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Statistical Model Calculations for (n,γ) Reactions

Mary Beard[1,2,a], Ethan Uberseder[3], and Michael Wiescher[1]

[1] *Department of Physics, University of Notre Dame, Notre Dame, Indiana, 46556, USA*
[2] *ExtreMe Matter Institute EMMI, GSI Helmholtzzentrum für Schwerionenforschung, Planckstraße 1, 64291 Darmstadt, Germany*
[3] *Cyclotron Institute, Texas A & M University, Collage Station, Texas 77843, USA*

Abstract. Hauser-Feshbach (HF) cross sections are of enormous importance for a wide range of applications, from waste transmutation and nuclear technologies, to medical applications, and nuclear astrophysics. It is a well-observed result that different nuclear input models sensitively affect HF cross section calculations. Less well known however are the effects on calculations originating from model-specific implementation details (such as level density parameter, matching energy, back-shift and giant dipole parameters), as well as effects from non-model aspects, such as experimental data truncation and transmission function energy binning. To investigate the effects or these various aspects, Maxwellian-averaged neutron capture cross sections have been calculated for approximately 340 nuclei. The relative effects of these model details will be discussed.

1 Introduction

Nuclear reaction rates are crucial to a spectrum of applications, including waste transmutation, nuclear technologies, and the production of isotopes for medical applications. Nuclear reactions are also the primary ingredient in nucleosynthesis studies. Not only are they of the utmost importance for understanding how stars produce energy, they are also the key to understanding the origin and observed abundance pattern for the vast majority of elements. Of all the various types of reactions that can occur in stellar environments, neutron capture rates are of particular importance. Neutron capture is by far the most dominant method for synthesizing nuclei heavier than iron. Indeed, virtually all of the heavy nuclei above iron in the Solar system were produced via either the s(low)- or r(apid)- capture of neutrons [1].

A huge amount of cross section data is required to understand nucleosynthetic processes, the vast majority of which has not been experimentally measured. Consequently nucleoastrophysical models heavily rely on theoretical methods to fill in the missing cross sections. One approach which is commonly used to calculate cross sections is the Hauser-Feshbach (HF) statistical model [2, 3]. For this approach to be valid firstly the compound framework must be applicable, i.e., the compound must fully equilibriate before breaking apart, and secondly the level density must be sufficiently large such that the individual resonances overlap all quantities can be treated in terms of averaged quantities.

Ground state properties, such as masses and deformations, level density descriptions, particle optical models, and γ-strength functions, which characterize the emission and absorption of photons, are all required for a statistical model calculation. It has long been known that the success of the statistical model depends sensitively on the details of these so called nuclear input models, specifically the details of the level density, optical model and γ-strength function models. It is generally accepted that over an energy range of 10 keV–10 MeV, the HF model is valid to within a factor of about 3 [4, 5]. A frequent approach to improve on the reliability of the statistical model is to compare experimental data to HF calculations obtained with various combinations of nuclear input models, the hope being to test the applicability of a particular model or to identify successful model combinations. Less explored however are the uncertainties in the calculations arising not from nuclear input model selections, but from code implementation details (e. g., how much data is used in a calculation) as well as non-model sources, such as truncation effects.

A study was recently performed to explore these effects using radiative neutron capture cross sections [6]. The study used results from 4 HF codes, including 1) TALYS (version 1.6) [7]; 2) NON-SMOKER [4, 8]; 3) CIGAR (Capture Induced GAmma-ray Reactions); 4) SAPPHIRE (Statistical Analysis for Particle and Photon capture and decay of HIgh energy REsonances) [9]. In each case, the results from the codes were compared to approximately 340 Maxwellian-averaged cross section data (MACS) compiled in the KADoNiS [10] database. Of these 4 codes, CIGAR and SAPPHIRE have been developed to use identical nuclear input models, implemented with exactly the same details (e.g., identical level density and back shift parameter, identical spin-cut off model etc). Developing the two codes to contain exactly the same for-

[a] e-mail: mbeard@nd.edu

malisms means that effects from non-model and coding details can be easily investigated.

2 Statistical model

In the HF framework, the cross section for a reaction $i^{\mu} + j \rightarrow o + m^{\nu}$ depends essentially on the transmission functions and is given by

$$\sigma(i^{\mu}(j,o)m^{\nu}, e_{ij}) = \frac{\pi}{k_{ij}^2(2J_i^{\mu}+1)(2J_j+1)} \times \sum_{J,\pi}(2J+1)\frac{T_j^{\mu}T_o^{\nu}}{T_{tot}}, \quad (1)$$

where target nucleus i is in excited state μ, and residual nucleus m is left in excited state ν. The spin, parity and excitation energy of the compound nucleus are given by J, π and E. Spin, parity and energy for a specific state in i (m) are represented by J_i^{μ} (J_m^{ν}), π_i^{μ} (π_m^{ν}) and E_i^{μ} (E_m^{ν}) respectively, whereas the spin, parity and energy of j (o) are denoted by J_j (J_o), π_j (π_o) and E_j (E_o). k_{ij} is the wave-number of the projectile and is equal to $k_{ij} = \sqrt{2\hat{A}_{ij}E_{c.m.}}/\hbar$, where $\hat{A}_{ij}$ is the reduced mass and $E_{c.m.}$ is the centre of mass energy. The transmission functions for the formation and decay channels, as well as the total transmission function for the decay of the compound nucleus, are represented by T_j^{μ}, T_o^{ν} and T_{tot} respectively. For particles the transmission functions are found by solving the Schrödinger equation with an optical nucleon-nucleus potential. Historically the nuclear potential has been described by the Woods-Saxon shape, however use of a Wood-Saxon equivalent square well (ESqW) also has a long history [11], as does the JLM semi-microscopic optical model of Ref. [12]. The photon transmission function, on the other hand, is obtained by parametrising the giant dipole resonance in terms of a Lorentzian. There are a few phenomenological descriptions of the giant dipole resonance that are commonly used, including the Kopecky-Uhl generalized, energy-damped Lorentzian [13] (GLO), and the energy-damped double Lorentzian [14] (DLO).

For astrophysical applications, the total cross section $\sigma(i^{\mu}(j,o)m)$, i. e., summed over all possible residual excitation states ν, is frequently of more interest than cross sections to specific J_m^{ν}, π_m^{ν}, E_m^{ν} states. In this case, T_o replaces T_o^{ν} in Eq. 1 where T_o^{ν} is summed over ν for all excited states in m. Since the sum over ν can involve a huge number of terms, whenever excitation states at energies greater than E_m^{max}, the maximum experimentally known energy, spin and parity become important, the sum over ν is replaced with an integral over the level density, $\rho(E_m, J_m, \pi_m)$. Two descriptions of level density ρ are frequently used, often in combination and matched at some energy. The first is the well-known back-shifted Fermi gas (BSFG) formula [15], which requires the level density a and back-shift parameters. The second is the constant temperature (CT) model [15], which is based on the observation that at low energy the number of excitation levels in the nucleus scales exponentially.

3 Statistical model codes

There are several, well-established HF code packages for cross section and reaction rate calculation available on the market including TALYS, NON-SMOKER, EMPIRE [16], MOST [17] and SMARAGD [18]. In each case the code package requires a user to select between the various available options for nuclear input model. It is often the case however that for any two code packages the user is presented with a different selection of nuclear input models to choose between. Even when the models are identical, such as back-shifted Fermi gas for the level density, specific implementation details can still be at variance between codes. Example of this include the level density parameter, which is defined differently in the TALYS and NON-SMOKER packages, as well as the definition of spin-cut off and the parameters used to describe the giant dipole resonance. Such differences make it very hard to directly compare the calculations from different codes. Though for the sake of brevity the effects on statistical model cross section calculations stemming from implementation details are not discussed here, they have been investigated in detail in Ref. [6].

As well as the various input models that can be used in a HF calculation, statistical model codes also contain inherent non-model aspects, which can affect the calculations. Examples of such aspects include the coarseness of the transmission function energy binning and J^{π} data truncation, i. e., how many levels are used before the level scheme is considered complete and a level density model is used.

To investigate the impact of non-model aspects, two HF codes have recently been developed. The first, CIGAR is based on the SMOKER [19] code and is specifically tailored for large scale astrophysical reaction rate calculations using the statistical model. The second, SAPPHIRE has been designed primarily to simulate the decay of excited nuclei via the Monte Carlo technique. Since the transmission functions needed to form the probability distribution functions for Monte Carlo are identical to those required to calculate Hauser-Feshbach cross sections however, the code can also be used to calculate astrophysical reaction rates. Although CIGAR and SAPPHIRE have been specifically developed to contain an overlapping set of identically implemented nuclear input models there are still non-model differences between the two codes. For instance whereas CIGAR truncates J^{π} data usage to a maximum of just 20 levels before considering the scheme complete, SAPPHIRE uses all existing level data before resorting to a level density model. Also, because SAPPHIRE is designed as a Monte Carlo code, it requires fine transmission function energy binning. CIGAR on the other hand has been designed with speed in mind, and so uses coarser binning.

4 Results

4.1 Non-model aspects

To investigate the effects of non-model aspects, approximately 340 MACS calculations were performed with the

codes CIGAR and SAPPHIRE. In both cases calculations were performed using the CT+BSFG level density model, the JLM OMP and the GLO γ-strength function. Parameters for the giant dipole resonance were supplied by Ref. [20]. Only ground state contributions to the MACS were considered. Since these two codes have been developed to use an identically implemented set of models, any differences between the calculation sets must arise from non-model sources.

Shown in Fig. 1 in red and blue respectively, are the ratio of CIGAR and SAPPHIRE MACS, at kT=30 keV, to the KADoNiS values. Both codes reproduce the experimental MACS to within a factor of roughly 3, though larger deviations are visible around the closed shells. In these regions the Q-values are lower and the assumption of many closely spaced resonances in the compound nucleus may not be valid. Though the calculations were performed using identical models, there are some minor differences visible between the calculations from the respective codes. As mentioned above, some of these differences are arising because of the different transmission function energy binning. The impact of the coarser energy binning in CIGAR is particularly visible for nuclei with neutron numbers less than 40, where large differences between SAPPHIRE and CIGAR calculations are evident. In these cases, where it may not be wholly appropriate to use CIGAR with the GLO γ-strength function.

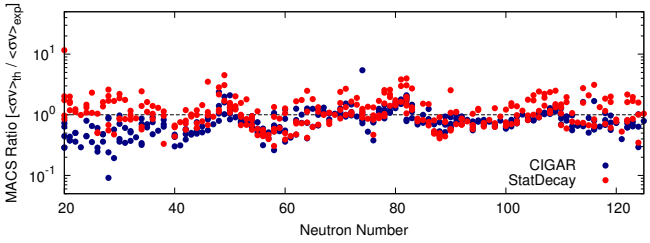

Figure 1. (Color online) Ratio of MACS at kT=30 keV obtained using CIGAR (blue) and SAPPHIRE (red) to KADoNiS [10].

An additional difference between CIGAR and SAPPHIRE is the truncation of J^π data. To investigate this effect, two sets of identical calculations were performed using the SAPPHIRE code. In the first set of calculations, the truncation on J^π was dictated by the total amount of experimental data, i. e., all of the data in the RIPL-3 data base [20] was used. In the second set of calculations, the J^π data was truncated at 20 levels to mirror the CIGAR code. The results from these two sets of calculations are compared in Fig. 2. The impact of the truncation is particularly evident for reactions involving low level densities, located around closed shells and N<40. For these cases, where the statistical model is known to be less reliable, restricting the amount of J^π data used in calculations can affect the value of the theoretical MACS by almost 20%.

4.2 Nuclear model combinations

Though it is well-established that various combinations of nuclear input models for level density, optical potential and γ-ray strength function yield significantly different cross section results, it can still be of general interest to investigate this aspect. To perform this investigation, calculations were carried out using the CIGAR code for eight level density, optical model and γ-strength function parameter combinations. Combinations included two γ-strength function models: the generalized Lorentzian (GLO) of Ref. [13] and the double Lorentzian (DLO) of [14]; two level density models: RTK [21] and HWFZ [5]; and two optical potentials: the microscopic JLM [12] and the phenomenological equivalent square well (ESqW) [5, 11]. Plotted in Fig. 3 are the MACS results at kT=30 keV for the eight nuclear model combinations.

The RTK level density model is based on the CT+BSFG models, whereas the HWFZ model is just a BSFG model. However, even though both models contain the BSFG, there are large differences in the definition of the level density parameter and the back-shift term. Inspection of Fig. 3 indicates that the choice of γ-strength function has a more significant impact on the MACS than the level density model. Within the framework of HF

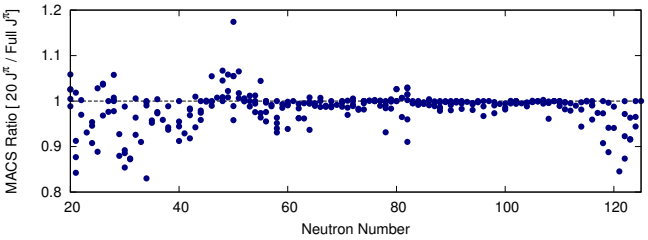

Figure 2. (Color online) Ratio of MACS at kT=30 keV obtained using different J^π truncation. Calculations were performed using the SAPPHIRE code with 1) no J^π truncation and 2) J^π truncated to 20 levels. Reproduced from Ref. [6].

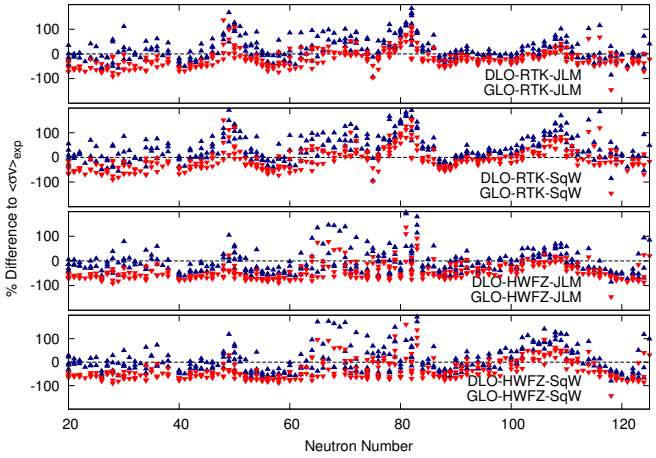

Figure 3. (Color online) Red and blue triangles correspond to the percentage difference of kT=30 keV MACS, calculated with CIGAR using the GLO and DLO γ-strength functions respectively, to the KADoNiS database. Calculations have been performed with the model combinations given in the text.

theory, $\sigma(n,\gamma) \propto \frac{T_n T_\gamma}{T_{tot}}$, where T_{tot} represents the transmission to all possible energetically accessible channels. The transmission co-efficients can be related to the average widths via $T = 2\pi\rho\langle\Gamma\rangle$, so that $\sigma(n,\gamma) \propto \frac{\langle\Gamma_n\rangle\langle\Gamma_\gamma\rangle}{\Gamma_{tot}}$. In general, $\langle\Gamma_n\rangle > \langle\Gamma_\gamma\rangle$ so that the neutron width dominates the photon width in the numerator. However the neutron width is also the major constituent of the total transmission, so $\langle\Gamma_n\rangle$ cancels out with Γ_{tot} in the denominator leaving $\sigma(n,\gamma) \propto \langle\Gamma_\gamma\rangle$. Consequently for the (n,γ) reactions considered here, knowledge of the γ-strength function is more crucial than information on the neutron optical model, and cross sections tend to be insensitive to choice of partial OMP. This effect can be seen in Fig. 3, where comparison of results obtained using identical models but for the neutron OMP (e. g. DLO-RTK-JLM and DLO-RTK-ESqW) show much less variation than calculations obtained with identical OMP but different γ-strength function (i. e. DLO-RKT-JLM and GLO-RTK-JLM).

5 Conclusions

In an attempt to identify and investigate the effects on the cross section uncertainties arising from non-model and implementation details, two codes have been developed CIGAR, SAPPHIRE. Though both codes have been designed to present the user with absolutely identical nuclear input model choices for e. g., level density, γ-ray strength function and particle optical model, implemented with identical details for, e. g. back-shift, level density parameter, giant dipole resonance parameters, etc., there are still differences between the cross section results from these two codes. These differences highlight that not all uncertainties in HF calculations stem from nuclear model input combinations. Non-model aspects, such as truncated data use and coarse transmission function energy binning, can also effect the calculations. In particular, it was found that truncating the quantity of excitation level data in the SAPPHIRE calculation could result in as much as a 20% decrease in the calculated MACS. It was also observed that the speed optimized, but coarse, energy binning can underestimate MACS, particularly for nuclei with low level densities.

Effects on the cross sections from non-model parameters are a less explored effect in statistical model calculations, presumably because the scale of the effects are less than the generally accepted factor of 3 usually associated with HF uncertainties. Various nuclear input model combinations can give rise to a significantly difference in the cross section calculations. Using the CIGAR code, it was found that model combinations using the DLO γ-strength function were in general larger than identical calculation using the GLO strength function, reflecting the difference in the two γ-strength function models.

References

[1] F. Käppeler *et al.*, Rev. Mod. Phys. **83**, 157 (2011)

[2] L. Wolfenstein, Phys. Rev. **82**, 690 (1951)

[3] W. Hauser and H. Feshbach, Phys. Rev. **87**, 366 (1952)

[4] T. Raucher and F.-K. Thielemann, At. Data Nucl. Data Tables **75**, 1 (2000)

[5] J. A. Holmes *et al.*, At. Data Nucl. Data Tables **18**, 305 (1976)

[6] M. Beard *et al.*, Phys. Rev. C **90**, 034619 (2014)

[7] A. J. Koning, S. Hilaire and M. Duijvestijn, *International Conference on Nuclear Data for Science and Technology*, edited by O. Bersillon, F. Gunsing, E. Bauge, R. Jacqmin and S. Leray (EDP Sciences, Les Ulis, France 2008) p. 211. URL: http://www.talys.eu/

[8] T. Rauscher and F.-K. Thielemann, *Stellar Evolution, Stellar Explosions and Galactic Chemical Evolution*, edited by A. Mezzacappa (IOP, Bristol, 1998), p. 519

[9] E. Uberseder *et al.*, Phys. Rev. Lett. **112**, 211101 (2014)

[10] I. Dillmann *et al.*, *EFNUDAT Fast Neutrons: Scientific Workshop on Neutron Measurements, Theory and Applications* (JRC-IRMM, Geel, 2009)

[11] G. Michaud *et al.*, Phys. Rev. C **1**, 864 (1970)

[12] J.-P. Jeukenne *et al.*, Phys. Rev. C **16**, 80 (1977)

[13] J. Kopecky and M. Uhl, Phys. Rev. C **41**, 1941 (1990)

[14] F.-K. Thielemann and M. Arnould *Proceedings of the International Conference on Nuclear Data for Science and Technology*, edited by K. Böchoff (Reidel, Dordrecht, 1983) p. 762

[15] A. Gilbert and A. G. W. Cameron, Can. J. Phys, **43**, 1446 (1965)

[16] M. Herman *et al.*, Nucl. Data Sheets **108**, 2655 (2007)

[17] S. Goriely, *Nuclei in the Cosmos V*, edited by N. Prantzos and S. Harissopulos (Editions Frontieres, Paris, 1999), p. 314

[18] T. Rauscher, Int. J. Mod. Phys. E **20**, 1071 (2011). URL: http://www.nucastro.org/smaragd.html

[19] F.-K. Thielemann, M. Arnould and J. W. Truran, *Advances in Nuclear Astrophysics*, edited by E. Vangioni–Flam (Editions Frontiere, Gif sur Yvette, 1987) p. 525

[20] R. Capote *et al.*, Nucl. Data Sheets **110**, 3107 (2009)

[21] T. Rauscher *et al.*, Phys. Rev. C **56**, 1613 (1997)