC and the hybrid method. The DBRC angular result was already seen in Figure 3. The mubars were estimated by averaging the mubar-weighted energy and angular dependent fluxes over all angles at each outgoing energy.

Of course, the contribution of each element of the nested integration in the hybrid method to the final output quantities in the lab system is not uniform. Scattering resonances distort the free gas scattering results significantly in the near vicinity of the scattering peak. The effective range of the scattering resonance effect is generally taken to be:

$$v_{res} \pm 4 / \beta \qquad (14)$$

where β was defined earlier after Equation (3), and
v_{res} is the relative neutron velocity which corresponds to the energy of the resonance.

At relative velocities beyond these limits, the Maxwellian distribution used in the integration falls off very rapidly to 0.0. The scattering cross section also asymptotes back to a flat distribution. Therefore, the usual free-gas scattering approach may be used for neutron incident energies not very close to the actual resonance energies.

Another insight is that if the desired multi-group neutron cross sections are fairly coarsely gridded, then the angular behavior near the resonance can be swallowed up by a broad energy group and the overall dependence will become isotropic (or nearly isotropic) in that group. So the angular dependence of Doppler-Broadened scattering cross sections will only be significant for cross section group widths which are smaller than or comparable in width to the effective range of the scattering resonance. The same phenomenon is also true for the energy dependence of the Doppler-Broadened scattering cross sections. The effects will only be seen in multi-group cross section sets where the energy resolution is sufficient to resolve the effects in the effective range of the scattering resonances.

Possible Acceleration of the Hybrid Approach to Resonance Scattering

For a given incident neutron energy, v, the largest contributions to the output energy and angular bins come from combinations of target nucleus velocity, V, and the angle between the incident neutron velocity direction and the target nucleus velocity direction, μ_t, which give values of the relative neutron velocity corresponding to the energies of the scattering resonances: (and it is here assumed that the scattering cross section at the resonance peak is much higher than the rest of the nearby in energy scattering cross sections)

$$\text{Scattering Resonance Energy} = ½\, m_n v_r^2 \qquad (15)$$

Therefore, combinations of V and μ_t which are related in the following way (derived from Equation 2) contribute the most:

$$\text{Constant1} = V^2 - 2\, \mu_t\, v\, V \qquad (16)$$

where Constant1 is an arbitrary constant which is related to the resonance energy.

And if the neutron velocity, v, is significantly larger that the target nucleus velocity, V, (which is usually true for high Z target nuclei, even at elevated material temperatures) this may be simplified by dropping the V^2 term:

$$\text{Constant2} = \mu_t V \tag{17}$$

This suggests that an efficient, though approximate, integration could be carried out along "lines" (i.e., the contours) of constant μ_t * V instead of along the cardinal axes of V and μ_t.

Figure 8 shows two typical contour curves along lines of constant μ_t * V. In this case, there is scattering resonance just below and another scattering resonance just above the incident neutron energy. The front axis is the cosine of the angle between the incident neutron motion and the target velocity motion – divided into 401 points between cosine values of -1 and 1. The axis going into the paper represents the velocity of the target nucleus in terms of 1/β *100. The vertical axis is the logarithmic value of the scattering cross section. It is clear that any integral quantity involving the scattering cross section as a function of angle and target nucleus velocity will be determined largely by the points along the 2 elevated curves. Notice that the curves asymptote at the midpoint of the front axis – which corresponds to a scattering cosine angle of 0.0. The 2 steep valleys correspond to the very low scattering cross sections seen just below a scattering resonance energy.

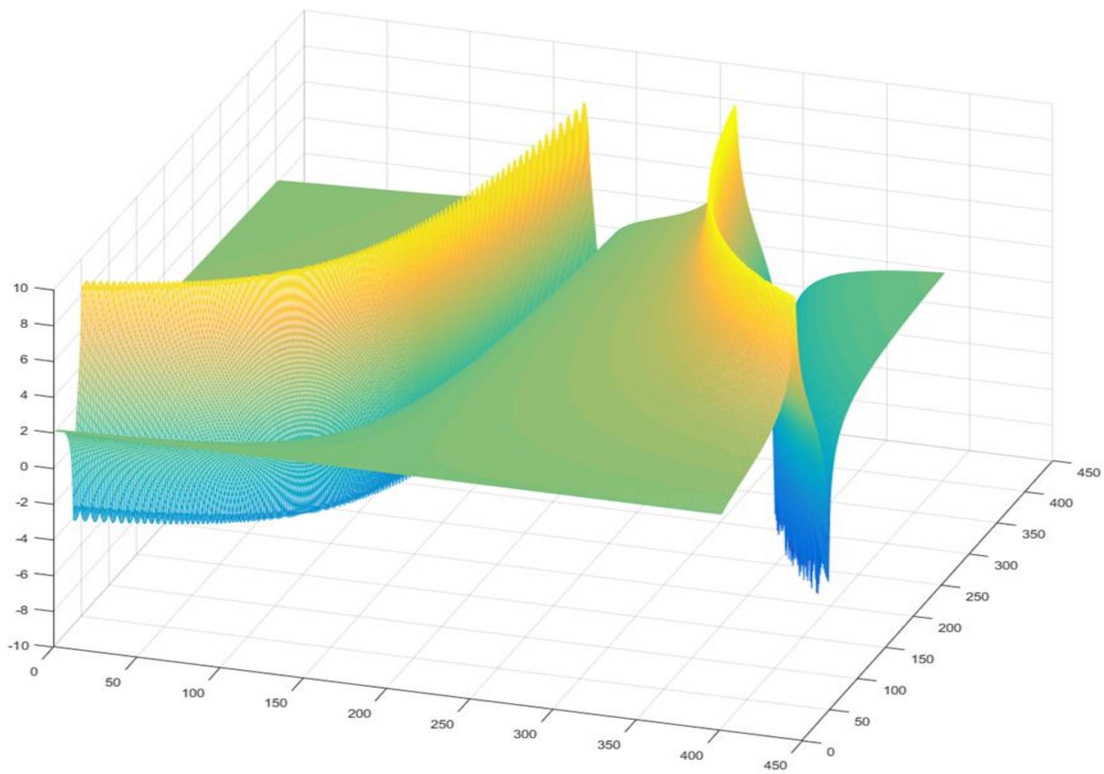

Figure 8: Typical Contour Curves from Resonance Scattering

Summary

Development of a Doppler-Broadening capability for scattering resonances in high Z target nuclei is underway at Los Alamos in the nuclear data team of XCP-5. This effort includes a thorough review of current capabilities, current documentation, and an extensive literature review. Implementation of the Doppler-Broadening capability for high-Z scattering resonances into the THERMR module will occur in the ongoing NJOY21 efforts.

Since the calculation of Doppler-Broadening of Resonance Scattering is somewhat cumbersome, it is anticipated that this capability will become a user option in NJOY – to be used only in the near vicinity of high-Z scattering resonances.

References

The following is a Topical Outline of References on Doppler Broadening of High Z Elastic Scattering of Incident Neutrons in the Vicinity of Resonances. (*Some references are listed more than once.)*

A. Theoretical Background to Resonance Scattering:

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