Global Microscopic Models for Nuclear Reaction Calculations

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Abstract. Important effort has been devoted in the last decades to measuring reaction cross sections. Despite such effort, many nuclear applications still require the use of theoretical predictions to estimate experimentally unknown cross sections. Most of the nuclear ingredients in the calculations of reaction cross sections need to be extrapolated in an energy and/or mass domain out of reach of laboratory simulations. In addition, some applications often involve a large number of unstable nuclei, so that only global approaches can be used. For these reasons, when the nuclear ingredients to the reaction models cannot be determined from experimental data, it is highly recommended to consider preferentially microscopic or semi-microscopic global predictions based on sound and reliable nuclear models which, in turn, can compete with more phenomenological highly-parameterized models in the reproduction of experimental data. The latest developments made in deriving such microscopic models for practical applications are reviewed. It mainly concerns nuclear structure properties (masses, deformations, radii, etc.), level densities at the equilibrium deformation, γ-ray strength, as well as fission barriers and level densities at the fission saddle points.

INTRODUCTION

Strong, weak and electromagnetic interaction processes play an essential role in many different applications of nuclear physics, such as accelerator-driven waste incineration, production of radioisotopes for therapy and diagnostics, charged-particle beam therapy, and material analysis as well as nuclear astrophysics. Although important effort has been devoted in the last decades to measuring reaction cross sections, experimental data only cover a minute fraction of the whole set of data required for such nuclear physics applications. Reactions of interest often concern unstable or even exotic (neutron-rich, neutron-deficient, superheavy) species for which no experimental data exist. Given applications (in particular, nuclear astrophysics and accelerator-driven systems) involve a large number (thousands) of unstable nuclei for which many different properties have to be determined. Finally, the energy range for which experimental data are available is restricted to the small range reachable by present experimental setups. To fill the gaps, only theoretical predictions can be used. For such demanding applications, two major features of the nuclear theory must be contemplated, namely its accuracy, which obviously has always been for most of the application the major (and some time unique) criterion in the model selection, but also its reliability. A microscopic description by a physically sound model based on first principles ensures a reliable extrapolation away from experimentally known region. For these reasons, when the nuclear ingredients to the reaction models (e.g., Hauser-Feshbach) cannot be determined from experimental data, use is made preferentially of microscopic or semi-microscopic global predictions based on sound and reliable nuclear models which, in turn, are accurate enough to compete with more phenomenological highly-parameterized models in the reproduction of experimental data. Global microscopic approaches have been developed for the last decades and are now more or less well understood. However, they are almost never used for practical applications, because of their lack of accuracy in reproducing experimental data, especially when considered globally on a large data set. Different classes of nuclear models can be contemplated according to their reliability, starting from local parametric systematics up to global microscopic approaches. We find in between these two extremes, approaches like the classical (e.g., liquid drop, droplet), semi-classical (e.g., Thomas-Fermi), macroscopic-microscopic (e.g., classical with microscopic corrections), semi-microscopic (e.g., microscopic with phenomenological corrections) and fully microscopic (e.g., mean field, shell model, QRPA) approaches. In a very schematic way, historically, the higher the degree of reliability, the less accurate the model used to reproduce the bulk set of experimental data. The classical or phenomenological approaches are highly parameterized and therefore are often successful in reproducing experimental data, or at least are much more accurate than microscopic calculations. The low accuracy obtained with microscopic models mainly originates from computational complications making the
determination of free parameters by fits to experimental data difficult and computerwise time-consuming. Nowadays, microscopic models can be tuned at the same level of accuracy as the phenomenological models, and therefore could replace the phenomenological inputs little by little in practical applications. In the present paper, we describe the latest developments made to estimate the major nuclear ingredients of relevance in reaction cross-section calculations on the basis of global microscopic models. These concern the ground state properties (Sect. 2), nuclear level densities (NLD) (Sect. 3), fission properties (Sect. 4), and the γ-ray strength (Sect. 5).

MICROSCOPIC MASS PREDICTIONS

Among the ground state properties, the atomic mass \( M(Z,A) \) is obviously the most fundamental quantity (for a review, see [1]). The calculation of the reaction cross section also requires the knowledge of other ground-state properties, such as the deformation, density distribution, and single-particle level scheme. When not available experimentally, these quantities are traditionally extracted from a mass formula that aims at reproducing measured masses as accurately as possible, i.e., typically with an rms deviation of about 700 keV. The importance of estimating all ground-state properties reliably should not be underestimated. For example, the NLD of a deformed nucleus at low energies (typically at the neutron separation energy) is predicted to be significantly (about 30 to 50 times) larger than of a spherical one due principally to the rotational enhancement. An erroneous determination of the deformation can therefore lead to large errors in the estimate of radiative capture cross sections.

Until recently the atomic masses were calculated on the basis of one form or another of the liquid-drop model, the most sophisticated version being the FRDM model [2]. Despite the great empirical success of this formula (it fits the 2149 \( Z \geq 8 \) measured masses [3] with an rms error of 0.656 MeV), it suffers from major shortcomings, such as the incorrect link between the macroscopic part and the microscopic correction, the instability of the mass prediction to different parameter sets, or the instability of the shell correction. It was demonstrated recently [4] that Hartree-Fock (HF) calculations in which a Skyrme force is fitted to essentially all the mass data are not only feasible, but can also compete with the most accurate droplet-like formulas available nowadays. Such HF calculations are based on the conventional Skyrme force of the form

\[
\psi_{ij} = t_0 \left( 1 + x_0 p_0 \right) \delta(r_{ij}) + t_1 \left( 1 + x_1 p_0 \right) \frac{1}{2\hbar^2} \left\{ p_{ij}^2 \delta(r_{ij}) + h.c. \right\} + t_2 \left( 1 + x_2 p_0 \right) \frac{1}{\hbar^2} p_{ij} \cdot \sigma_{ij} \delta(r_{ij}) + \frac{1}{6} t_3 \left( 1 + x_3 p_0 \right) \rho^2 \delta(r_{ij}) + \frac{i}{\hbar^2} W_0 = \frac{(\sigma_i + \sigma_j)}{A} \rho_{ij} \cdot \delta(r_{ij}),
\]

and a δ-function pairing force acting between like nucleons,

\[
v_{\text{pair}}(r_{ij}) = V_{\text{pair}} \left[ 1 - \eta \left( \frac{\rho}{\rho_0} \right)^{\alpha} \right] \delta(r_{ij}).
\]

where \( \rho \) is the density and \( \rho_0 \) the saturation value of \( \rho \). A density-independent (\( \eta = 0 \)) zero range pairing force was originally adopted with a strength parameter \( V_{\text{pair}} \) allowed to be different for neutrons and protons, and also to be slightly stronger for an odd number of nucleons (\( V_{\text{pair}}^N \)) than for an even number (\( V_{\text{pair}}^P \)).

The latest Skyrme forces are derived on the basis of HF calculations with pairing correlations taken into account in the Bogoliubov approach and lead to rms errors with respect to the measured masses of all the 2149 nuclei included in the 2003 atomic mass evaluation [3] with \( Z,N \geq 8 \) of about 0.630 to 0.730 MeV. Despite the success of the HFB mass formula, uncertainties remain in relation to the large parameter space made by the coefficient of the Skyrme and pairing interactions. For this reason, a series of studies of possible modifications to the basic force model and to the method of calculation were initiated all within the HFB framework [4, 5, 6, 7, 8]. The most obvious reason for making such modifications would be to improve the data fit, but there is also a considerable interest in being able to generate different mass formulas even if no significant improvement in the data fit is obtained, since, in the first place, it is by no means guaranteed that mass formulas giving equivalent data fits will extrapolate in the same way out to the neutron-drip line: the closer that such mass formulas do agree in their extrapolations the greater will be our confidence in their reliability. But there is another reason to study different HFB mass models, and that concerns the fact that masses are not the only property of highly unstable nuclei that one might wish to determine by extrapolation from measured nuclei. In particular, many nuclear applications requires also a knowledge of the fission barriers, β-decay strength functions, giant dipole resonances, nuclear level densities, and neutron optical potential of highly unstable nuclei, and it may be that different models that are equivalent from the standpoint of masses may still give different results for other properties. The construction of different HFB mass models is thus motivated also by the quest for a universal framework within which all the different nuclear quantities can be treated.

A set of nine mass tables, referred to as HFB-1 to HFB-9 were designed so far [4, 5, 6, 7, 8] and
the sensitivity of the mass fit and extrapolations towards the neutron drip line analysed. These tables consider modified parameterizations of the effective interaction. In particular HFB-3,5,7 [5, 6] are obtained with a density dependence of the pairing force as inferred from the calculations of the pairing gap in infinite nuclear matter at different densities [9] using a realistic nucleon-nucleon interaction (corresponding to $\eta = 0.45$ and $\alpha = 0.47$ in Eq. 2). For the mass tables HFB-4,5 (HFB-6,7) [6], a low isoscalar effective mass $M_s = 0.92$ ($M_s = 0.8$) is adopted as prescribed by microscopic (Extended Brückner-Hartree-Fock) nuclear matter calculations [10]. The last improvement considered in the HFB-8 and HFB-9 models restores the particle number symmetry by applying the projection-after-variation technique to the HFB wave function [7]. Finally, in the HFB-9 parameterization, the nuclear-matter symmetry coefficient $J$ is constrained to the value of 30 MeV to conform with realistic calculation of neutron matter at high densities [8].

All new mass tables reproduce the experimental masses with the same level of accuracy as the FRDM mass model, i.e., with a rms error of about 0.630 to 0.730 MeV. The HFB rms charge radii as well as the radial charge density distributions are also in excellent agreement with experimental data [7]. In addition, it is found that globally the extrapolations out to the neutron drip line of all these different HFB mass formulas are essentially equivalent. Figure 1 compares the HFB-2 and HFB-9 masses for all nuclei with $8 \leq Z \leq 110$ lying between the proton and neutron drip lines. Although HFB-2 and HFB-9 are obtained from significantly different Skyrme forces, deviations smaller than about 3 MeV are obtained for all nuclei with $Z \leq 110$. In contrast, higher deviations are seen between HFB-9 and FRDM masses (Fig. 1), especially for the heaviest nuclei. For lighter species, the mass differences remain below 5 MeV, but locally the shell and deformation effects can differ significantly. Most interestingly, the HFB mass formulas show a weaker (though not totally vanishing) neutron-shell closure close to the neutron drip line with respect to droplet-like models as FRDM.

Although complete mass tables have now been derived within the HFB approach, further developments that could have an impact on mass extrapolations towards the neutron drip line need to be studied. Most particularly, all HFB mass fits show a strong pairing effect that needs to be re-estimated within the renormalization procedure of [11]. Rotational as well as vibrational correlations need to be studied in more detail. More fundamentally, mean field models need to be improved, so that all possible observables (such as giant dipole, Gamow-Teller excitations, nuclear matter properties, fission barriers) can be estimated coherently on the basis of one unique effective force. These various nuclear aspects are extremely complicated to reconcile within one unique framework and this quest towards universality will most certainly be an important challenge for future fundamental nuclear physics research.

**NUCLEAR LEVEL DENSITIES**

In a similar way to the determination of the nuclear ground-state properties, until recently, only classical analytical models of NLD were used for practical applications. Although reliable microscopic models (in the statistical and combinatorial approaches) have been developed in recent years, the back-shifted Fermi gas model (BSFG) approximation—or some variant of it—remains the most popular approach to estimate the spin-dependent NLD, particularly in view of its ability to provide a simple analytical formula. However, it is often forgotten that the BSFG model essentially introduces phenomenological improvements to the original analytical Fermi gas formulation, 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 shortcomings in matching experimental data are overcome by empirical parameter adjustments. It is well accepted that the shell correction to the NLD cannot be introduced by either an energy shift or a simple energy-dependent level-density parameter, and that the complex BCS pairing effect cannot be reduced to an odd-even energy back-shift (e.g., [12]). A 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, especially because of the high sensitivity of NLD to the different empirical parameters. For these reasons, large uncertainties
HFB (right panel) to experimental \( D_{\text{exp}} \) deformation energy to spherical shapes at excitation energies exceeding the dependent factor describes the transition from deformed takes two specific effects into account. First, an energy-a phenomenological deformation damping function that NLD of deformed nuclei has been solved by introducing parameter and energy. The difficulty in describing the model provides in a consistent way the single-particle of accuracy as the global BSFG formulas. The HFBCS to reproduce experimental data with the same degree improvements to an accurate and reliable determination of NLD.

are expected in the BSFG prediction of NLD, especially when extrapolating to very low (a few MeV) or high energies \( (U \gtrsim 15\text{MeV}) \) and/or to nuclei far from the valley of \( \beta \)-stability.

Several approximations used to obtain the NLD expressions in an analytical form can be avoided by quantitatively taking into account the discrete structure of the single-particle spectra associated with realistic average potentials. This approach has the advantage of treating in a natural way shell, pairing, and deformation effects on all the thermodynamic quantities. The computation of the NLD by this technique corresponds to the exact result that the analytical approximation tries to reproduce, and remains by far the most reliable method for estimating NLD (despite inherent problems related to the choice of the single-particle configuration and pairing strength).

The NLD estimated within the statistical approach based on a HFBCS ground-state description was shown [13] to reproduce experimental data with the same degree of accuracy as the global BSFG formulas. The HFBCS model provides in a consistent way the single-particle level scheme, pairing strength, as well as the deformation parameter and energy. The difficulty in describing the NLD of deformed nuclei has been solved by introducing a phenomenological deformation damping function that takes two specific effects into account. First, an energy-dependent factor describes the transition from deformed to spherical shapes at excitation energies exceeding the deformation energy \( E_{\text{def}} = E_{\text{ sph}} - E_{\text{ eq}} \) (where \( E_{\text{eq}} \) is the energy at the equilibrium deformation and \( E_{\text{ sph}} \) the energy in the spherical configuration). Second, the slightly deformed nuclei are described by including in the damping function a smooth deformation-dependent transition.

NLDs at low energies are remarkably sensitive to the pairing interaction. In [13], the pairing correction is introduced in the constant-G approximation where the strength is renormalized with respect to the original one derived from the mass fit. This inconsistent treatment of the pairing strength is found necessary to ensure an accurate description of the experimental s-neutron resonance spacings, as shown in Fig. 2. The quality of the NLD formula can be described by the rms deviation factor defined as

\[
f_{\text{rms}} = \exp \left( \frac{1}{N_{e}} \sum_{i} \ln^{2} \frac{D_{\text{th}}}{D_{\text{exp}}} \right)^{1/2},
\]

where \( D_{\text{th}}(D_{\text{exp}}) \) is the theoretical (experimental) resonance spacing and \( N_{e} \) is the number of nuclei in the compilation. For the microscopic HFBCS formula, \( f_{\text{rms}} = 2.17 \) on the 295 experimental data [14], which is comparable with the value of \( f_{\text{rms}} = 1.78 \) obtained with the phenomenological BSFG formula [15] on the same data set. The microscopic NLD formula also gives reliable extrapolation at low energies where experimental data on the cumulative number of levels is available [13]. Furthermore, the microscopic HFBCS model has been renormalized on experimental (neutron resonance spacings and low-lying levels) data to account for the available experimental information. NLDs are provided in a tabular form in order to avoid the loss of precision with analytical fits. The complete set of HFBCS-based NLD tables on a large energy and spin grid is available at http://www-astro.ulb.ac.be.

A similar formulation can also be derived on the basis of the HFB ground state, as described in the previous section. The Skyrme force BSk8 corresponding to the HFB-8 masses [7] has been used to estimate the resonance spacing at the neutron separation energy. As seen in Fig. 2, the agreement with experimental data is rather good, though less satisfactory than within the HFBCS approach. This is principally due to the low effective mass \( M^{*}/M = 0.8 \) characterizing the BSk8 force and leading to a rather low single-particle level density at the Fermi energy. The HFB NLD formula based on the BSk8 force has the advantage of being possibly applied to the estimate of the NLD at the fission saddle points determined within the same coherent framework (see next section).

Important effort still has to be made to improve the microscopic description of collective (rotational and vibrational) effects, and the disappearance of these effects at increasing energies. Coherence in the pairing treatment of the ground- and excited-state properties also needs to be worked out in more detail. Further exploration of the combinatorial method (e.g., [16]) will also bring new improvements to an accurate and reliable determination of NLD.
FISSION PROPERTIES

So far, extended tables of fission barriers have mainly been constructed in the microscopic-macroscopic framework of the liquid drop model (e.g., [17]) or the Extended Thomas-Fermi plus Strutinsky Integral (ETFSI) method [18]. In order to increase the predictive power, the HFB method based on the BSk8 effective Skyrme interaction has been used to study the fission properties of heavy nuclei. The same framework as the one described above is used, i.e., the full HFB model corrected for the restoration of broken symmetries (translation, particle number, rotation) and constrained on the quadrupole, octupole, and hexadecapole moments. In addition to the axial deformation considered for equilibrium shapes, the reflection asymmetry (including the projection on the good parity quantum number) is taken into account at large deformations, where it is known to affect the outer barrier height. The energy surfaces are analysed using the flooding method [18]. More details can be found in [19]. The resulting HFB fission barriers are found to be in agreement with experimental data within roughly 1 MeV. This level of accuracy, though far from being satisfactory for many applications, is similar to the one obtained by previous global models [17, 18]. Future microscopic investigations will be needed to improve the accuracy. The HFB energy surface is also analysed to estimate the static fission path and the corresponding widths at both the inner and outer saddle points, assuming that the barrier shape can be well described by an inverted parabola. Interestingly, the shape of the fission barriers often deviates from a simple inverted parabola and a wide third barrier at large deformations is required. Details are given in [20].

The NLD at the fission saddle points is a fundamental quantity needed to estimate fission transmission coefficients. So far, only parametric modifications of the BSFG formula have been adopted to estimate the local increase of the NLD at the saddle point relative to the one at the equilibrium deformation. This empirical approach is exclusively guided by an experimental cross section, so that for unknown reactions the lack of a reliable theory makes the determination of the transition state NLD highly uncertain. In the global microscopic approaches described in the present paper, a sound determination of the NLD at the fission saddle point can also be derived. Based on the constrained HFB model, the single-particle level scheme at both the inner and saddle points is estimated and used within the partition function model to generate the NLD at the saddle point deformations. No damping of the collective effects at increasing excitation energies is taken into account for the NLD at the saddle points. It is also found that the NLD calculated without pairing interaction gives a better description of the low-energy fission cross section. The $a_{fp}/a$ ratio of the NLD $a$-parameter at the (inner or outer) saddle point to the value in the equilibrium ground-state configuration is displayed in Fig.3 for $^{235}$U and $^{240}$Pu. Note that the plotted intrinsic $a_{fp}/a$ ratio corresponds to the entropy $S_{fp}/S$ ratio. As seen in Fig. 3, the $a_{fp}/a$ ratio can reach relatively large values at low energies and the energy dependence can be different for the inner or outer barriers.

As far as the neutron-induced fission cross sections are concerned, some results within the statistical model can be found in [20]. The major uncertainty obviously lies in the exact determination of the fission barrier height. A 1 MeV uncertainty affects drastically the fission cross section, especially at low energies close to the fission threshold. However, if the fission barrier height is adjusted and the spherical microscopic optical potential of [21] is renormalized (globally) to take deformation effects into account, the fission cross section can be in rather good agreement with experiment, taking into account that all inputs (except the fission barrier height) are derived from global microscopic models. Furthermore, it should be added that all these inputs at equilibrium and saddle point deformations are coherently determined within the same HFB model obtained with the same effective interaction.

$\gamma$-RAY STRENGTH FUNCTION

The total photon transmission coefficient from a compound nucleus excited state is also one of the key ingredients for statistical cross section evaluation. The photon transmission coefficient is most frequently described in the framework of the generalized Lorentzian model of the giant dipole resonance (GDR) [22, 23]. Until recently, this model has even been the only one used for practical applications, and more specifically when global predictions are requested for large sets of nuclei.

The Lorentzian GDR approach suffers, however, from...
shortcomings of various sorts. It is unable to predict the enhancement of the $E1$ strength at low energies and even if a Lorentzian function provides a suitable representation of the $E1$ strength, the location of its maximum and its width remain to be predicted from some underlying model for each nucleus. This approach clearly lacks reliability when dealing with exotic nuclei.

In view of this situation, combined with the fact that the GDR properties and low-energy resonances may influence substantially the predictions of radiative capture cross sections, it is clearly of substantial interest to develop models of the microscopic type, which are hoped to provide a reasonable reliability and predictive power for the $E1$-strength function. Attempts in this direction have been conducted within the QRPA model based on a realistic Skyrme interaction. The QRPA $E1$-strength functions obtained within the HFBCS [24] as well as HFB framework [25] have been shown to reproduce satisfactorily the location and width of the GDR and the average resonance capture data at low energies [22]. The aforementioned QRPA calculations have been extended to all the $8 < Z < 110$ nuclei lying between the two drip lines. In the neutron-deficient region as well as along the valley of $\beta$-stability, the QRPA distributions are very close to a Lorentzian profile. However, significant departures from a Lorentzian are found for neutron-rich nuclei. In particular, QRPA calculations [24, 25] show that the neutron excess affects the spreading of the isovector dipole strength, as well as the centroid of the strength function. The energy shift is found to be larger than predicted by the usual $A^{-1/6}$ or $A^{-1/3}$ dependence given by the phenomenological liquid drop approximations. In addition, some extra strength is predicted to be located at sub-GDR energies, and to increase with the neutron excess. Even if it represents only about a few percents of the total $E1$ strength, it can be responsible for an increase by more than an order of magnitude of the radiative capture cross section by exotic neutron-rich nuclei [24, 25].

**CONCLUSIONS**

Many nuclear applications involve a large number of unstable nuclei and therefore require the use of global approaches. The extrapolation to exotic nuclei or energy ranges far away from experimentally known regions constrains the use of nuclear models to the most reliable ones, even if empirical approaches sometimes present a better ability to reproduce experimental data. A subtle compromise between the reliability, accuracy, and applicability of the different theories available has to be found according to the specific application considered. A continued effort to improve the prediction of the reaction, and more particularly fission cross sections will require a better coherent description of the ground-state as well as fission properties, i.e., in particular masses, radii, deformations, and fission barrier heights. Nuclear level densities and $\gamma$-ray strength functions remain also on the fundamental input in reaction theory that need to be further explored within microscopic approaches.

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