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Recent progress in mass predictions

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Abstract. We review the latest efforts devoted to the global prediction of atomic masses. Special attention is paid to the new developments made within the Hartree-Fock-Bogolyubov framework. So far, 9 HFB mass tables based on different parametrizations of the effective interactions in the Hartree-Fock and pairing channels have been published. We analyze their ability to reproduce experimental masses as well as nuclear-matter and giant-resonance properties. The possibility to derive within the HFB framework a universal effective interaction that can describe all known properties of the nuclei (including their masses) and of asymmetric nuclear matter is critically discussed.

PACS. 21.30.Fe Forces in hadronic systems and effective interactions – 21.60.Jz Hartree-Fock and random-phase approximations

1 Introduction

Attempts to develop formulas estimating the nuclear masses of nuclei go back to the 1935 "semi-empirical mass formula" of von Weizsäcker [1]. Improvements have been brought little by little to the original liquid-drop mass formula, leading to the development of macroscopic-microscopic mass formulas, where microscopic corrections to the liquid drop part are introduced in a phenomenological way (for a review, see [2]). In this framework, the macroscopic and microscopic features are treated independently, both parts being connected exclusively by a parameter fit to experimental masses. Later developments included in the macroscopic part properties of infinite and semi-infinite nuclear matter and the finite-range character of nuclear forces. 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 [3]. Despite the great empirical success of this formula (it fits the 2149 $Z \geq 8$ measured masses [4] with an r.m.s. error of 0.656 MeV), it suffers from major shortcomings, such as the incoherent 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. The quality of the mass models available is traditionally estimated by the r.m.s. error obtained in the fit to experimental data and the associated number of free parameters. However, this overall accuracy does not imply a reliable extrapolation far away from the experimentally known region in view of the possible shortcomings linked to the physics theory underlying the model. The reliability of the mass extrapolation is a second criterion of first importance when dealing with specific applications such as astrophysics, but also more generally for the predictions of experimentally unknown ground- and excited-state properties. Generally speaking, the more microscopically grounded is a mass formula, the better one would expect its predictive power to be. In the present paper, we describe the latest developments made to estimate nuclear masses on the basis of global mean-field models and the ability of such models to reproduce some nuclear-matter and giant-resonance properties.

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2 The Hartree-Fock mass formulas

It was demonstrated recently [5] 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

$$\begin{aligned} v_{ij} &= t_0(1+x_0P_\sigma)\delta(\mathbf{r}_{ij}) \\ &\quad + t_1(1+x_1P_\sigma)\frac{1}{2\hbar^2}\{p_{ij}^2\delta(\mathbf{r}_{ij}) + \text{h.c.}\} \\ &\quad + t_2(1+x_2P_\sigma)\frac{1}{\hbar^2}\mathbf{p}_{ij}\cdot\delta(\mathbf{r}_{ij})\mathbf{p}_{ij} \\ &\quad + \frac{1}{6}t_3(1+x_3P_\sigma)\rho^\gamma\delta(\mathbf{r}_{ij}) \\ &\quad + \frac{i}{\hbar^2}W_0(\boldsymbol{\sigma}_i+\boldsymbol{\sigma}_j)\cdot\mathbf{p}_{ij}\times\delta(\mathbf{r}_{ij})\mathbf{p}_{ij}\,, \end{aligned} \tag{1}$$

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

$$v_{\mathrm{pair}}(\mathbf{r}_{ij}) = V_{\pi q} \left[1 - \eta \left(\frac{\rho}{\rho_0}\right)^{\alpha}\right] \delta(\mathbf{r}_{ij}), \qquad (2)$$

where ρ is the density and ρ_0 the saturation value of ρ. The strength parameter $V_{\pi q}$ is allowed to be different for neutrons and protons, and also to be stronger for an odd number of nucleons ($V_{\pi q}^-$) than for an even number ($V_{\pi q}^+$). The HF formula adds to the energy corresponding to the above forces the Coulomb energy and a phenomenological Wigner term of the form

$$E_{\mathrm{W}} = V_{\mathrm{W}} \exp\left\{-\lambda\left(\frac{N-Z}{A}\right)^2\right\} \qquad (3)$$

$$+ V'_{\mathrm{W}}|N-Z| \exp\left\{-\left(\frac{A}{A_0}\right)^2\right\}. \qquad (4)$$

A completely microscopic HF mass formula, known as HFBCS-1, was constructed for the first time in [5]. It consists of a tabulation of the masses of all nuclei lying between the drip lines over the range $Z, N \geq 8$ and $Z \leq 120$, calculated by the HF method with a Skyrme-type force, together with a BCS treatment of pairing. In order to improve the description of highly neutron-rich nuclei, the BCS approach was later replaced by the full HF-Bogoliubov (HFB) calculation [6]. These two mass formulas give comparable fits (typically with a r.m.s. deviation of about 0.75 MeV) to the 1888 measured masses of nuclei with $N, Z \geq 8$ that appear in the 1995 compilation [7]. A comparison between HFB and HFBCS masses shows that the HFBCS model is a very good approximation to the HFB theory provided both models are fitted to experimental masses. The extrapolated masses never differ by more than 2 MeV below $Z \leq 110$. The reliability of the HFB predictions far away from the experimentally known region, and in particular towards the neutron drip line, is however increased thanks to the improved Bogoliubov treatment of the pairing correlations.

The new data made available in 2001 [8] (with 382 "new" nuclei out of which only 45 are neutron rich) revealed significant limitations in both the HFBCS-1 and HFB-1 models. This defiency was cured in the subsequent HFB-2 mass formula [9], where considerable improvement was obtained by modifying the prescription for the cutoff of the spectrum of s.p. states over which the pairing force acts. The r.m.s. error with respect to the measured masses of all the 2149 nuclei included in the latest 2003 atomic mass evaluation [4] with $Z, N \geq 8$ is 0.659 MeV [9]. Despite the success of the HFB-2 mass formula, it was not regarded as definitive, in particular in relation to the large and uncertain 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 [10,11,12,13]. 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. An understanding of the r-process nucleosynthesis, in particular, requires also a knowledge of the nuclear-matter equation of state, as well as fission barriers, β-decay strength functions, giant dipole resonances, nuclear level densities and neutron optical potential of highly unstable nuclei. It may be that different models that are equivalent from the standpoint of masses may still give different results for other properties. Our intention to develop different HFB mass models is thus motivated also by the quest for a universal framework within which all the different nuclear aspects can be estimated.

For this reason, a set of additional 7 new mass tables, referred to as HFB-3 to HFB-9, and the corresponding effective forces, known as BSk3 to BSk9, respectively, were designed and the sensitivity of the mass fit and extrapolations towards the neutron drip line analysed. These new tables consider modified parametrizations of the effective interaction. In particular HFB-3, 5, 7 [10,11] 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 [14] using a "bare" or "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) [11], 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 [15]. The 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 [12]. Finally, while in all calculations prior to the HFB-9, the nuclear-matter symmetry coefficient J was kept to the lowest acceptable value (*i.e.* $J = 28$ MeV) to avoid the collapse of neutron matter at densities above saturation, in the HFB-9 parameterization [13], J is constrained to the value of 30 MeV to conform with realistic calculation of neutron matter at high densities (see below). All new mass tables reproduce the 2149 experimental masses [4] with a high level of accuracy, *i.e.* with a r.m.s. error of about 0.65 MeV, except in the case of HFB-9, for which the constraint on $J = 30$ MeV rises the r.m.s. value to 0.73 MeV.

The HFB r.m.s. charge radii as well as the radial charge density distributions are also in excellent agreement with experimental data [12]. More specifically, the deviation between the theoretical HFB-9 and experimental r.m.s. charge radii for the 782 nuclei with $Z, N \geq 8$ listed in the 2004 compilation [16] amounts to only 0.027 fm. The Skyrme forces were also tested on their ability to reproduce excited state properties. In particular, the giant

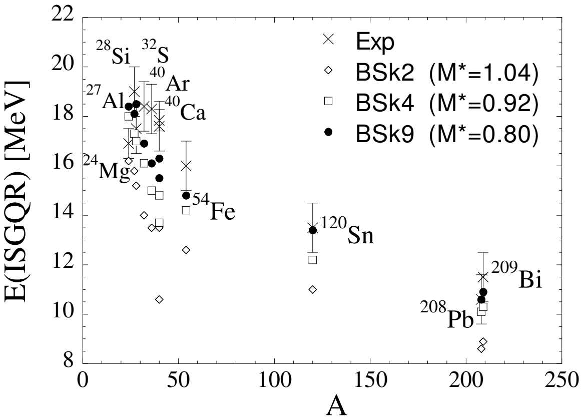

Fig. 1. Comparison of experimental and HFB+QRPA ISGQR energies for spherical nuclei. The HFB + QRPA results are shown for 3 forces (BSk2, BSk4 and BSk9) characterized by different nucleon effective mass M^*.

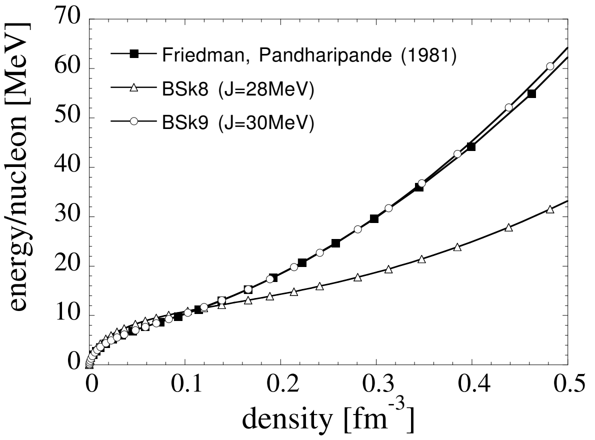

Fig. 2. Energy per nucleon as a function of density of neutron matter for the forces BSk8 and BSk9, and for the calculations of ref. [24].

dipole resonance properties obtained within the HFB plus Quasi-particle Random Phase Approximation (QRPA) framework with the BSk2-7 forces were found to agree satisfactorily with experiments [17]. As far as isoscalar giant quadrupole resonance (ISGQR) is concerned, a comparison with experiments provides a stringent test for the adopted values of the nucleon effective mass (M_s^*). Figure 1 compares the experimental [18,19,20,21,22,23] and theoretical ISGQR excitation energies obtained in the framework of the HFB+QRPA for 3 of our forces, namely BSk2 ($M_s^* = 1.04$), BSk4 ($M_s^* = 0.92$) and BSk9 ($M_s^* = 0.80$). The agreement is seen to be excellent for the BSk9 force characterized by the low effective mass $M_s^* = 0.80$, as also inferred from realistic nuclear-matter calculations.

All our original HFB forces lead to a neutron matter that was a little softer than the prediction of realistic neutron matter calculations, as, for example, in the work of Friedman and Pandharipande [24]. The situation is well represented in fig. 2 by the case of BSk8; all our earlier forces lead to essentially the same curves. In fact, there

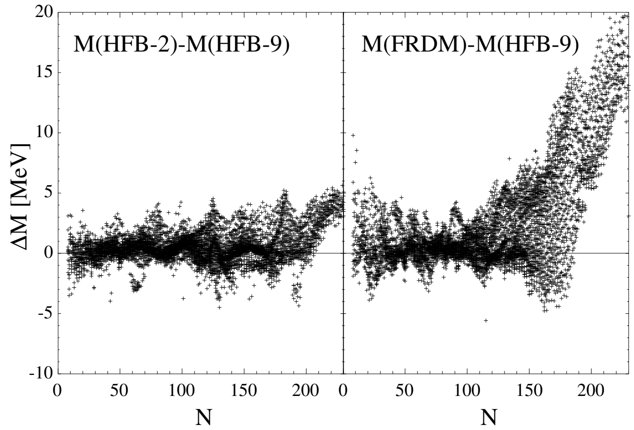

Fig. 3. Differences between the HFB-2 masses and the HFB-9 (left panel) or FRDM (right panel) masses as a function of the neuton number N for all nuclei with $8 \le Z \le 110$ lying between the proton and neutron drip lines.

was a general tendency in our mass fits for neutron matter to be still softer, with an optimal mass fit leading to an unphysical collapse of neutron matter at sub-nuclear densities. We were able to avoid this contradiction with the known stability of neutron stars by imposing a nuclear-matter symmetry coefficient $J = 28$ MeV. To conform with the calculations of neutron matter at high densities [24], the latest BSk9 force was constrained in such a way that $J = 30$ MeV. As seen in fig. 2, this constraints leads to a neutron matter energy per nucleon in excellent agreement with the Friedman and Pandharipande curve. As explained above, this constraint inevitably rises the r.m.s. error. This compromise on the mass accuracy is however essential for a correct description of the transition from nuclear matter to nuclei, as required in particular during the decompression of nuclear matter composing the inner crust of neutron stars [13,25]. Future accurate measurements of the neutron skin thickness of finite nuclei will hopefully help in further constraining the value of J (for more details, see [13]).

3 Extrapolations

Globally the extrapolations out to the neutron drip line of all these different HFB mass formulas are, so far, essentially equivalent. Figure 3 compares the HFB-2 and HFB-9 masses for all nuclei with $8 \le Z \le 110$ lying between the proton and neutron drip lines. Although HFB-2 and HFB-9 masses are obtained from significantly different Skyrme forces, deviations not larger than 5 MeV are obtained for all nuclei with $Z \le 110$. In contrast, higher deviations are seen between HFB-9 and FRDM masses (fig. 3), 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 (*e.g.* [10,11]).

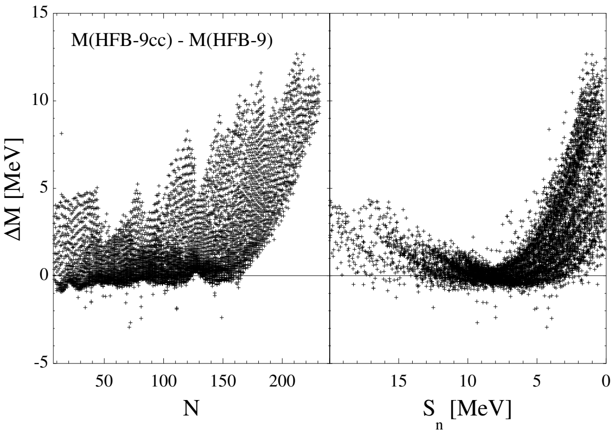

Fig. 4. Differences between the HFB-9cc and HFB-9 masses as a function of N (left panel) and the neutron separation energy S_n (right panel) for all nuclei with $8 \leq Z \leq 110$ lying between the proton and neutron drip lines.

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 most probably accounts in part for extra correlations that have not been explicitly included in our calculation of the total binding energy (note, however, that the good mass fits shows that these correlations are included implicitly in a way or another through the adjustement of the force parameter). In particular, our HFB calculation should also explicitly include the correction for vibrational zero-point motion. To the best of our knowledge, there exists no strategy to estimate the vibrational correction properly and at the same time include them in a global mass fit as ours with current computing resources. Finally, some specific effects still need to be worked out in detail. In particular, the interplay between the Coulomb and strong interactions was shown [26] to lead to an enhancement of the Coulomb energy in the nuclear surface that could solve the Nolen-Schiffer anomaly, *i.e.* the systematic reduction in the estimated binding energy differences between mirror nuclei with respect to experiment. This Coulomb correlation effect could in fact significantly affect the nuclear-mass predictions close to the neutron drip line. To analyse its impact, we have refitted the BSk9 Skyrme force excluding the contribution from the Coulomb exchange energy, since, as shown by [26], in a good approximation the Coulomb correlation energy cancels the Coulomb exchange energy. The final force leads to an r.m.s. error on all the 2149 experimental masses of 0.73 MeV, *i.e.* a value identical to the HFB-9 one. The resulting HFB-9cc masses are seen in fig. 4 to differ by more than 10 MeV from the HFB-9 masses close to the neutron drip line. This effect is actually larger than the one studied so far (see fig. 3) and will need to be further scrutinized.

More fundamentally, mean-field models still need to be studied coherently and confronted to all possible observables (such as giant resonances, nuclear-matter properties, fission barriers, ...) on the basis of one unique effective force. These various nuclear aspects are extremely complicate to reconcile within one unique framework and this quest towards universality will most certainly be an important challenge for future fundamental nuclear-physics research.

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