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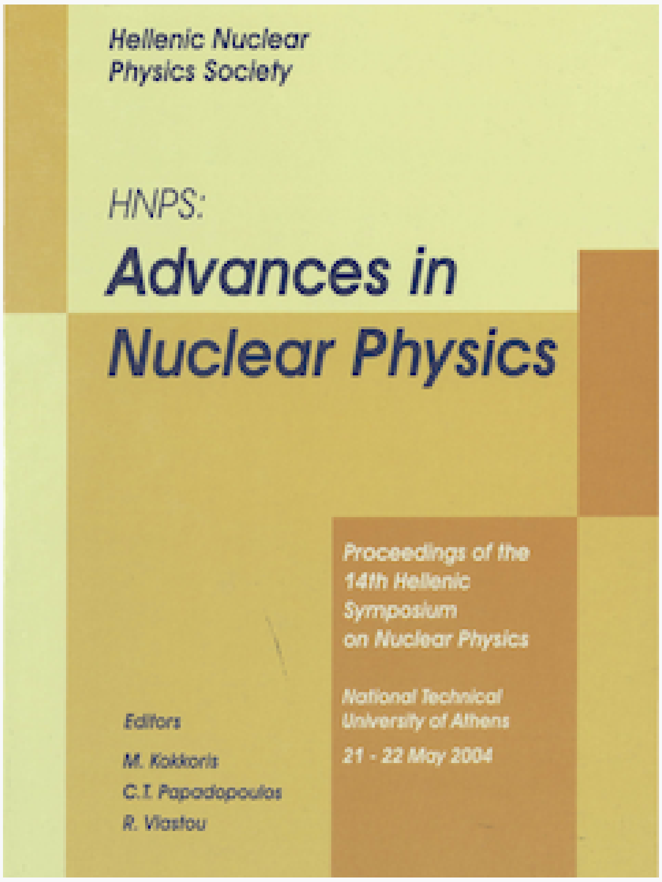

Global predictions for astrophysics applications

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Abstract

Nuclear reaction rates play a crucial role in nuclear astrophysics. In the last decades there has been an enormous effort to measure reaction cross sections and extensive experimental databases have been compiled as a result. In spite of these efforts, most nuclear reaction network calculations still have to rely on theoretical predictions of experimentally unknown rates. In particular, in astrophysics applications such as the s-, r- and p-process nucleosynthesis involving a large number of nuclei and nuclear reactions (thousands). Moreover, most of the ingredients of the calculations of reaction rates have to be extrapolated to energy and/or mass regions that cannot be explored experimentally. For this reason it is important to develop global microscopic or semi-microscopic models of nuclear properties that give an accurate description of existing data and are reliable for predictions far away from the stability line. The need for more microscopic input parameters has led to new developments within the Hartree-Fock-Bogoliubov method, some of which are presented in this paper.

1 Introduction

Nuclear physics plays a major role in the study and description of a large number of energetic astrophysical environments, where the temperatures and densities allow for interactions among particles that lead to nuclear reactions. Strong, electromagnetic and weak interactions (fusion, exchange reactions, photo-disintegrations, beta decays, electron/positron captures, neutrino scattering and captures) can produce nuclei far from stability and thus, require extended knowledge of nuclear structure near and far from stability, as well as decay and fission properties. In particular the s-, p- and r-processes of nucleosynthesis, involve a large number (thousands) of stable and unstable nuclei

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for which reaction rates need to be determined. In spite of the enormous effort to measure reaction cross sections in the past decades, the existing experimental data correspond to only a very small fraction of the data required for the reaction network calculations for such applications. To compensate for the lack of data, theoretical models have been developed with the aim to provide nuclear data for all the nuclides globally. The main requirements for these global models is that they reproduce existing data with accuracy and that at the same time, they give reliable predictions in the experimentally unknown region. For this reason, microscopic or semi-microscopic global models are the preferred choice since they are based as much as possible on first principles, and therefore they are expected to give more reliable extrapolations away from the known region. Many global microscopic approaches have been developed in the last decades, however they are seldom used for practical applications, mainly because of their lack of accuracy in reproducing the existing data. The problem of low accuracy is mainly related to the fact that the computational implementation of these models is rather involved and time-consuming and hence, the adjustment of free parameters on experimental data impracticable. However, with the advent of powerful processors and the availability of more and more CPU power, nowadays global microscopic models can be adjusted with the same ease and accuracy as the phenomenological models. In this work, we present the latest efforts in this direction and give a brief review of the most accurate global microscopic models developed for the description of ground-state properties, nuclear level densities and fission properties.

2 Microscopic mass predictions

Until recently, most atomic masses were obtained from models based, one way or another, on the liquid-drop model, the most updated and successful version being the Finite Range Droplet model (FRDM) [1] (it fits the 2149 $Z \geq 8$ measured masses [2] with an rms error of 0.656 MeV). However, it has now been well demonstrated [3], that Hartree-Fock (HF) calculations using a Skyrme-type force that is fitted to all the mass data, are also feasible and can provide the same accuracy as the most accurate droplet-like formulas. Among the first most accurate microscopic mass formulas was the one derived on the basis of a Skyrme force with pairing correlations taken into account in the BCS approach that lead to an rms error of 0.738 MeV for all the then known 1888 masses [3]. The latest Skyrme mass formulas treat pairing correlations in the Bogoliubov approach (HFB) and have been able to fit all 2149 masses [2] with an rms error from 0.638 to 0.730 MeV [4,5]. The uncertainties in the parameterization of the Skyrme force lead to a series of studies of different forces and methods of calculation within the HFB framework. The main reason for such a study was the realization that a) mass formulas with equivalent data fits do not necessarily give identical extrapolations out to the drip-lines and b) HFB models that give equivalent mass predictions may give rather different results for other nuclear properties such as fission barriers, giant dipole resonances, nuclear level densities, nucleon optical potential etc., that enter in the reaction cross section calculations.

3 Nuclear level densities

In a first attempt to treat properties of excited nuclei on the same footing as ground-state properties, microscopic nuclear level densities based on the statistical model were calculated [6]. The statistical calculations used the deformed HF-BCS predictions of the ground-state properties [3] mentioned in the previous section. The microscopic model enables a consistent treatment of shell effects, pairing correlations, deformation effects and collective excitations. It predicts the 278 experimental neutron resonance spacings [7] with a degree of accuracy ($f_{rms} = 2.14$) comparable to that of the phenomenological back-shifted Fermi-gas-type formulas ($f_{rms} = 1.92$), as can be seen in Fig. 1.

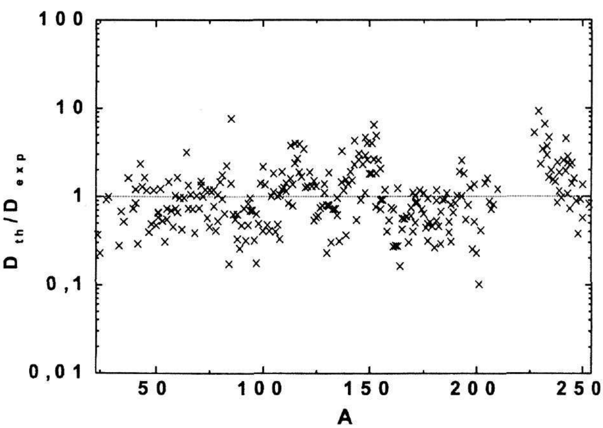

Fig. 1. Ratio of the theoretical D_{th} to experimental D_{exp} [7] s-neutron resonance spacings as a function of the mass number A.

The microscopic level densities have been renormalized to the existing data, namely the s-wave neutron resonance spacings and the cumulative number of low-lying levels. Level densities for more than 8000 nuclei have been made available in a table format (URL:www-astro.ulb.ac.be) for practical applications. These level densities have be used together with the HF-BCS masses to give consistent predictions of radiative capture cross sections for astrophysics applications (see Ref. [8]).

4 Fission properties

Fission properties, such as barriers and paths, spontaneous fission half-lives have also been widely studied within the macroscopic-microscopic FRDM [1]. Recently, an attempt has been made to treat all aspects of fission on a microscopic basis, using a Skyrme-Hartree-Fock approach for the calculation of masses, fission barriers and fission level densities. The potential energy surface of the nucleus has been calculated within the HF-Bogoliubov (HFB) approach with the appropriate restoration of broken symmetries using the force labelled BSk-8 [5,10]. The calculations are constrained with respect to the multipole moments (Q, O, H) and the barriers are determined by the *flooding method* [9]. For the determination of the fission paths we use the multi-dimensional potential energy surfaces in the (β_2, β_3, β_4) deformation space. Starting from the location of the saddle-points, we apply the method of steepest descent to generate the paths leading downhill to the minima. The details of the calculations can be found in [10,11]. The resulting static fission paths are plotted in Fig. 2 with respect to one of the three deformation coordinates, namely β_2. One can see that the inner barrier is in general narrow and symmetric while the outer barrier tends to be broader and more asymmetric.

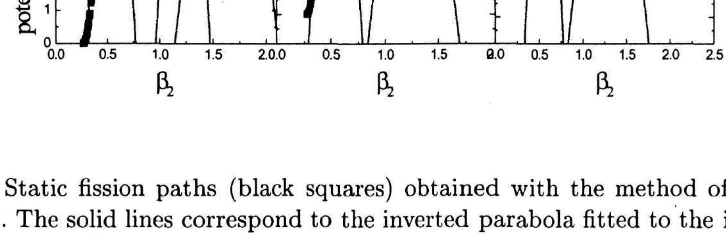

Fig. 2. Static fission paths (black squares) obtained with the method of steepest descent. The solid lines correspond to the inverted parabola fitted to the inner and outer barriers.

For the sake of comparison with experimental values, we also simulate the barriers along the resulting static fission paths with inverted parabolas and extract values for the respective widths $\hbar\omega$. In the present analysis we consider single- and double-humped barriers. The results of the fitting procedure are also shown in Fig. 2. The overall uncertainty in the determination of the barrier heights was estimated to be $\Delta B \approx 1$ MeV and of the widths $\Delta\hbar\omega$ of about 30%. From Fig. 2 one sees that the shape of the outer barrier tends to deviate from an inverted parabola. In the case of ^{238}U, a third hump, comparable to the first two barriers, appears at larger deformations. The assumption of a double-humped fission barrier is therefore, not always an adequate one. In such a case the barrier is considered as triple-humped and the contribution of the inner lower hump is taken to be of minor importance.

The extracted barrier heights and widths are subsequently used to calculate spontaneous fission half-lives T_{SF} in terms of the Hill-Wheeler transmission coefficients. The resulting T_{SF} of several even-even actinides are compared with measured half-lives in Fig. 3. Overall, the deviations between theory and experiment do not exceed 1-2 orders of magnitude. In the case of ^{236,238}U, in particular, the consideration of the third barrier (Fig. 2) leads to a significant improvement of the predicted T_{SF}. However, for ^{242}Pu and ^{250}Cm, the discrepancies amount to several orders of magnitude. The T_{SF} is extremely sensitive to the uncertainties ΔB and $\Delta\hbar\omega$ (exponential dependence). For a given value of $\hbar\omega = 0.6$ MeV, for example, the global uncertainty of $\Delta B \approx 1$ MeV results in $\Delta T_{SF} \approx 10^4$. The deviations from experimental data observed in Fig. 3 therefore, lie within the uncertainties affecting B and $\hbar\omega$.

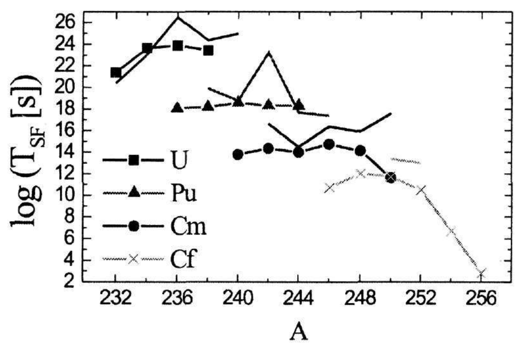

Fig. 3. T_{SF} (s) of even-even nuclei (solid lines) obtained with the HFB barriers are compared with measured ones (symbols) [12].

5 Conclusions

A systematic effort to calculate ground-state properties, as well as nuclear level densities and fission properties of the nucleus within a global, microscopic model has been undertaken in the past decade. Significant improvements in the HF-BCS or HFB models have lead to mass formulas that can compete with the more phenomenological ones, and has opened the way for more accurate and reliable global predictions of levels densities, fission barriers and half-lives among others. The aim is to use the global and consistent calculations of the different nuclear properties to obtain sound and reliable predictions of all nuclear reactions relevant to astrophysics applications.

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