

PAPER • OPEN ACCESS

## The mass of odd-odd nuclei in microscopic mass models

To cite this article: W. Ryssens *et al* 2023 *J. Phys.: Conf. Ser.* **2586** 012097

View the [article online](#) for updates and enhancements.

You may also like

- [Nonadiabatic quasiparticle description of rotation-particle coupling in triaxial odd-odd nuclei](#)  
Pooja Siwach, P Arumugam, S Modi et al.
- [The predictive accuracy of analytical formulas and semiclassical approaches for decay half-lives of superheavy nuclei](#)  
T L Zhao, X J Bao and S Q Guo
- [Microscopic study of ground state bands in  \$N = 45\$  and  \$46\$  isotones in mass region  \$A = 70-80\$](#)   
Preeti Verma, Suram Singh, Arun Bharti et al.

# The mass of odd-odd nuclei in microscopic mass models

W. Ryssens<sup>1</sup>, G. Scamps<sup>2</sup>, G. Grams<sup>1</sup>, I. Kullmann<sup>1</sup>, M. Bender<sup>3</sup> and S. Goriely<sup>1</sup>.

<sup>1</sup>Institut d'Astronomie et d'Astrophysique, Université Libre de Bruxelles, Campus de la Plaine CP 226, 1050 Brussels, Belgium

<sup>2</sup>Department of Physics, University of Washington, Seattle, Washington 98195-1560, USA

<sup>3</sup>Université de Lyon, Université Claude Bernard Lyon 1, CNRS, IP2I Lyon / IN2P3, UMR 5822, F-69622, Villeurbanne, France

E-mail: wouter.ryssens@ulb.ac.be

**Abstract.** Accurate estimates of the binding energy of nuclei far from stability that cannot be produced in the laboratory are crucial to our understanding of nuclear processes in astrophysical scenarios. Models based on energy density functionals have shown that they are capable of reproducing all known masses with root-mean-square error better than 800 keV, while retaining a firm microscopic foundation. However, it was recently pointed out in [M. Hukkanen et al., arXiv:2210.10674] that the recent BSkG1 model fails to account for a contribution to the binding energy that is specific to odd-odd nuclei, and which can be studied by using appropriate mass difference formulas. We analyse here the (lacking) performance of three recent microscopic mass models with respect to such formulas and examine possibilities to remedy this deficiency in the future.

## 1. Introduction

The modelling of nuclear processes that impact stellar evolution and nucleosynthesis relies on our knowledge of the properties of atomic nuclei. Astrophysical applications require reliable values for many different quantities, but the central observable in this context is the nuclear mass or binding energy [1]. For many relevant nuclei far from stability, however, the experimental difficulties of producing and handling unstable isotopes preclude mass measurements in the foreseeable future.

This knowledge gap can only be filled through the development of models, which should provide reliable extrapolations for the masses of exotic nuclei. Our confidence in such extrapolations naturally increases if such models can provide a faithful description of known experimental data, not only for nuclear masses but also with respect to other quantities such as charge radii and nuclear deformations. Models based on energy density functionals (EDFs) [2] are the most promising avenue in this respect, since they have a microscopic foundation in an effective (pseudo-)potential between individual nucleons while their application to thousands of nuclei remains feasible. However, the analytical form of the EDF is phenomenological and its coupling constants are adjusted to experimental data. Many forms of the EDF and parameter adjustment strategies have been proposed [2]. We focus here on those developed by the Brussels group: the BSk [3] and BSkG [4, 5] series are based on EDFs of the Skyrme type and are fitted to essentially all known nuclear masses. These models describe the known nuclear masses with a root-mean-square (rms) error that is below 0.8 MeV [3, 4, 5], an accuracy that is competitive with more phenomenological microscopic-macroscopic approaches [6].



Experimentally, the mass of a nucleus with an odd number of neutrons  $N$  and an odd number of protons  $Z$  is somewhat smaller than would naively be expected from the masses of its neighbouring even-even, odd- $Z$  and odd- $N$  isotopes. This additional binding energy is visible in the systematics of mass differences and is often taken as evidence for the existence of a residual interaction between the odd proton and odd neutron. This effect has been discussed at length in the literature, see for example [7, 8, 9, 10, 11, 12], but without reaching a consensus about its microscopic origin and nature. We ask here the pragmatic question: do microscopic mass models account for the effect of this interaction on the binding energies of odd-odd nuclei? Through the use of appropriate mass difference formulas, we will show that the answer is "no", confirming the discussions in Ref. [13, 5]. We discuss possibilities to improve future models by accounting for this effect in a microscopic way.

## 2. Mass differences

Leaving aside shell effects, the (positive) binding energies  $B(N, Z)$  of even-even atomic nuclei are rather smooth functions of both neutron number  $N$  and proton number  $Z$ . Adjacent odd-mass nuclei follow almost identical trends with nucleon number, but are systematically less bound than the average of their even-even neighbours, an effect that is attributed to the presence of pair correlations in nuclei [14, 15]. Using  $\Delta_q$  ( $q = p, n$ ) for the distance between the curves that interpolate the masses of even-even and odd-mass nuclei, this can be schematically written as

$$B(N, Z) \simeq \frac{1}{2} [B(N-1, Z) + B(N+1, Z)] + (-1)^N \Delta_n, \quad (1)$$

$$B(N, Z) \simeq \frac{1}{2} [B(N, Z-1) + B(N, Z+1)] + (-1)^Z \Delta_p, \quad (2)$$

where  $\Delta_n$  and  $\Delta_p$  vary only slowly with particle number when away from closed shells. Values of these shifts can be extracted approximately from experiment with suitable mass difference formulas, such as the three- and five-point gaps  $\Delta_q^{(3)}$  and  $\Delta_q^{(5)}$  [14, 15]. The experimental values determined this way typically range between 0.5 and 1.5 MeV.

The evolution of the binding energy of odd-odd nuclei with nucleon number is also similar to that of the even-even nuclei. However, the distance between the mass surface of even-even and odd-odd nuclei is generally *smaller* than  $\Delta_n + \Delta_p$ , which is what one would expect naively from Eqs. (1) and (2). Schematically, we write for odd values of  $N$  and  $Z$ :

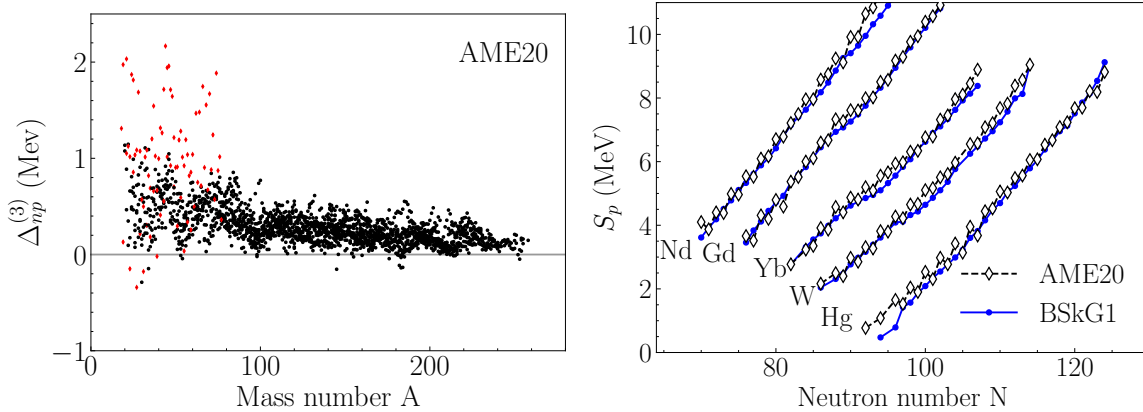
$$B(N, Z) \simeq \frac{1}{2} [B(N+1, Z-1) + B(N-1, Z+1)] - \Delta_n - \Delta_p + \Delta_{np}. \quad (3)$$

As we will show below, measured nuclear masses systematically point to values of  $\Delta_{np}$  that are on the order of a few hundred keV. Different mass formulas have been suggested to quantify this effect based on the measured masses [11, 12], but we focus on the following quantity:

$$\Delta_{np}^{(3)}(N, Z) = (-1)^Z \left[ \Delta_n^{(3)}(N, Z) - \Delta_n^{(3)}(N, Z-1) \right] = -(-1)^{Z+N} S_{p2n}. \quad (4)$$

where  $S_{p2n}$  characterizes the odd-even staggering of the proton separation energy  $S_p$  along an isotonic chain, i.e.  $S_{p2n}(N, Z) \equiv S_p(N, Z) - \frac{1}{2}[S_p(N+1, Z) + S_p(N-1, Z)]$  [9]. An alternative definition of  $\Delta_{np}^{(3)}$  in terms of proton three-point gaps energies leads to similar conclusions.  $\Delta_{np}^{(3)}$  is closely related, but not identical, to the quantity  $\delta_{np}$  studied in Ref. [11].

In the left panel of Fig. 1, we show the  $\Delta_{np}^{(3)}$  values calculated from the experimental masses tabulated in the AME20 compilation [16]. Essentially all values are positive: of the 1993  $(N, Z)$  pairs for which we can evaluate  $\Delta_{np}^{(3)}$ , only 28 result in negative values. Positive values of  $\Delta_{np}^{(3)}$  indicate that the three-point neutron gaps along odd- $Z$  isotopic chains are smaller than the gaps along neighbouring even- $Z$  chains. We observe several outliers larger than one MeV, but these



**Figure 1.** (Color online) Left:  $\Delta_{np}^{(3)}$  values for nuclei with  $Z \geq 8$  calculated from the known masses [16]. Red diamonds indicate nuclei with  $|N - Z| \leq 1$ . Right: Proton separation energies  $S_p$  along the Nd, Gd, Yb, W and Hg isotopic chains. We show experimental values (empty black diamonds) [16] and BSkG1 values (blue circles).

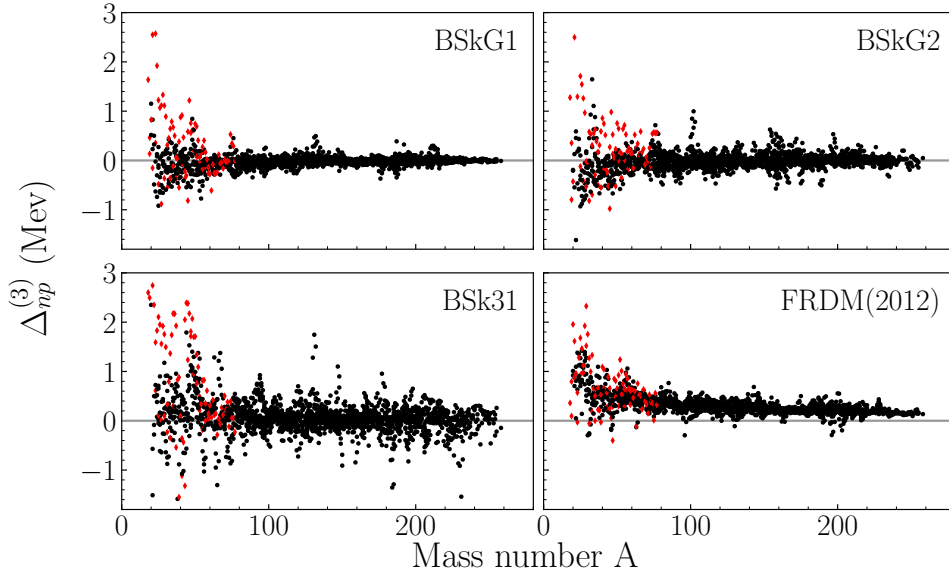
occur almost exclusively for nuclei with  $|N - Z| \leq 1$ , whose binding energies follow more complex patterns than those outlined above [12]. For all other nuclei, the typical effect amounts to a few hundred keV, decreasing slowly with increasing mass. The overall trend can be fitted with a simple  $A$ -dependence [7, 9, 12], but the large scatter seems to indicate that shell structure also plays an important role. For the purpose of simple comparison, the average of all experimental values is 305 keV.

As pointed out in Ref. [13] for the example of Ru, Rh and Pd isotopes, this empirical trend of the  $\Delta_{np}^{(3)}$  is not necessarily described by microscopic mass models. To illustrate how this deficiency is already visible for a more conventional mass difference, the right panel of Fig. 1 shows the proton separation energies along the Nd, Gd, Yb, W and Hg isotopic chains. BSkG1 produces rather smooth curves that reproduce the overall trends of experimental data, but the clearly visible odd-even staggering of the experimental data is absent from the model. Similar conclusions apply to neutron separation energies along isotonic chains. The actual  $\Delta_{np}^{(3)}$  values obtained from the BSkG1 model (for the same set of nuclei as in Fig. 1) are shown in the top left panel of Fig. 2. The difference with experimental information is obvious: about half of all calculated values are negative and the average value is very close to zero.

Other microscopic mass models face similar problems, which is illustrated in Fig. 2 for BSkG2 [5] and BSk31 [3]. We also compare with the macroscopic-microscopic FRDM(2012) model [6] that explicitly includes a phenomenological term proportional to  $A^{-2/3}$  for odd-odd nuclei that models  $\Delta_{np}$ . All models we consider offer an excellent global description of AME20 masses [16]: the rms deviations for BSkG1 and BSkG2 are 741 and 678 keV respectively, while BSk31 and FRDM(2012) achieve slightly smaller values, 588 and 606 keV, respectively.

To the best of our knowledge, the recent BSkG2 is the only microscopic mass model so far that consistently included the so-called ‘time-odd’ terms during the parameter adjustment. In principle, said terms contribute to the binding energy of odd-mass and odd-odd nuclei, but are omitted by all other models through the means of the equal filling approximation [17], which greatly simplifies the solution of the mean-field equations. Even though this approximation is, in general, quite accurate [5], one might expect that BSkG2 achieves an above-standard description of the binding energies of odd-odd nuclei.

We also show results for BSk31, which differs from the more recent BSkG-series in several ways. Most of these differences do not directly impact our discussion, except for the approach to



**Figure 2.** (Color online)  $\Delta_{np}^{(3)}$  values for nuclei with  $Z \geq 8$  whose masses are known [16] calculated from four different mass models: BSkG1 (top left), BSkG2 (top right), BSk31 (bottom left) and FRDM(2012) (bottom right). Red diamonds indicate nuclei with  $|N - Z| \leq 1$ .

the proton and neutron pairing strengths. Both BSkG1 and BSkG2 employ a single parameter to characterize the pairing strength for each nucleon species. For reasons outlined in Ref. [18], BSk31 generalizes this approach by taking two parameters for each species, depending on whether the corresponding particle number is even or odd. Through this mechanism, the proton (neutron) pairing strength in odd- $Z$  (odd- $N$ ) nuclei is enhanced by 6% (4%) compared to even- $Z$  (even- $N$ ) ones. Both pairing strengths are increased in odd-odd systems, providing the possibility for additional binding energy in these nuclei [18].

The  $\Delta_{np}^{(3)}$  values obtained from these models are shown in Fig. 2. As expected, FRDM(2012) describes the overall size and trend of the experimental data; the average calculated  $\Delta_{np}^{(3)}$  among this set of nuclei is about 306 keV. The microscopic models fare much worse: in all of them, about half of the values come out negative, resulting in average values of  $\Delta_{np}^{(3)}$  of almost precisely 0 keV for BSkG1 and BSkG2, respectively, and about 100 keV for BSk31. While the calculated average  $\Delta_{np}^{(3)}$  is at least positive for BSk31, this model yields stronger scattering than BSkG1 and BSkG2, which are closer to experimental data in this respect.

For the BSkG2 and BSk31 models, the rms error on the 585 known masses of odd-odd nuclei amounts to 704 and 616 keV, i.e. about 40 keV above their respective rms deviation on all masses. It is tempting to interpret this as a consequence of the missing physics discussed here. However, model deficiencies that affect a subset of nuclei feed back on the parameter adjustment which targets an optimal description of all masses. The incomplete description of the binding energy of odd-odd nuclei thus need not result in an increased rms for such systems. For example, the BSkG1 model has an rms deviation for odd-odd nuclei that is equal to its rms error on all masses.

### 3. Perspectives

We have established that BSkG1, BSkG2 and BSk31 do not reproduce the enhanced binding energies of odd-odd nuclei observed experimentally. For BSkG1, there is no clear mechanism that could have produced the desired effect. BSkG2 and BSk31 provide a similar (lacking)

description of the data, despite the presence of time-odd terms in the former and the alternating pairing strength in the latter. This conclusion comes with the caveat that none of these models included observables in their fitting protocols that are sensitive to this small effect.

Although we only show results for three models, we are under the impression that the failure to describe this additional binding of odd-odd nuclei is universal among EDF-based approaches. There are several possible reasons for this. First, the form of the EDF might not contain the necessary degree of freedom needed to describe the additional binding energy. Even if the structure of the EDF would be sufficiently rich, the fit protocol might not constrain this specific mass difference or the effect might be related to a broken symmetry that is not explored in the calculations. Finally, there here also is the possibility that the modeling of this effect requires considering a specific type of correlations in a beyond-mean-field approach.

The failure we observe might be due to a combination of all of the above, but we will limit our considerations to modifications of the current state-of-the-art models that could generate additional binding energy in odd-odd nuclei without abandoning the mean-field description. It is likely that the problem we discuss here is linked to another known problem: EDF-based models do not reproduce the energy splitting of states in odd-odd nuclei that are obtained from coupling the same two quasiparticles with either aligned or anti-aligned spins [10]. Whatever is the mechanism that generates the extra binding energy, it is clear that it has to be sensitive to the relative orientation of the angular momenta of the two odd nucleons and has to favour the parallel alignment of their intrinsic spins as suggested by the Gallagher-Moszkowski (GM) rule [10].

One mechanism at the origin of the extra binding might be the formation of spin-aligned proton-neutron pairs in odd-odd nuclei, whose mean-field description requires breaking the conserved isospin projection of the single-particle states and the introduction of proton-neutron pairing terms in the EDF. As argued in Ref. [9] however, this is unlikely to generate the desired effect in a pure mean-field approach, where the formation of a static neutron-proton pair condensate usually only occurs near the  $N = Z$  line. On the other hand, it is also known that dynamical proton-neutron pairing is a necessary ingredient for the QRPA modeling of the  $\beta$ -decay of even-even to odd-odd nuclei across the chart of nuclei [19], pointing to an inherent limitation of the mean-field approach to capture all relevant pairing correlations simultaneously.

If the modeling of the enhanced binding of odd-odd nuclei is a beyond-mean-field effect, one might attempt to include it through a phenomenological correction similar to the ones for collective motion that are employed in the BSk and BSkG models [4, 5, 3]. The simplest possibility is the adoption of an analytical formula such as the one included in the FRDM(2012) model, which works well for the global trends of the known nuclear masses. More microscopic correction formulas in the form of sums over matrix elements of a residual interaction can be designed as well [9], but might double-count contributions already included in the EDF.

This brings us to a third possibility: tuning the proton-neutron spin-spin interaction terms in the Skyrme EDF that only contribute when time-reversal symmetry is broken, meaning that it vanishes for even-even nuclei. The most simple one among these terms contains the scalar product of the proton and neutron spin densities  $\mathbf{s}_p(\mathbf{r}) \cdot \mathbf{s}_n(\mathbf{r})$  [5]. The spin densities encountered in ground-state configurations are usually dominated by the single-particle contribution of the odd nucleons,<sup>1</sup> such that terms involving  $\mathbf{s}_n(\mathbf{r}) \cdot \mathbf{s}_p(\mathbf{r})$  will only significantly impact the ground states of odd-odd nuclei. The scalar product of the pseudovector spin densities also introduces a dependence on the relative orientation of the nucleon's spins as expected from the GM rule. The fine-tuning of the spin-spin terms to the enhanced binding of odd-odd nuclei, however, should not be made at the expense of other qualities of the model. For example, changes in the proton-neutron spin terms might spoil the realistic values of the Landau parameters  $G_0$  and

<sup>1</sup> Polarisation effects will also induce a small spin density for the nucleons of the other species, such that the spin density of the nucleon species with even number will not vanish exactly in odd-mass nuclei.

$G'_0$  that BSkG1, BSkG2 and BSk31 all exhibit, which then would call for higher-order spin terms such as tensor interactions that were already evoked in earlier attempts to model the GM splitting [20]. In any case, since BSkG2 already incorporates time-odd terms yet fails to describe the experimental values of  $\Delta_{np}^{(3)}$ , progress along this line will require amending the fit protocol with suitable observables.

#### 4. Conclusions

The binding energy of odd-odd nuclei is slightly, but systematically, larger than what would be expected from estimates based on the masses of their even-even and odd-mass neighbours. We have investigated whether large-scale microscopic mass models describe this effect through the  $\Delta_{np}^{(3)}$  mass difference. As could be suspected from the discussion in Ref. [13], the BSkG1 model produces values for this observable that are scattered around zero while experiment indicates systematically positive values. BSk31 and BSkG2 possess mechanisms that could generate additional binding energy in odd-odd nuclei, but in practice do not offer a better description of the data. The macroscopic-microscopic FRDM(2012) model employs a phenomenological ingredient that explicitly accounts for the additional binding. We have discussed perspectives to improve future microscopic models and, for models based on EDFs of the Skyrme type, have pointed out that specific time-odd terms could be used to generate additional binding energy in odd-odd nuclei.

#### Acknowledgments

This work was supported by the Fonds de la Recherche Scientifique (F.R.S.-FNRS) and the Fonds Wetenschappelijk Onderzoek-Vlaanderen (FWO) under the EOS Project nr O022818F. The present research benefited from computational resources made available on the Tier-1 supercomputer of the Fédération Wallonie-Bruxelles, infrastructure funded by the Walloon Region under the grant agreement nr 1117545. The funding for G.S. from the US DOE, Office of Science, Grant No. DE-FG02-97ER41014 is greatly appreciated. S.G. and W.R. acknowledge financial support from the F.R.S.-FNRS (Belgium). Work by M.B. has been supported by the French Agence Nationale de la Recherche under grant No. 19-CE31-0015-01 (NEWFUN).

#### References

- [1] Arnould M and Goriely S 2020 *Prog. Part. Nucl. Phys.* **112** 103766
- [2] Bender M, Heenen P-H and Reinhard P-G 2003 *Rev. Mod. Phys.* **75** 121
- [3] Goriely S, Chamel N and Pearson J M 2016 *Phys. Rev. C* **93** 034337
- [4] Scamps G, Goriely S, Olsen E, Bender M and Ryssens W 2021 *Eur. Phys. J. A* **57** 333
- [5] Ryssens W, Scamps G, Goriely S and Bender M 2022 *Eur. Phys. J. A* submitted (arXiv:2208.06455).
- [6] Möller P, Sierk A J, Ichikawa T, and Sagawa H 2016 *At. Data Nucl. Data Tables* **109–110** 1
- [7] Basu M K and Banerjee D 1971 *Phys. Rev. C* **3** 992
- [8] Jensen A S, Hansen P G, and Jonson B 1984 *Nucl. Phys. A* **431** 393
- [9] Friedman W A and Bertsch G F 2007 *Phys. Rev. C* **76** 057301
- [10] Robledo L M, Bernard R N, and Bertsch G F 2014 *Phys. Rev. C* **89** 021303
- [11] Wu Z, Changizi S A and Qi C, 2016 *Phys. Rev. C* **93** 034334
- [12] Le Yang G, Qi B, Wang X D and Qi C, 2022 *Phys. Rev. C* **106** 024325
- [13] Hukkanen M *et al.* 2022 *Phys. Rev. C* submitted (arXiv:2210.10674)
- [14] Bender M, Rutz K, Reinhard P-G and Maruhn J A 2000 *Eur. Phys. J. A* **8** 59
- [15] Duguet T, Bonche P, Heenen P-H and Meyer J 2001 *Phys. Rev. C* **65** 014311
- [16] Wang M, Huang W J, Kondev F G, Audi G, and Naimi S 2021 *Chin. Phys. C* **45** 3
- [17] Perez-Martin S and Robledo L M 2008 *Phys. Rev. C* **78** 014304
- [18] Nayak R C and Pearson J M 1995 *Phys. Rev. C* **52** 2254
- [19] Engel J, Bender M, Dobaczewski J, Nazarewicz W and Surman R 1999 *Phys. Rev. C* **60** 014302
- [20] Boisson J P, Piepenbring R and Ogle W 1976 *Phys. Rep.* **26** 99