Nuclear Mass Predictions within the Skyrme HFB Theory

M. Samyn*, S. Goriely* and J. M. Pearson†

*Institut d’Astronomie et d’Astrophysique, ULB - CP226, 1050 Brussels, Belgium
†Département de Physique, Université de Montréal, Montréal (Québec), H3C 3J7 Canada

Abstract. To increase the reliability of predictions of highly neutron-rich nuclear masses we systematically analyze the sensitivity of Hartree-Fock-Bogoliubov (HFB) mass formulae to various physical inputs, such as a density dependence of the pairing interaction, a low effective mass, the particle-number projection, the symmetry energy, . . . We typically use a 10-parameter Skyrme force and a 4-parameter δ-function pairing force. The 14 degrees of freedom are adjusted to the masses of all measured nuclei with \(N, Z \geq 8\) given in the 2001 and 2003 Audi et al. compilations. The masses of light and proton-rich nuclei are corrected by a 4-parameter phenomenological Wigner term. With more than ten such parameter sets complete mass tables are constructed, going from one drip line to the other, up to \(Z = 120\).

INTRODUCTION

In the last few years we have been able to construct complete mass tables by the Hartree-Fock-Bogoliubov (HFB) method [1, 2, 3, 4, 5], with the parameters of the underlying forces being fitted to essentially all of the available mass data. This contribution is an overview of the major modifications made since the HFB-2 mass formula [2], the first of our models that was able to give a satisfactory fit to the new data that had accumulated since the 1995 Atomic Mass Evaluation [6]. The most obvious reason for making such changes would be to improve the data fit, but there is also a considerable astrophysical interest in being able to generate different mass formulae even if no significant improvement in the data fit is obtained. The main point here is that the r-process of stellar nucleosynthesis proceeds through the formation of nuclei that are so highly neutron rich that their properties cannot be measured but must be inferred by extrapolating the properties of known nuclei, and there is no guarantee that mass formulae giving equivalent mass-data fits will still give the same masses out towards the neutron drip line. Moreover, even if they do, it is still possible that the underlying model (forces) will give different results for other properties relevant to the r-process (see Section 1 of [3]). Predictions for the equation of state of neutron star matter could likewise differ.

Basically, we discussed in [3] the role of a possible density dependence of the pairing interaction, while in [4] we examined the question of the effective nucleon mass to be imposed on the Skyrme force. In [5] we extended our HFB model by the restoration of the particle-number symmetry. In a coming paper [7], the symmetry energy coefficient will be set to reproduce the energy per nucleon of neutron matter at high densities.

After recalling the main features of our HFB model, we will discuss our mass fit procedure and the ability of our last parameter set BSk8 (obtained including the particle-number projection) to predict masses and radii. The corresponding mass table, HFB-8, is finally compared with the earlier HFB-6 and HFB-2 mass tables.

THE HFB MODEL

For convenience we recall some of the essential features of these HFB models. They are based on conventional Skyrme forces of the form

\[
v_{ij}^{ph} = t_0(1 + x_0 P_0) \delta(r_{ij}) + t_1(1 + x_1 P_0) \frac{1}{2\hbar^2} \left\{ p_{ij}^2 \delta(r_{ij}) + h.c. \right\} + t_2(1 + x_2 P_0) \frac{1}{\hbar^2} p_{ij} \times p_{ij} \times \delta(r_{ij}) + t_3(1 + x_3 P_0) P_0^2 \Delta \delta(r_{ij})
\]

(1)

in the particle-hole (ph) channel, and in the particle-particle (pp) channel a δ-function pairing force acting between like nucleons treated in the full Bogoliubov framework

\[
v_{ij}^{pp} = V_{\sigma_{ij}} \left[ 1 - \eta \left( \frac{\rho}{\rho_0} \right)^\eta \right] \delta(r_{ij}),
\]

(2)

where \(\rho \equiv \rho(r)\) is the local density, and \(\rho_0\) is its equilibrium value in symmetric infinite nuclear matter (INM).
Actually, it was only with models HFB-3 [3], HFB-5 [4], and HFB-7 [4] that the possibility of a density dependence in the pairing force was admitted; in all our other HFB models, HFB-1 [1], HFB-2 [2], HFB-4 [4], and HFB-6 [4] we had \( \eta = 0 \), as will be the case in the present paper.

An important aspect relating to \( \delta \)-function pairing forces concerns the cutoff to be applied to the space of single-particle (s.p.) states over which the force is allowed to act: both BCS and Bogoliubov calculations diverge if this space is not truncated [8, 9]. However, making such a cutoff is not simply a computational device but is rather a vital part of the physics, pairing being essentially a finite-range phenomenon. To represent such an interaction by a \( \delta \)-function force is thus legitimate only to the extent that all high-lying excitations are suppressed, although how exactly the truncation of the pairing space should be made will depend on the precise nature of the real, finite-range pairing force. It was precisely our ignorance on this latter point that allowed us in [2] to exploit the cutoff as a new degree of freedom: we found there an optimal mass fit with the spectrum of s.p. states \( \epsilon_i \) confined to lie in the range

\[
E_F - \epsilon_\Lambda \leq \epsilon_i \leq E_F + \epsilon_\Lambda, \tag{3}
\]

where \( E_F \) is the Fermi energy of the nucleus in question, and \( \epsilon_\Lambda \) is a free parameter. We shall adopt the same parameterization in the present paper.

**Restoration of Broken Symmetries**

Mean-field approaches, such as the HFB used here, establish an intrinsic frame of the nucleus and consequently break several symmetries of the Hamiltonian and the wave function in the laboratory frame [10, 11]. In particular, finite nuclei break translational invariance, deformed nuclei rotational invariance, reflection-asymmetric shapes the parity symmetry, and the HFB framework the particle-number symmetry. These symmetry breakings are required to include the desired correlations to the modeling (as multi-particle-multi-hole states), but at the same time gives rise to an admixture of excited states to the calculated ground state. The broken symmetries can be restored rigorously by projecting the wave function on the exact quantum numbers. A simpler procedure aims at estimating the contribution to the binding energy in a suitable approximation, and to add the resulting correction to the binding energy. We adopted such a procedure in some of our previous mass formulas, in particular to estimate the center-of-mass (cm) correction from the recoil energy, and the rotational correction within the cranking model [12].

**Center-of-mass motion.** As far as the cm correction is concerned, the approximate prescription of Butler et al. [13] was replaced in [4] by a more fundamental calculation of the recoil energy.

**Particle-number projection.** The particle-number symmetry has been very recently restored and taken into account in the global mass fit [5]. The so-called PLN method is used. It consists of an approximate Lipkin-Nogami projection before variation, followed by the exact projection on the good particle number after variation. We present here its impact on the mass fit.

**Rotational correction.** As suggested and discussed in [5], we adopt for the rotational energy the phenomenological prescription

\[
E_{\text{rot}} = bE_{\text{rot}}^{\text{rank}} \tanh(c|\beta_2|), \tag{4}
\]

where \( E_{\text{rot}}^{\text{rank}} \) is the rotational energy obtained with the cranking value of the moment of inertia and \( \beta_2 \) is the dimensionless quadrupole moment defined as a function of the quadrupole moment \( Q_2 \) and the reduced radius \( R_0 \) by \( \beta_2 = \sqrt{\frac{\pi}{3}}Q_2/(3AR_0^2) \). Experimental information on the mass of well deformed nuclei, but also the energy of the shape isomers in the actinide region is used to determine the free parameters \((b, c)\). For HFB-8, we adopt \( b = 0.65 \) and \( c = 4.5 \).

**Vibrational correction.** The rotational correction should be accompanied by corrections for vibrational zero-point motion. To the best of our knowledge, there exists no strategy to estimate them properly and at the same time include them in a global mass fit as ours with current computing resources. Common strategies are to calculate RPA correlations [14, 15], usually restricted to spherical nuclei, or to use the generator coordinate method [16]. More research in this direction is necessary in the future.

**THE MASS FIT WITH THE PARTICLE-NUMBER PROJECTION**

To study the impact of the PLN framework, we start from the BSk6 force [4], keeping some of its characteristics: an isoscalar effective mass \( M_1^1/M \) constrained to 0.8, the symmetry energy \( J \) to 28 MeV, a density-independent pairing interaction (i.e., \( \eta = 0 \)) and the \( \gamma \) exponent in the \( t_2 \) term of Eq.( 1) to 1/4 for the incompressibility coefficient \( K_v \) to conform with the experimental value of 231\( \pm \)5 MeV extracted from breathing-mode measurements [17]. The results of the mass fit within the new HFB+PLN framework are presented in Table 1 (all details about the corresponding BSk8 Skyrme force can be found in [5]). For comparison, Table 1 also includes the results obtained with the BSk6 Skyrme force. Since the latter was fitted to the 2135 nuclei with \( Z, N \geq 8 \) whose masses had been measured and compiled in the unpublished 2001 Atomic Mass Evaluation (AME) of Audi and...
TABLE 1. Rms ($\sigma$) and mean ($\bar{\varepsilon}$) errors (in MeV) in the predictions of masses $M$ obtained with the BSk6 and BSk8 forces with respect to the 2135 nuclei in the 2001 AME [18] and the 2149 nuclei in the 2003 AME [19]. The last two lines correspond to the rms and mean errors (in fm) in the predictions of the 523 measured charge radii ($r_c$).

<table>
<thead>
<tr>
<th>Force</th>
<th>2135 nuclei</th>
<th>2149 nuclei</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\sigma(M)$</td>
<td>0.684</td>
<td>0.666</td>
</tr>
<tr>
<td>$\bar{\varepsilon}(M)$</td>
<td>0.021</td>
<td>0.014</td>
</tr>
<tr>
<td>$\sigma(r_c)$</td>
<td>0.0262</td>
<td>0.0250</td>
</tr>
<tr>
<td>$\bar{\varepsilon}(r_c)$</td>
<td>-0.0028</td>
<td>0.0047</td>
</tr>
</tbody>
</table>

FIGURE 1. Differences between experimental and calculated mass excesses as a function of the neutron number $N$ for the HFB-8 mass tables.

Wapstra [18] we show results for both this data set and the 2149 measured masses of the updated AME that was released and published at the end of 2003 [19]. Experimental and calculated mass excesses are compared in Fig. 1.

EXTRAPOLATIONS

With the BSk8 Skyrme force determined as described we constructed a complete mass table, labeled HFB-8, for the same nuclei as were included in the HFB-6 and HFB-2 tables, i.e., all the nuclei lying between the two drip lines over the range of $Z$ and $N \geq 8$ and $Z \leq 120$. We recall here that the only formal difference between HFB-2 and HFB-6 lies in the isoscalar effective mass that was imposed in the mass fit: 1.05 and 0.80 respectively.

The HFB-8 masses are compared in Fig. 2 with the HFB-6 (upper panels) and HFB-2 (lower panels) masses, as a function of the neutron number $N$ (left panels) and the neutron separation energy $S_n$ (right panels).

Differences seldom exceed some 2 MeV, even close to the neutron dripline; the largest deviations are found for open shell nuclei. Shell effects far away from stability are found to be very similar for the two mass tables. Moreover, the HFB-8 shell gaps are very similar to the shell gaps obtained with the HFB-6 mass formula so that they are not shown here. These results once again confirm the relative stability of the HFB mass predictions with respect to different parameterizations or frameworks, as already emphasized in [4].

OUTLOOK

The HFB treatment of pairing correlations is known to break the particle-number symmetry. The restoration of the exact particle number is done on the basis of the projection technique, i.e., by projecting the wave function on the exact number of particles after a variation that includes the approximate LN projection before variation. Doing so, we have constructed a new Skyrme force, labelled BSk8, the parameters of which reproduce the 2149 measured masses with an rms error of 0.635 MeV. The final table, referred to as HFB-8, includes all the 9200 nuclei lying between the two drip lines over the range of $Z$ and $N \geq 8$ and $Z \leq 120$. The extrapolations of this new mass formula out to the drip lines do not differ significantly from the previous HFB-6 mass formula obtained without the restoration of the particle-number symmetry.

ACKNOWLEDGMENTS

M.S. and S.G. are FNRS Research Fellow and Associate, respectively. J.M.P. acknowledges financial support from NSERC (Canada).

REFERENCES

FIGURE 2. Differences between calculated HFB-8 and HFB-6 (upper panels) or HFB-2 (lower panels) mass excesses shown as a function of the neutron number \(N\) (left panels) or the neutron separation energy \(S_n\) (right panels), for all nuclei with \(N, Z \geq 8\) and \(Z \leq 110\), and ranging between the two drip lines.