EMPIRE-II: APPLICATION TO RADIATIVE NEUTRON CAPTURE

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Large-scale calculations of radiative neutron capture have been performed with the EMPIRE-II code for all stable nuclei, starting with ^{27}Al and using nine combinations of optical model parameters and level densities. Comparison with experimental data data shows that calculations with EMPIRE-specific level densities and optical model potential derived by Koning and Delaroche describe 70% of existing experimental results adequately. These approaches retain their validity up to about 200 MeV, providing for a consistent treatment of the radiative capture and more complex nuclear reactions.

1. Introduction

EMPIRE-II belongs to a new generation of statistical model codes, intended as a general theoretical tool to be used in basic research and nuclear data evaluation for the calculation of nuclear reactions over a broad range of incident energies and projectiles. This code was designed to contain up to date nuclear reaction models as well as being easy to use. EMPIRE-2.18 (Mondovi)[1] includes major nuclear reaction mechanisms, such as optical model (SCAT2[2]), coupled channels (ECIS[3]), Multistep Direct[4] (ORION + TRISTAN), NVWY Multistep Compound[5], Monte Carlo pre-equilibrium emission[6,7], and the full featured Hauser-Feshbach model with widths fluctuation correction (HRTW[8]). A comprehensive library of input parameters covers nuclear masses, optical model parameters, ground state deformations, discrete levels and decay schemes, level densities, fission barriers (BARFIT[9]), moments of inertia (MOMFIT[9]), and γ-ray strength functions. Effects of the dynamic deformation of a fast rotating nucleus can be taken into account in the calculations. The results can be converted into the ENDF-6 format using the accompanying code EMPEND as developed by A. Trkov. The package includes the full EXFOR library of experimental data. Relevant EXFOR entries are automatically retrieved during the calculations. By default, plots comparing experimental results with the calculated data are produced using the extended PLOTC4[10] code linked to the rest of the system through a series of pre-processing codes[11] and bash-shell scripts. Interactive plotting is possible through the powerful ZVView package[12]. Simple operation of the whole system is ensured by the graphic user interface, which has been rewritten and extended substantially in the 2.18 version.

The purpose of this work was to study the global predictive power of the EMPIRE-II code for neutron capture, and to select the best set of global parameters. Large-scale calculations were performed with the statistical model and including widths fluctuation effects. Below we give a short description of the γ-strength functions and level densities used in the calculations, followed by the results and conclusions.

2. γ-ray emission

The M1, E1 and E2 transitions are taken into account in the statistical model (Hauser-Feshbach) calculations. Introducing the γ-ray strength function $f_{Xl}(E_\gamma)$, the transmission coefficient can be written as:

$$T_{Xl}^{GMR} = 2\pi f_{Xl}(E_\gamma) E_\gamma^{2l+1} \,. \tag{1}$$

According to Kopecky and Chrien[13] the γ-ray strength function is given by the expression:

$$f_{Xl}(E_\gamma) = \sum_{i=1}^{2} \sigma_i \Gamma_i \left[E_\gamma \frac{\Gamma_i(E_\gamma, T)}{(E_\gamma^2 - E_i^2)^2 + E_\gamma^2 \Gamma_i(E_\gamma, T)^2} + 0.7 \frac{\Gamma_i(E_\gamma = 0, T)}{E_\gamma^3} \right] , \tag{2}$$

where σ_i, Γ_i, and E_i are the peak cross section, the width, and the energy of the i-th hump of the GDR respectively, and the energy dependent width is given by:

$$\Gamma_i(E_\gamma, T) = \Gamma_i \frac{E_\gamma^2 + 4\pi T^2}{E_i^2} \,. \tag{3}$$

By default, the GDR parameters are estimated from the systematics based on the Dietrich and Berman compilation[14], which contains 150 experimental data for nuclei ranging from mass $A = 51$ up to 239.

3. Level densities

EMPIRE-II accounts for various models describing level densities, and includes several respective parameterizations. Equal parity distribution $\rho(E, J, \pi) = \frac{1}{2}\rho(E, J)$ is assumed.

3.1. *Gilbert-Cameron*

The Gilbert-Cameron approach[15] is well known, and will not be explained in details. We only mention that EMPIRE tries to reproduce the discrete levels and that the general expression for the a-parameter as proposed by Ignatyuk *et al.*[16] is used:

$$a(U) = \widetilde{a}[1 + f(U)\frac{\delta W}{U}], \tag{4}$$

where δW is the shell correction, $\widetilde{a}$ is the asymptotic value of the a-parameter and

$$f(U) = 1 - exp(-\gamma U). \tag{5}$$

The systematics used in the present calculations is the one developed by Iljinov *et al.*[17]: $\widetilde{a} = 0.114A + 9.80 \cdot 10^{-2} A^{2/3}$ and $\gamma = -0.051$

3.2. *EMPIRE-specific*

The default approach adopted in EMPIRE takes into account collective enhancements of the level densities due to nuclear vibration and rotation. The formalism uses the super-fluid (BCS) model[18] below the critical excitation energy, and the Fermi gas model above. Unlike other formulations, the adopted Fermi gas model accounts explicitly for the rotation induced deformation of the nucleus, which becomes spin dependent.

Assuming that the prolate nuclei rotate along the axis perpendicular to the symmetry axis, the explicit level density formula above the critical energy is defined as:

$$\rho(E, J, \pi) = \frac{1}{16\sqrt{6\pi}} \left(\frac{\hbar^2}{\Im_{\parallel}}\right)^{\frac{1}{2}} a^{1/4} \sum_{K=-J}^{J} \left(U - \frac{\hbar^2 K^2}{2\Im_{eff}}\right)^{-\frac{5}{4}}$$

$$\exp\left\{2\left[a\left(U - \frac{\hbar^2 K^2}{2\Im_{eff}}\right)\right]^{\frac{1}{2}}\right\}. \tag{6}$$

For the oblate nuclei which are assumed to rotate parallel to the symmetry axis, we have:

$$\rho(E, J, \pi) = \frac{1}{16\sqrt{6\pi}} \left(\frac{\hbar^2}{\Im_{\parallel}}\right)^{\frac{1}{2}} a^{1/4}$$

$$\sum_{K=-J}^{J} \left(U - \frac{\hbar^2 \left[J(J+1) - K^2\right]}{2|\Im_{eff}|}\right)^{-\frac{5}{4}} \tag{7}$$

$$\exp\left\{2\left[a\left(U-\frac{\hbar^2\left[J\left(J+1\right)-K^2\right]}{2|\Im_{eff}|}\right)\right]^{\frac{1}{2}}\right\}.$$

a is a level density parameter, J is a nucleus spin with projection K, E is the excitation energy, and U is the excitation energy less pairing (Δ). The effective moment of inertia $\Im_{eff}$ is defined in terms of the perpendicular $\Im_{\|}$and parallel $\Im_{\perp}$moments through the difference of their inverses. It should be stressed that Eqs. 6 and 7 account automatically for the rotational enhancement. In addition, the vibrational enhancement is applied as a multiplication factor.

By default, a-parameter is assumed to be energy (temperature) dependent, and is calculated by the method of Ignatyuk *et al.*[16]. Values at the neutron binding energy were extracted from average neutron resonance spacings D_{obs} as compiled by Iljinov et al.[17].

3.3. *Hartree-Fock-BCS*

EMPIRE can use pre-calculated level densities from the RIPL-2 library, which contains tables of level densities[19] for more than 8000 nuclei calculated via the Hartree-Fock-BCS approach. These microscopic results include a consistent treatment of shell corrections, pairing correlations, deformation effects and rotational enhancement. The results were normalized to the experimental s-wave neutron resonance spacings and adjusted to the cumulative number of discrete levels, so that the degree of accuracy can be comparable to the phenomenological formulae.

Using the partition function method, the state density can be expressed as:

$$\omega(U)=\frac{e^{S(U)}}{(2\pi)^{3/2}\sqrt{Det(U)}}. \tag{8}$$

Entropy S and excitation energy U are derived from the summation over single particle levels, and Det represents the determinant. Pairing correlations are treated within the standard BCS theory in the constant-G approximation with blocking. Consequently single-particle energies are replaced by their quasi-particle equivalents with BCS equations determining gap parameter Δ and the chemical potential λ. The calculations under discussion are based on schemes obtained using the Hartree-Fock method, with MSk7 Skyrme type force.

There are certain affinities between the HF-BCS and the default, EMPIRE-specific level densities. Both approaches use the BCS model at low energies, incorporate rotational enhancement directly into the level density formula, and apply phenomenological (although functionally different) damping of rotational effects. Furthermore, they take into account deformation effects (in EMPIRE-specific densities these are not only temperature but also spin dependent), and are adjusted to the available experimental information. The EMPIRE-specific densities also include a vibrational enhancement factor. However, the essential difference between the two approaches is the use of a phenomenological a-parameter and closed formula in the EMPIRE-specific approach, while HF-BCS level densities are derived directly from the microscopic single-particle schemes. The latter approach is expected to be more reliable away from valley of stability.

4. Calculations and results

Large-scale calculations of neutron capture on all stable isotopes starting with ^{27}Al (263 isotopes) were performed using 3 optical model parameter sets (Koning-Delaroche[20], Wilmore-Hodgson[21], and Moldauer[22]) and 3 different level densities approaches (Empire, Gilbert-Cameron, and HF-BCS) in order to test code performance and find the best set of global parameters. All-together 2367 calculations from 1 keV up to 4 MeV with default input have been performed. The results have been compared with suitable experimental data available for 193 isotopes. Inspection of the plots showed that the three optical model potentials (omp) provide similar results (see Fig.1). Calculations using Wilmore-Hodgson and Moldauer omp agree remarkably in most cases, while those with Koning-Delaroche tend to be somewhat lower in a certain energy range below 1 MeV. There is no strong evidence that one potential set is the best; however, there seems to be a slight preference for the Koning-Delaroche set. Therefore, further analyses have been carried out for this omp, which is also applicable up to incident energies of 200 MeV.

The role of the level densities turned out to be more significant than that of the optical model potentials. Plots comparing calculations using the three level density approaches against experimental data were analyzed, and the following rating was ascribed:

- excellent (at least 2/3 of the calculated excitation function are within experimental errors or within data spread) - 3 points
- good (at least 2/3 are within 50% of experiment) - 2 points
- fair (at least 2/3 within a factor of 2) - 1 point
- none - 0 points

An example is shown in Fig. 2, and results of this analysis are sum-

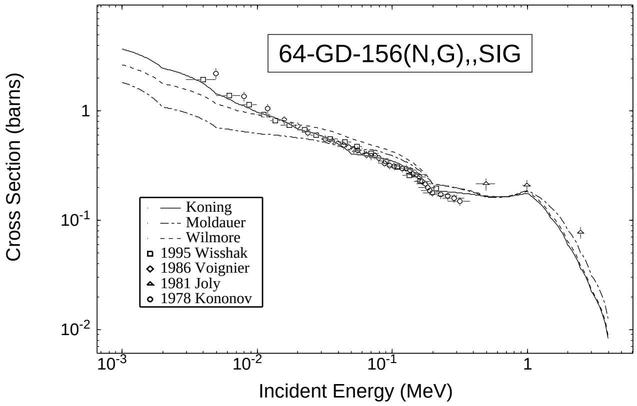

Figure 1. Capture cross sections calculated with three different optical model parameter sets.

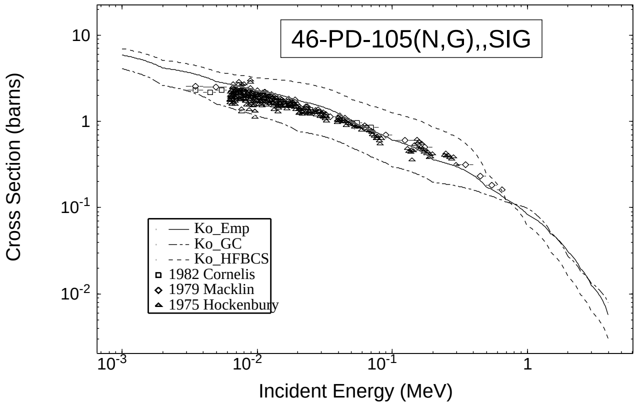

Figure 2. Capture cross sections calculated with three different level density approaches. In this example results with Empire-specific level densities are rated 'excellent' while the remaining two as 'fair'.

marized in Table 1. Overall, EMPIRE-specific level densities appear to be clearly superior compared to the remaining two approaches, providing good or excellent agreement for 70% of cases. Significant exceptions are tin isotopes for which Gilbert-Cameron formulation appears to be the best. We also note, that the results of the phenomenological Gilbert-Cameron approach and the microscopic HF-BCS approach are of comparable quality, although the first exhibits more excellent-fits and less failures. This is very encouraging since the HF-BCS approach is theoretically more sound and is more suited to extrapolation to unstable nuclei. Generally, HF-BCS calculations tend to overestimate the data, suggesting that their overall normalization might bring improvement.

Table 1. Average score and number of excellent, good, fair and bad fits for the three level density approaches used in the present calculations.

level density	av. score	excellent	good	fair	none
EMPIRE	1.96	58	80	45	10
GC	1.46	27	64	68	31
HF-BCS	1.24	13	67	67	46

Agreement for all three models could be further improved, without free adjustment of the parameters, by making use of the independent information available for particular isotopes. First of all, completeness of the adopted level schemes should be checked against level densities. Current calculations involve the use of the number of levels as recommended by RIPL-2, which is not always correct for the particular level density approach. In fact, the same numbers derived within the HF-BCS approach are considerably lower. Furthermore, no normalization of the γ-strength functions to the experimental Γ_γ, which is a standard practice in the neutron capture evaluations, has been performed. Finally, individual optical model potentials, particularly Coupled-Channels potentials for deformed nuclei, could bring additional improvement. Taking into account these shortcomings, the agreement achieved with the present parameter-free calculations can be considered remarkable.

5. Conclusions

Large-scale calculations have been performed for neutron capture reactions on all stable isotopes with Z>12 using 9 combinations of global model parameters (without any adjustment). These studies proved that EMPIRE-II (version 2.18) is able to reproduce 70% of existing experimental data within about 50% or better. Calculations are very sensitive to nuclear level densities, and are less affected by optical model potentials. Best results are obtained when using EMPIRE-specific level densities and the optical model potential of Koning and Delaroche (somewhat surprising since both methods were developed for much higher energies). Therefore, nuclear reaction calculations can be performed from 1 keV up to about 200 MeV with the same set of parameters. Such a uniform treatment is not only physically desirable but also important for nuclear data development with the limitation of discontinuities.

Encouraging results have also been obtained for the microscopic HF-BCS level densities. While the agreement for the stable isotopes is slightly worse than with the phenomenological Gilbert-Cameron model, the microscopic approach should be much more reliable when applied to nuclei far from the stability line (important for astrophysics, Heavy Ions reactions and ADS).

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