I. INTRODUCTION

Many physical applications require a precise and accurate knowledge of nuclear binding energies. A typical case is that of astrophysical simulations used to describe explosive scenarios where the goal is to understand how chemical elements heavier than iron are formed [1, 2]. The nuclear reactions involved take place along the "r-process" path that evolves in neutron rich nuclei regions well away from the stability line. Those nuclei are not within reach in the present day or near future experimental facilities [3] and therefore astrophysical simulations require theoretical input. A consistent framework working with the same accuracy all over the nuclide chart involves mean field techniques with effective interactions [4]. For the later it is common to used the family of Gogny forces [5] focusing on D1M [6] for its good reproduction of masses. The parameters of D1M were fitted to reproduce the binding energies of all known nuclei using as input a Hartree-Fock-Bogoliubov (HFB) calculation [7] supplemented with an approximate rotational energy correction and an approximate zero point energy correction from quadrupole motion. In this way an impressive rms deviation for the binding energy of 0.7 MeV was obtained. Recently, additional correlation energies including Projection on Particle Number (PNP), exact angular momentum projection (AMP) of axial states and quadrupole configuration mixing with the projected states have been computed with Gogny D1M [8]. Unfortunately none of these effects seem to improve the agreement with experimental data in a significant way [2, 8] but can have a strong impact on astrophysical scenarios where an accuracy of a couple hundred keV is required [2].

This paper is a follow up of Ref [13] where a systematic calculation of octupole properties over a large set of 818 even-even nuclei was carried out. In the accompanying material of [13] three tables with the relevant quantities obtained with three parametrizations of the Gogny force were included. In those tables the correlation energies discussed here were already included but never discussed. Given the renewed interest on nuclear binding energies [2, 8] we consider now timely to discuss them in detail.

II. CALCULATIONAL METHOD

The computational procedure is the same as in Ref [13] where a thorough account of the properties of negative parity excited states was given using the HFB, parity projection and configuration mixing. Therefore we will give here only a sort description for the convenience of the reader. The constrained HFB equation with a constraint on the axial octupole moment is solved using the approximate second order gradient method [14, 15] in order to generate a set of axially symmetric HFB wave functions |Φ(Q30)⟩. For the interaction we use the parametrization D1M of the Gogny force [5, 6]. The location of the minimum of the HFB energy curve $E_{\text{HFB}}(Q_{30})$ determines whether the ground state is octupole deformed or not. The energy difference $E_{\text{HFB}}(Q_{30}) - E_{\text{HFB}}(0)$ is the mean field correlation energy gained by breaking reflection symmetry. This calculation is carried out for a set of 818 even-even nuclei from oxygen to Z=112 nuclei. In the next step, the octupole deformed HFB states are projected to good parity $\pi = \pm 1$ and the corresponding projected energies

$$E_\pi(Q_{30}) = \frac{\langle \Phi(Q_{30}) | \hat{H} \hat{P}_\pi | \Phi(Q_{30}) \rangle}{\langle \Phi(Q_{30}) | \hat{P}_\pi | \Phi(Q_{30}) \rangle}$$

are computed (paying special attention to the consistency problems associated to the use of density depen-
nate Method (GCM) calculation using the set of collective coordinate. In panel a) of Fig. 1 the HFB results \( \Delta E_{\text{HFB}} \) are depicted: just a few nuclei in the Ra, Ba and Zr regions show a non-zero correlation energy that never exceeds 1.2 MeV. Those are the regions where both proton and neutron numbers are close to the numbers favoring octupole correlations [11]. Parity projection on top of both reflection symmetric as well as octupole deformed HFB ground states produce a negligible energy gain as discussed in ref. [13]. However, the consideration of parity RVAP leads to a non zero value of the octupole correlation energy in all the nuclei considered and as large as 1.5 MeV. The parity RVAP produces the largest correlation energies for octupole soft nuclei and gives almost negligible ones for those nuclei which are octupole deformed at the HFB level. Finally, the GCM correlation energy includes in its definition the HFB correlation energy, the parity RVAP one as well as the correlation energy gained by the fluctuating octupole degree of freedom. This correlation energy is largest in those regions showing octupole deformation at the HFB level as observed in panel c) of Fig. 1. The GCM correlation energy can be as large as 2.5 MeV. In the regions in between the correlation energy is not as large and is typically of the order of 1 MeV with slow variations as a function of proton and neutron number.

In order to understand the impact of the octupole correlation energy in the description of experimental binding energies we have plotted in Fig. 2 the binding energy difference between the theoretical (GCM) result and the experimental data (as in the 2012 compilation [18]) as a function of neutron number for each \( Z \) value considered in the calculation (from oxygen to \( Z = 112 \)). In each panel corresponding to a given \( Z \) value two curves are shown: one corresponds to the HFB with octupole deformation (black) and the other to the calculation including the GCM correlations. The inclusion of the GCM octupole correlations represents in most of the cases a mere displacement upwards of the curves and little improvement is observed. A comment is in order: in our calculations we do not have access to the zero point energy correction of the quadrupole degrees of freedom as computed in [6] and therefore this quantity has not been added. It is typically of the order of 2-3 MeV and explain the overall shift observed in the D1M HFB predictions. Another interesting aspect of this plot is the fact that the most severe discrepancies always take place around magic numbers and is specially remarkable for \( Z = 48 - 52 \) and \( Z = 80 - 84 \). In those cases the inclusion of the octupole correlation energy improves the discrepancies but is far from being enough to provide a good description of experimental data. When away from those magic numbers the behavior of the binding energy differences is quite horizontal in most of the cases.

Another quantity connected to binding energies and of interest in astrophysics is the two neutron separation

\[
\Delta E_{\text{GCM}} = E_{\text{GS, GCM}} - E_{\text{HFB}}(0).
\]

### III. RESULTS

First an HFB calculation preserving reflection symmetry is carried out for a set of 818 even even nuclei from oxygen to \( Z = 112 \). The choice is made as to include the 520 even-even nuclei with known binding energies as given in the 2012 binding energy compilation [18] plus a few more. The binding energy obtained will be used as a reference in Fig. 1 where the binding energy obtained in the approaches described above are plotted with the reflection symmetric HFB ones subtracted. The three approaches are the reflection symmetric breaking HFB, the parity RVAP and finally the GCM with \( Q_{30} \) as collective coordinate. The minima of the two curves \( E_{++}(Q_{30}) \) and \( E_{++}(Q_{30}) \) determine the optimal intrinsic states for each parity in the spirit of the restricted variation after projection (RVAP) method. In even-even nuclei the ground state is always positive parity and the RVAP correlation energy is given by \( \Delta E_{\text{RVAP}} = E_{++}(Q_{30}, P_{\text{min}}) - E_{\text{HFB}}(0) \). Finally, a Generator Coordinate Method (GCM) calculation using the set \( \Phi(Q_{30}) \) of HFB wave function as basis states is performed. The solution of the Hill-Wheeler equation with the minimum energy corresponds to the positive parity ground state. The correlation energy is defined in this case as \( \Delta E_{\text{GCM}} = E_{\text{GS, GCM}} - E_{\text{HFB}}(0) \).
energy $S_{2N}$. The reaction rates of nuclear reactions depend on the Q value of the reaction which is related to the $S_{2N}$. For neutron numbers equal to magic this quantity shows a sudden drop that is not well reproduced by HFB mass models: before the drop the theoretical models provide too high values and after the drop the $S_{2N}$ values are too small. The expectation is that correlations beyond the mean field will reduce the discrepancy by quenching the "shell gap" (see [2] for a discussion in the astrophysical context) but the amount of quenching associated to each improvement on top of HFB is still under debate [8]. The difference $\Delta S_{2N} = S_{2N,\text{th}} - S_{2N,\text{exp}}$ is plotted in Fig. 3 in separated panels for each $Z$ value and as a function of $N$. As theoretical models we consider the HFB results and the octupole GCM numbers. To help reading the results the zero is marked by a horizontal line and vertical lines are placed at magic neutron numbers. The conclusion extracted from the plot is that the extra correlation energies associated to the octupole GCM do not modify in a substantial way the HFB $\Delta S_{2N}$ values (the two curves are almost indistinguishable for most $Z$ values) and therefore octupole correlations do not help to quench the "shell gaps".

The present discussion has focused on the results of the D1M parametrization of the Gogny force but similar conclusions can be drawn for the D1S and D1N parametrizations of the force (see [13] for definitions and the accompanying material of that reference for the specific data).

IV. CONCLUSIONS

The ground state octupole correlation energy computed at three levels of approximation: the octupole deformed HFB, the parity RVAP and the octupole GCM are computed with the Gogny D1M effective interaction. Although non negligible and as large as 2.5 MeV the octupole GCM correlation energy does not improve substantially the agreement between theory and experiment for the binding energies. This is a consequence of the rather smooth behavior of the correlation energy as a function of $Z$ and $N$ as well as the theory-experiment discrepancies that accumulates around magic numbers. The impact on the "shell gaps" is also imperceptible. We con-

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**FIG. 2.** (Color online) Binding energy difference between the theoretical predictions and the experimental data (2012 compilation [13]) plotted as a function of neutron number differences N-N$_0$ where N$_0$(Z) is a reference neutron number specific of each Z value. In each panel the corresponding values of Z and N$_0$(Z) are given in the label. The horizontal lines correspond to a perfect agreement theory-experiment. The vertical lines in this reference horizontal line signal magic neutron numbers. The black curves correspond to the theoretical binding energy computed with D1M using the HFB energy plus the rotational energy correction. The red curves include additionally the octupole correlation energy of the GCM calculation. The energy range for the y axis is from -6.5 to 6.5 MeV. For the x axis goes from 0 to 40 with major ticks every 5 units and minor ticks every 1 unit.
FIG. 3. (Color online) The two neutron separation energy difference between the theoretical predictions and the experimental values $\Delta S_{2N} = S_{2N,\text{th}} - S_{2N,\text{exp}}$ is plotted for each $Z$ value as a function of $N-N_0$ (see Fig 2). Black (red) curves correspond to the HFB (GCM) results. The $y$ axis range is from -5 to 5 MeV and the $x$ one from 0 to 45.

Conclude that the ground state octupole correlation energies only contribute to minor improvements in the description of binding energies and can be neglected at the present level of accuracy of the theoretical description.

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