Assessment of Approximate Methods for Width Fluctuation Corrections

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Abstract. Using the exact triple-integral expression for compound nucleus cross sections as a benchmark, the accuracy of the HRTW and Moldauer approximation methods is compared for a wide range of physically plausible cases. The Moldauer method is found to give superior results, although still with significant errors for weak elastic cross sections. An improved formula for the elastic-enhancement factor is presented and assessed, and is shown to improve the accuracy of both methods. Finally, the convergence to exactness of the approximate methods in the high-absorption limit is investigated.

INTRODUCTION

The original Hauser-Feshbach formula for the compound-nucleus cross section is known to be inaccurate when only a few reaction channels are involved, due to the obvious correlation between incoming and outgoing channels in the case of elastic scattering. This deficiency is usually cured with the multiplicative factor called the width-fluctuation correction. Two approximate but computationally fast methods, one by Moldauer [1] and the other one called HRTW [2], are typically used in reaction calculations. More recently, the exact formula for the compound-nucleus cross section, known as the triple integral, was formulated by the Heidelberg group [3]. Due to much more involved calculations the latter is used only exceptionally but can be exploited for benchmarking approximate expressions ubiquitous in the reaction codes.

Fröhner reported typical differences of 1%-3% between the triple-integral and the Moldauer formula [4]. Hilaire et al. [5] compared the two formulae in a number of physical cases and similarly found a typical error of less than 3%, although up to 6% was seen in the case of elastic \((n,n)\) reactions. Both exercises involved realistic ‘observable cross sections,’ i.e., cross sections summed over many physical channels. In this paper we extend previous analyses by investigating the accuracy of the approximate methods for explicit physical channels. In doing so we are able to study cases that would not show up in the previous papers (such as weak-weak cross sections). In addition, we derive improved expressions for the elastic-enhancement factor that improve robustness of both approximate methods.

FORMULAE FOR CROSS SECTIONS

HRTW Method

The compound nucleus cross section \(\sigma_{ab}\) is expressed as

\[
\sigma_{ab} = \left(1 + \delta_{ab} (W_a - 1) \right) \frac{V_a V_b}{\sum_i V_i},
\]

where \(W_a\) is the elastic enhancement factor and \(V_i\) are related to optical-model transmission coefficients \(T_i\).

\[
V_a = T_a \left(1 + \frac{(W_a - 1) V_a}{\sum_i V_i} \right)^{-1}.
\]

The latter formula allows calculation of the \(V_i\) by starting with \(V_i = T_i\) and iterating. The HRTW original empirical formula for \(W_a\) was improved in [6] and results obtained with the latter one will be referred as HO in the rest of this paper.

Moldauer Method

The Moldauer expression involves an integral and is more complicated than the HRTW formula. It reads

\[
\sigma_{ab} = \frac{T_a T_b}{\sum_i T_i} \left(1 + \delta_{ab} \frac{2}{V_a} \right) \int_0^\infty dx \prod_k \left(1 + \frac{2T_k x}{\gamma_k \sum_i T_i} \right)^{-\delta_a - \delta_b - \gamma_i/2}.
\]

The coefficient \(\gamma_i\) is the number of degrees of freedom of the \(\chi^2\) distribution from which the channel widths...
are assumed to be drawn. It is related to the elastic-enhancement factor by the relation

\[ W_a = 1 + \frac{2}{\nu_a}. \]  

(4)

From a set of randomly generated \( S \)-matrices Moldauer derived the following empirical formula [1]

\[ \nu_a = 1.78 + (T_a^{1.212} - 0.78) \exp(-0.228 \Sigma T_j). \]  

(5)

### Triple Integral Formula

The exact and computationally tractable solution, based on the assumption that the nuclear Hamiltonian belongs to the Gaussian Orthogonal Ensemble (GOE), was published by Verbaarschot, Weidenmüller, and Zirnbauer [3]. Their expression contains three integrals irrespective of the number of open channels and has consequently become known as the \textit{triple-integral formula}. In the case of a diagonal \( \langle S \rangle \)-matrix it takes the form

\[
\sigma_{ab} = \frac{T_a T_b}{8} \int_0^\infty \int_0^\infty \int_0^1 d\lambda_1 \, d\lambda_2 \, d\lambda \frac{\lambda(1-\lambda) |\lambda_1 - \lambda_2|}{\sqrt{\lambda_1(1+\lambda_1)} \sqrt{\lambda_2(1+\lambda_2)} (\lambda + \lambda_1)^2 (\lambda + \lambda_2)^2} \times \left( \prod_j \frac{1 - T_j \lambda}{\sqrt{1 + \frac{1}{T_j \lambda}}} \right)^2 \left\{ \delta_{ab} (1 - T_a) \left( \frac{\lambda_1}{1 + T_a \lambda_1} + \frac{\lambda_2}{1 + T_b \lambda_2} + \frac{2 \lambda}{1 - T_a \lambda} \right) \right. \\
+ \left(1 + \delta_{ab} \right) \left( \frac{\lambda_1 (1 + \lambda_1)}{(1 + T_a \lambda_1) (1 + T_b \lambda_2)} + \frac{2 \lambda (1 - \lambda)}{(1 - T_a \lambda) (1 - T_b \lambda)} \right) \right\},
\]

where the product is taken over all open channels. Being exact, this formula will serve as a benchmark against which the approximate methods will be compared.

### CALCULATIONS

The integrand in Eq. (6) is singular for \( \lambda_i \to 0, \ i = 1,2 \). Part of this singularity was removed by a change of variables. Each two integrals to infinity were mapped onto a finite interval by breaking them into two and using the substitution \( \lambda_i \to 1/\lambda_i \) on the remaining integral to infinity.

The resulting nested integrals were then calculated using a Romberg integration routine [7]. For each of the (nested) integrals the algorithm was set to yield an estimated fractional error of no more than $10^{-7}$.

A total of 8931 quasi-random sets of \( T_j \), corresponding to more than 50,000 cross sections, were generated and the various methods compared for each one using the triple-integral result as a benchmark. For computational ease the number of separate \( T_j \) was fixed at four but each was assigned a multiplicity, allowing it to represent a large number of physical channels. The selection of \( T_j \) and their multiplicities was such as to resemble physical cases at low incident energies.

For each set of \( T_j \), the following six cross sections were calculated: \( \sigma_{11} \) (weak elastic), \( \sigma_{12} \) (weak-strong inelastic), \( \sigma_{13} \) (weak-weak inelastic), \( \sigma_{14} \) (weak-weak inelastic) \( \sigma_{23} \) (strong-weak inelastic), and \( \sigma_{33} \) (strong elastic).

### IMPROVED FORMULA FOR \( \nu \)

Moldauer arrived at Eq. (5) by fitting data obtained by calculating cross sections from generated \( S \)-matrices corresponding to cases in which all \( T_j \) were equal. The cross-section ratio \( \sigma_{11}/\sigma_{12} \) then gives the elastic enhancement factor \( W_1 \) and we have

\[
\nu_a = 2 - \frac{2}{W_1 - 1} = \frac{2}{(\sigma_{11}/\sigma_{12}) - 1}.
\]

(7)

We have used the triple integral to construct a data set similar to the one employed by Moldauer but with more (and more evenly spaced) data points, including also the case of very low \( T \) that was not included in original data. The range of \( \sum T_j \) was extended up to 50. The empirical prescription for \( \nu \) was found to be

\[
\nu_a = 2 - \frac{1}{1 + f(T_a) \cdot \sigma(T_a)},
\]

(7)

where

\[
f(T) = \frac{\alpha}{1 - T^\beta} \quad \text{and} \quad g(T) = 1 + (\gamma T)(1 - T),
\]

with \( \alpha, \beta, \) and \( \gamma \) being free parameters. Given the relation (4), this result can also be straightforwardly applied within the HRTW scheme.

While the coefficients must be obtained by fitting, the functional forms have been chosen so as to have the appropriate limits. Thus, the form (7) will, for \( f(T_a) > 0 \), ensure that \( \lim_{\sum T_j \to \infty} \nu_a = 2 \), while the form of \( f(T) \) imposes \( \lim_{T \to 1} \nu_a = 2 \).

Since Eq. (7) is a function of \( T_a \) and \( \sum T_j \) only, it is insensitive to the exact distribution of channel strengths.
and might fail under certain circumstances. However, comparison between cases with the same $\sum_i T_i$ but different channel types revealed only a slight dependence on the average of the $T_i$.

The parameters of Eq. (7) ($\alpha$, $\beta$, and $\gamma$) were determined by fitting the approximate methods across the full set of cross sections.

$$\rho_X^2 = \frac{1}{N} \sum_{i=1}^{N} \left( \frac{\sigma_X^i - \sigma_{X_{\rm TI}}^i}{\sigma_{X_{\rm TI}}^i} \right)^2,$$

(8)

where $N$ is the total number of cross sections; TI labels triple-integral results and X results obtained using approximation method X. As expected, the result depends on whether one fits Eq. (7) using cross sections generated by the HRTW or Moldauer methods. The optimal parameters are listed in Table 1. The improvement achieved by using these sets of parameters together with Eq. (7) will be assessed below.

**TABLE 1.** Coefficients in Eq. (7) found to reproduce triple-integral results when used with HRTW and the Moldauer method.

<table>
<thead>
<tr>
<th></th>
<th>$\alpha$</th>
<th>$\beta$</th>
<th>$\gamma$</th>
<th>$\rho^2$</th>
</tr>
</thead>
<tbody>
<tr>
<td>HRTW</td>
<td>0.139</td>
<td>15.247</td>
<td>4.081</td>
<td>2.86 $\times$ 10$^{-3}$</td>
</tr>
<tr>
<td>Moldauer</td>
<td>0.177</td>
<td>20.337</td>
<td>3.148</td>
<td>5.34 $\times$ 10$^{-4}$</td>
</tr>
</tbody>
</table>

**COMPARISON OF APPROXIMATE METHODS**

The Moldauer and HRTW methods using the original parameterization and the one developed in the preceding section were compared against the triple-integral. In the following they will be denoted as

- **HO**: HRTW with $W_a$ from [6]
- **HN**: HRTW with $\nu_a$ from Eq. (7)
- **MO**: Moldauer with $\nu_a$ from Eq. (5)
- **MN**: Moldauer with $\nu_a$ from Eq. (7)

The Moldauer method is markedly better than HRTW (irrespective of the formula used for $W_a$), both in total and across all individual cross sections. For strong-weak and strong-strong inelastic channels both methods are generally very precise, the typical errors being below 4% for HRTW and below 2% for Moldauer. These values are in agreement with the earlier results of Fröhner [4] and Hilaire [5].

However, the errors for the elastic ($\sigma_{11}$ and $\sigma_{33}$) and weak-weak channels ($\sigma_{14}$) are much more substantial for both the HRTW and Moldauer methods. This is particularly so for the weak-elastic channel; when using the traditional prescriptions for $\nu$ (or $W$), more than 40% of the HRTW results for $\sigma_{11}$ are off by more than 10% and even with the Moldauer method more than 9% differ by at least that much. For all of these channels, employing the improved prescription for $\nu$ yields a significant decrease in average errors. Similarly, with the new formula for $\nu$, the percentages of $\sigma_{11}$ results off by more than 10% goes down to around 10% and 2% for HRTW and Moldauer, respectively.

The improved formula has the additional advantage of giving a faster increase in precision with increasing $\sum_i T_i$ for both the HRTW and Moldauer methods.

On the other hand, we note that the improved formulae lead to a *loss* of precision for strong-weak channels. The overall effect is that the improved formulae yield a more even distribution of errors across a various combination of channels.

The distributions of errors are shown in Fig. 1. All distributions are centered on 0, but errors generally tend to fall on the low side (i.e., underestimating the cross section). However, HRTW with the old formula for $W_a$ also overestimates in a significant number of cases. The latter errors come almost exclusively from the weak-elastic cross section ($\sigma_{11}$).

For HRTW, the new formula eliminates the substantial ‘shoulder’ of overestimates, while in the case of the Moldauer method it makes the distribution visibly narrower on the low (underestimated) side.

The true outliers in the distribution are the ones in which only very few channels are open and elastic enhancement is important. In these cases, both HRTW and Moldauer used in conjunction with the old prescriptions for $\nu$ (or $W$) may yield errors of 50% or more, while the improved method does much better. For instance, the improved Moldauer method does not give errors above 35% on a single cross section in our set.

**TABLE 2.** Percentage errors of approximate methods. The total includes all cross sections indiscriminately.

<table>
<thead>
<tr>
<th></th>
<th>HO</th>
<th>HN</th>
<th>MO</th>
<th>MN</th>
</tr>
</thead>
<tbody>
<tr>
<td>Total</td>
<td>3.24</td>
<td>2.38</td>
<td>1.7</td>
<td>1.31</td>
</tr>
<tr>
<td>$\sigma_{11}$</td>
<td>9.77</td>
<td>4.15</td>
<td>3.77</td>
<td>1.87</td>
</tr>
<tr>
<td>$\sigma_{12}$</td>
<td>0.85</td>
<td>0.81</td>
<td>0.53</td>
<td>0.48</td>
</tr>
<tr>
<td>$\sigma_{13}$</td>
<td>0.87</td>
<td>0.84</td>
<td>0.54</td>
<td>0.49</td>
</tr>
<tr>
<td>$\sigma_{14}$</td>
<td>4.91</td>
<td>3.71</td>
<td>2.63</td>
<td>1.2</td>
</tr>
<tr>
<td>$\sigma_{23}$</td>
<td>0.6</td>
<td>2.05</td>
<td>0.58</td>
<td>1.48</td>
</tr>
<tr>
<td>$\sigma_{33}$</td>
<td>2.44</td>
<td>2.72</td>
<td>2.12</td>
<td>2.36</td>
</tr>
</tbody>
</table>
CONVERGENCE OF METHODS IN THE HIGH ABSORPTION LIMIT

The overall effect of elastic enhancement diminishes as the number of open channels increases i.e., as $\sum T_i \rightarrow \infty$. The approximate methods should therefore converge in this limit. In particular, even the simple Hauser-Feshbach (HF) formula should become exact for inelastic channels. This can be seen in Fig. 2, which shows the average fractional error as a function of $\sum T_i$.

While all methods give an error below 5% for $\sum T_i > 10$, the methods that use the updated $\nu$ formula [Eq. (7)] show a notably faster convergence. In particular, the fact that the original Moldauer method actually loses precision for $\sum T_i > 10$ while the improved method continues converging indicates that the updated formula provides a substantially better fit in the high-absorption case.

CONCLUSIONS

Our benchmarking of the approximate formulae for the width-fluctuation correction shows that the Moldauer approach is more precise than the HRTW method, especially if the sum of transmission coefficients is lower than 10. This confirms conclusions of [5]. We reckon that the accuracy of both methods (2% for Moldauer and 4% for HRTW) is sufficient for typical nuclear-reaction calculations since errors brought about by uncertainties of model parameters are substantially larger. In addition, observed quantities are often sums over a number of physical channels and eventual serious deviations for a few of them tend to be de-emphasized.

REFERENCES