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P. Demetriou, S. Goriely

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P. Demetriou[a] and S. Goriely[b]

[a]Institute of Nuclear Physics, N.C.S.R "Demokritos" , Aghia Paraskevi 15310, Athens, Greece

[b]Institut d'Astronomie et d'Astrophysique, CP-226, Univeristé Libre de Bruxelles, Campus de la Plaine, Boulevard du Triomphe, B-1050 Brussels, Belgium

Abstract

A new level density formula based on a microscopic calculation of the thermodynamic quantities using the deformed Hartree-Fock-BCS method is proposed. In the microscopic approach shell, pairing and deformation effects on the thermodynamic quantities are treated consistently. The final level density formula is shown to be in close agreement with experimental neutron resonance spacings and low energy states. The impact of the newly-determined level densities on nuclear reaction cross sections and rates of relevance in astrophysics applications is presented.

1 Introduction

Until recently, classical or semi-classical analytical models of nuclear level densities (NLD) were used for most of the practical applications. Although statistical and combinatorial approaches have lead to the development of reliable microscopic models, the back-shifted Fermi gas model (BSFG)-or some variant of it-remains the most usual approach for the calculation of spin-dependent NLD's, mainly due to the simple analytical formulae it provides. However, the BSFG model introduces phenomenological improvements to the original analytical formulae of Bethe and therefore, cannot be expected to describe any of the important shell, pairing and deformation effects. In particular, the shell correction to the NLD cannot be introduced by neither an energy shift, nor a simple energy-dependent level density parameter. On the other hand, the complex pairing effect in the BCS approach cannot be reduced to an odd-even energy back-shift(e.g [1]). A much more sophisticated formulation of NLD than the one used in the BSFG approach is required if one pretends to describe the excitation spectrum of a nucleus analytically.

2   Hartree-Fock-BCS method

A new NLD formula within the microscopic statistical approach and based on a Hartree-Fock-BCS method has been constructed. The HF-BCS method is described in detail in [2,3] so we shall just briefly mention some basic features. A conventional 10-parameter Skyrme force, along with a 4-parameter δ-function pairing force, are fitted using the HF-BCS (with blocking) method to 1772 nuclei with A$\geq$36. The rms error for the set of 1772 nuclei is found to be 0.683 MeV. The HF-BCS method is expected to work less well for very light nuclei. Nevertheless, the new mass table gives all 1888 nuclei with $Z, N \geq 8$ appearing in the 1995 compilation [5]. The rms error for the set of 1888 masses is 0.738 MeV, as compared with 0.689 MeV for the same set given by the finite-range-droplet-model predictions [6]. Other quantities, such as deformations and rms charge radii are also predicted in close agreement with experimental data.

3   Microscopic Nuclear Level Densities

The new NLD's obtained with the above-mentioned model also include the following improvements

(1) The density of levels with spin J at an excitation energy U in a nucleus (Z, A) is given by

$$\rho(U, J) = \left[1 - f_{dam}(U)\right]\rho_{sph}(U, J) + f_{dam}(U)\ \rho_{def}(U, J) \qquad (1)$$

where the damping function is divided into an energy damping part and a transitional deformation part given by

$$f_{dam}(U) = \frac{1}{1 + e^{(U - E_{def})/d_u}}\ \left[1 - \frac{1}{1 + e^{(\beta - \beta^*)/d_\beta}}\right]. \qquad (2)$$

The deformation energy $E_{def} = E_{sph} - E_{eq}$ is estimated within the HF-BCS method with the Msk7 Skyrme force. E_{eq} is the energy at the equilibrium deformation and E_{sph} the energy in the spherical configuration. The parameters are taken as $d_u = 2$ MeV, $\beta^* = 0.15$ and $d_\beta = 0.02$. At energies above the deformation energy the nucleus is assumed to become spherical. No shape barriers is assumed in this simple picture. Second, the unphysical sharp transition in the NLD formula from deformed to spherical shapes is avoided by including in the damping function a smooth deformation-dependent transition.

(2) The spherical approximation to the NLD is now estimated with the use of a spherical single-particle level scheme, while the deformed NLD is

derived from the deformed scheme at the equilibrium deformation.

(3) To avoid the unphysical divergence at low temperatures, the traditional formula at $T \to 0$ is corrected by the asymptotic limit given by [7].

4 Results

The new NLD formula has been applied to the calculation of s-neutron resonance spacings, cumulative numbers of low energy levels and the spectra of evaporated particles, all relevant to astrophysical applications.

For the s-neutron resonance spacings D_0 we define the rms deviation as

$$f_{rms} = \exp\left[\frac{1}{N_e}\sum_{i=1}^{N_e}\ln^2\frac{D_{th}^i}{D_{exp}^i}\right]^{1/2} \qquad (3)$$

where $D_{th}(D_{exp})$ is the theoretical (experimental) resonance spacing and N_e is the number of nuclei in the compilation (Fig. 1). The rms deviation found with the present microscopic HF-BCS formula is $f_{rms} = 2.17$ on the 281 experimental data [8] which is comparable with the value of $f_{rms} = 1.97$ obtained with the phenomenological BSFG formula [9] on the same data set.

The total number of observed levels $N(U)$ with excitation energy $\leq U$ (up to which the level scheme is complete) can be estimated and in Fig. 2 we show the results of the comparison of the theoretical predictions $N_{th}(U)$ with the experimental estimates $N_{exp}(U)$ of [10] for ^{208}Pb.
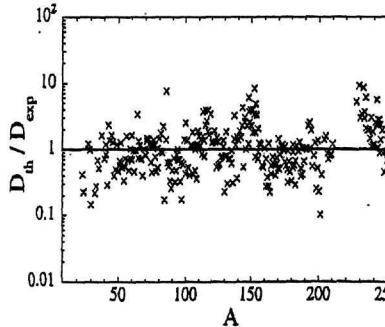

Fig. 1. Ratios of the HFBCS neutron resonance spacings to the experimental one [8].
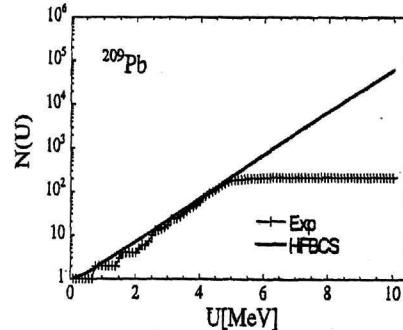
Fig. 2. Cumulative number of low-energy states in ^{209}Pb predicted by the present model and compared with the experimental data [8].

The microscopic NLD's have also been used to calculate low energy proton radiative capture cross sections relevant to the astrophysical p-process. The

modelling of the p-process requires extensive sets of (p, γ) and (γ, p) cross sections for nuclei in the $12 \leq A \leq 210$ mass range. For nuclei above Si theoretical calculations are based on the statistical theory of Hauser-Feshbach and depend strongly on the NLD formulae. In Figs. 3-4 we compare the results obtained with the statistical model code MOST, using the microscopic HF-BCS NLD's, with experimental cross sections. The nucleon-nucleus and alpha-particle-nucleus OP's used in the MOST calculations are those of [11] and [12] respectively, and the γ-ray strength functions are obtained from [13].
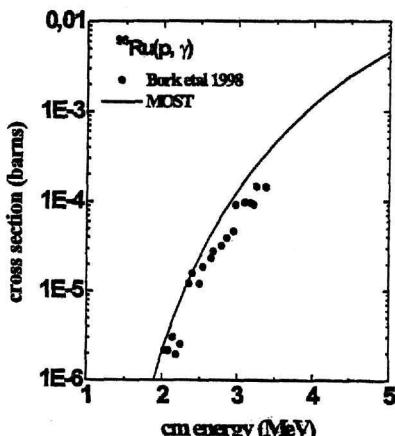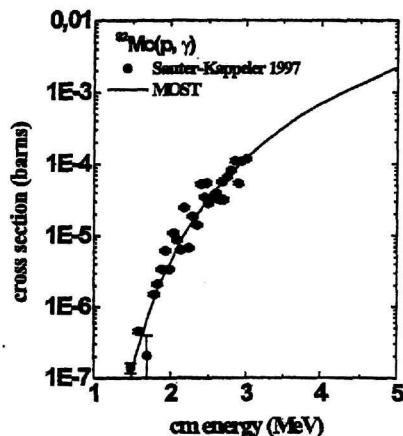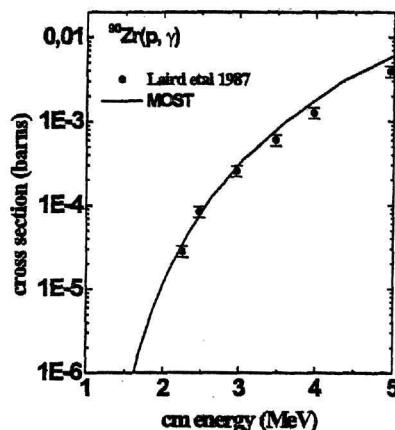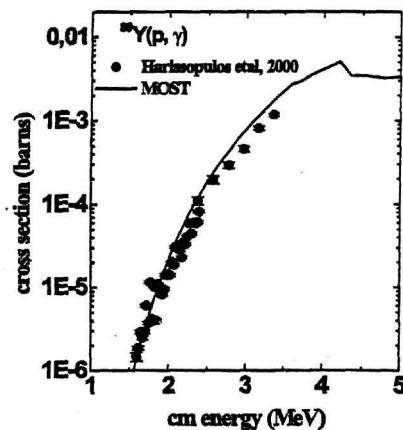

Fig. 3. Cross sections for the ^{89}Y(p, γ)^{90}Zr [14] and ^{92}Mo(p, γ)^{93}Tc [15] reaction compared with the predictions of MOST with HFBCS NLD's.

Fig. 4. The same as Fig. 3 but for the reaction ^{90}Zr(p, γ)^{91}Nb [16] and ^{96}Ru(p, γ)^{97}T [17].

Radiative neutron capture rates play an essential role in our understanding of the s- and r-processes that are responsible for the abundances of the vast

majority of nuclei heavier than Fe. In Fig. 5 we present a comparison of MOST maxwellian-averaged (n, γ) rates obtained with the HF-BCS NLD's, as well as those obtained with the BSFG model NLD's of [9], with experimental measurements at $T = 3 \cdot 10^8$K. All the other input parameters are as mentioned above.
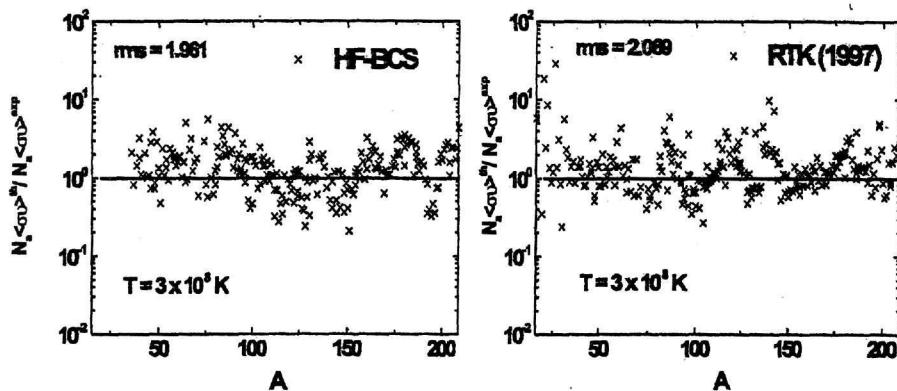

Fig. 5. Ratios of maxwellian-averaged (n, γ) rates, obtained with HFBCS NLD's and BSFG NLD's respectively, over the experimental ones.

5 Conclusions

A new NLD formula, based on the microscopic calculation of the thermodynamic quantities using a Hartree-Fock-BCS method, has been presented and applied to the calculation of neutron resonance spacings, cumulative number of low lying states for which the set is complete, reaction cross sections relevant to the astrophysical p-process and reaction rates relevant to the astrophysical s- and r-process.

The results are in reasonable agreement with the experimental data and comparable with the results of the widely used BSFG model NLD's. However, it is often forgotten that the BSFG model essentially introduces phenomenological improvements to the original analytical formula of Bethe, and consequently none of the important shell, pairing and deformation effects are properly accounted for in such a description. Drastic approximations are usually made in deriving analytical formulae and often their failure to reproduce experimental data is overcome by empirical parameter adjustments. For these reasons, large uncertainties are expected in the BSFG prediction of NLD's, especially when

extrapolating to very low energies (a few MeV) or high (U≥15 MeV) and/or to nuclei far from the valley of β-stability. On the other hand, in the microscopic approach shell, deformation and pairing effects are treated in a natural way, by taking into account the discrete structure of the single-particle scectra. The global microscopic NLD formula based on the Hartee-Fock-BCS ground state properties (single-particle level scheme and pairing strength) can therefore be considered more reliable to describe the yet experimentally unexplored energy and mass regions.

6   Numerical Tables

The NLD formula described in the present paper has been applied to the calculation of the spin-dependent NLD for more than 8000 nuclei ranging from Z=8 to Z=110 and tabulated in an energy and spin grid ($U = 0.25$ to 100 MeV and the lowest 15 spins). The corresponding tables can be found at the website http://www-astro.ulb.ac.be and are retrievable by typing on the atomic number Z of the isotope of interest. The availability of the miscroscopic NLD's in the form of numerical tables should simplify their implementation in any statistical model code making them just as easy to handle as the analytical formulae of the BSFG model. This would allow for an extensive application in reaction network calculations and also for a more detailed comparison with experimental data to explore the applicability and limitations of the HF-BCS model.

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