

Systematic study of infrared energy corrections in truncated oscillator spaces with Gogny energy density functionals

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We study the convergence properties of nuclear binding energies and two-neutron separation energies obtained with self-consistent mean-field calculations based on the Hartree-Fock-Bogolyubov (HFB) method with Gogny-type effective interactions. Owing to lack of convergence in a truncated working basis, we employ and benchmark one of the recently proposed infrared energy correction techniques to extrapolate our results to the limit of an infinite model space. We also discuss its applicability to global calculations of nuclear masses.

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I. INTRODUCTION

Nuclear physics properties like nuclear masses, decay and capture rates, fission, etc., constitute a key ingredient to study the formation of elements in stellar nucleosynthesis. For example, all current rapid neutron capture nucleosynthesis process (*r*-process) models require nuclear physics input for a large number of nuclei that have extreme neutron excess and stretch up to the limits of the nuclear chart. Such nuclei lie far beyond the capabilities of the experimental facilities in any foreseeable future, and hence performing *r*-process simulations one has to almost entirely rely on theoretical predictions. Since masses determine thresholds of all nuclear reactions, the calculated final *r*-process elemental abundances of any astrophysical model are very sensitive [1–3] to the employed nuclear mass tables.

Self-consistent mean-field theories based on the Hartree-Fock-Bogolyubov (HFB) variational approach with energy density functionals (EDF) were actively developing in the recent decades and have proven successful in the systematic study of low energy nuclear structure [4–6]. In particular, the recent HFB-based mass models [7,8] are now found to be on a similar accuracy level in describing experimental masses as the more phenomenological approaches [9–11]. Nonetheless, in order to further increase the predictive power of HFB-based models, particular attention must be paid to the following important issues inherent to all currently used HFB-models with either Skyrme, Gogny, or relativistic EDFs. First of all, there are missing correlations at the purely mean-field level, and one has to introduce the so-called beyond-mean-field (BMF) corrections, such as symmetry restorations and/or configuration mixing [8,12–14], in order to achieve a better compliance with experimental data. Furthermore, nuclei with an odd number of neutrons and/or protons are usually not treated at the same self-consistent level as the even-even isotopes [15–17], resulting in elevated uncertainties when describing such odd-mass nuclei. This aspect affects theoretical predictions of reaction *Q* values needed to describe nucleosynthesis processes. Finally, there are also purely numerical problems, such as an incomplete convergence of observables in practical calculations that can lead to numerical

noise in the form of artificial jumps in the calculated binding and neutron-separation energies [1,14,18]. In what follows, we discuss the issue of insufficient convergence of practical HFB calculations in more detail.

In particular, most of the current EDF calculations utilize for the many-body wave function expansion either a mesh with a given size of the box and a distance between neighbor points, or a finite number of harmonic oscillator single-particle states. Observables such as binding energies, radii, etc., should in principle be independent of a particular choice for the working basis. Nonetheless, such an independence is only obtained in calculations in a mesh if a sufficiently large and dense box is used. On the other hand, a large number of single-particle states have to be included in the calculation with harmonic oscillator bases. This is rarely the case in practical applications due to limited computational resources. Hence, increasing the size of the working basis usually leads to an emergence of a convergence pattern for the calculated observables. In the case of calculations in a mesh, such convergence studies have been systematically performed recently with Skyrme functionals (see Ref. [19] and references therein). For harmonic oscillator bases, extrapolations schemes to the limit of an infinite basis have been used [7,8,20–25] as well as modifications of the basis in the so-called transformed harmonic oscillator method [26].

One of the goals of this paper is to analyze the convergence of energies computed with an underlying harmonic oscillator single-particle basis using the variational HFB method. By doing this, we can directly test the global validity of the central ansatz for a widely implemented phenomenological extrapolation prescription in some of the previous large-scale HFB-based calculations [8,21,27]. To our best knowledge, none of the earlier publications addressed the accuracy of this approach across entire isotopic chains. Having performed the convergence analysis, we turn our attention to a more recent extrapolation method that was theoretically derived for calculations performed in harmonic oscillator basis [22–25]. However, previous studies have evaluated the performance of this extrapolation strategy on a couple of simple systems for which “exact” many-body calculations are possible. In this paper, we introduce necessary tools and establish appropriate

criteria for the systematic analysis of this extrapolation strategy applied to HFB calculations using the Gogny EDF.

In the first part of the paper (Sec. II A) we briefly discuss the HFB method and the general properties of the harmonic oscillator working basis (Sec. II B). In Sec. III we analyze the convergence patterns of HFB calculations with the variation of the numerical parameters of the basis. Then, we describe the most important aspects of an extrapolation scheme introduced by Furnstahl, Hagen, and Papenbrock in Ref. [22] and improved subsequently in Refs. [23–25] (Sec. IV A–IV B). In Sec. IV C, this method is applied to the nucleus ^{16}O as a benchmark. This analysis is generalized to the nucleus ^{120}Cd and the cadmium isotopic chain in Sec. IV D, where we identify the potential problems that could appear in the extrapolation. Finally, the main results are summarized in Sec. V.

II. THEORETICAL FRAMEWORK

A. Hartree-Fock-Bogolyubov (HFB) method

The HFB method is based on the variational principle, where the variational many-body space is spanned by the product-type HFB wave functions [28]

$$|\Phi\rangle = \prod_k \hat{\beta}_k |0\rangle, \quad (1)$$

with the property of being vacuum states with respect to the Bogolyubov quasiparticles, i.e.,

$$\hat{\beta}_k |\Phi\rangle = 0 \quad \forall k. \quad (2)$$

Bogolyubov quasiparticle creation and annihilation operators, $\hat{\beta}_k^\dagger$ and $\hat{\beta}_k$, are the most general linear transformation of arbitrary single-particle operators \hat{c}_i^\dagger and \hat{c}_i [28],

$$\hat{\beta}_k^\dagger = \sum_i U_{ik} \hat{c}_i^\dagger + V_{ik} \hat{c}_i, \quad (3)$$

where the matrices U_{ik} and V_{ik} are sought by the minimization of the total energy. Since the HFB states $|\Phi\rangle$ violate the particle-number symmetry, the minimization is performed with constraints on the desired expectation values of neutron and proton number operators \hat{N} and \hat{Z} , so that $\langle \Phi | \hat{N} | \Phi \rangle = N$ and $\langle \Phi | \hat{Z} | \Phi \rangle = Z$. Hence, the HFB equations that define the ground-state $|\Phi_0\rangle$ are found by the condition

$$\delta(E'_{\text{HFB}}[|\Phi\rangle])_{|\Phi\rangle=|\Phi_0\rangle} = 0 \quad (4)$$

with

$$E'_{\text{HFB}}[|\Phi\rangle] = \langle \Phi | \hat{H} - \lambda_N \hat{N} - \lambda_Z \hat{Z} | \Phi \rangle, \quad (5)$$

where λ_N, λ_Z are Lagrange multipliers to ensure the constraints above, while the \hat{H} is the effective nuclear Hamiltonian. In the present study, the Gogny D1S interaction [29] is used to define the energy density functional and the HFB equations are solved using the computer code developed at the Universidad Autónoma de Madrid [30] based on the gradient method. Here, all terms have been included in the Hartree-Fock (direct and exchange) and pairing fields except the pairing part from the spin-orbit term which is very small.

B. Spherical harmonic oscillator single-particle basis

A common choice of the single-particle working basis for the quasiparticles' expansion [Eq. (3)] is a set of spherical harmonic oscillator (SHO) functions. In this case there are two numerical parameters that define the basis itself. The first one is the total number of major oscillator shells included in the basis, N_{OS} , which defines its dimension d_{tot} , i.e., the number of single-particle states, as

$$d_{\text{tot}} = \sum_{N=1}^{N_{\text{OS}}} D(N) = \frac{1}{3} N_{\text{OS}} (N_{\text{OS}} + 1) (N_{\text{OS}} + 2), \quad (6)$$

where $D(N) = N(N+1)$ is the degeneracy of a single oscillator shell. Here, $N = 1, 2, \dots$ is the major oscillator number $N = 2n + l + 1$, with $n = 0, 1, 2, \dots$ and l being the radial and angular momentum quantum numbers, respectively.

The second parameter of the basis is the intrinsic oscillator length b of the SHO functions, which is connected to the oscillator energy $\hbar\omega$ as

$$b = \sqrt{\frac{\hbar}{m\omega}}. \quad (7)$$

In Fig. 1 we represent schematically the well-known spherical harmonic oscillator potential, $V(r) = -V_0 + (r/b)^2 \hbar\omega/2$, for two different values of the oscillator length $b = 1.65$ and 2.45 fm. The depth of the well is chosen to be the same for both schematic potentials, $V_0 = 60$ MeV. It is thus clear that, for a fixed number of N_{OS} , the maximum energy reached by a single-particle state will be larger when the intrinsic oscillator length b (and therefore the effective radius of the basis) is smaller. Nevertheless, both bases are equivalent and should yield identical results for calculated observables when an infinite value of N_{OS} is considered. However, due to basis truncations in practical calculations and an improper asymptotic behavior of the harmonic oscillator wave functions at long distances, such an independence from the numerical basis parameters (N_{OS}, b) is rarely reached.

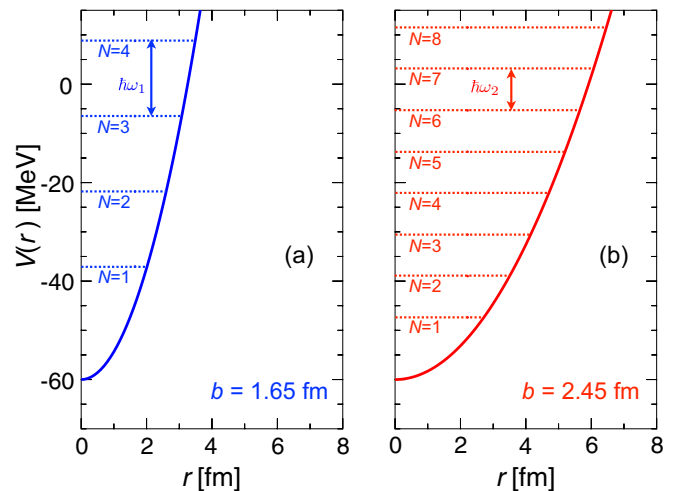


FIG. 1. Spherical harmonic oscillator levels for two different values of the oscillator length (a) $b = 1.65$ fm and (b) $b = 2.45$ fm.

III. CONVERGENCE ANALYSIS

Figure 2 shows the calculated ground-state (g.s.) HFB energies of ^{16}O and ^{120}Cd for bases $N_{\text{OS}} = 11, \dots, 21$ that are plotted against various oscillator length values b . One sees that going from $N_{\text{OS}} = 11$ to $N_{\text{OS}} = 13$, or from $N_{\text{OS}} = 13$ to $N_{\text{OS}} = 15$ yields noticeably deeper minima. Yet given a sufficiently large basis, g.s. energies of the ^{16}O nucleus are largely insensitive to the numerical parameters N_{OS} and b ; see Fig. 2(a). We can thus state that in this case the results are virtually converged to the true HFB energy, thereafter to be referred to as E_{∞} . However, as was already mentioned, a complete convergence is rarely achieved in practice. For example, the calculated g.s. energies of the neutron-rich ^{120}Cd in Fig. 2(b) are rather sensitive to the chosen intrinsic length of the basis b , even in larger bases with greater N_{OS} values. Hence, further energy gain is anticipated from expanding the

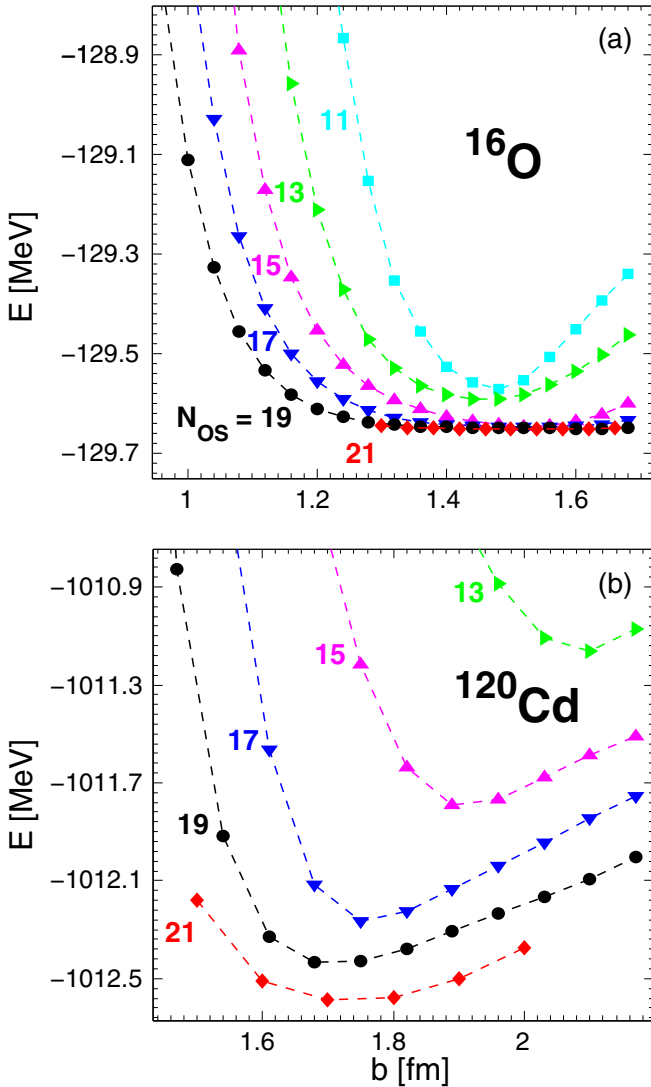


FIG. 2. HFB energies calculated in different bases $N_{\text{OS}} = 11, \dots, 21$ (see labels at each curve) as a function of oscillator length b for (a) ^{16}O and (b) ^{120}Cd .

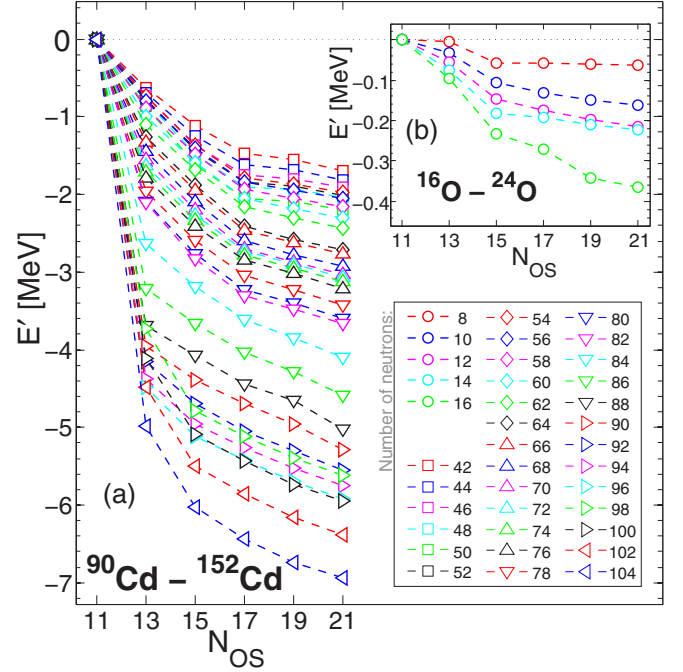


FIG. 3. Convergence patterns of HFB energies with enlargement of the basis dimension, defined as $E'(N_{\text{OS}}) = E_{\text{min}}(N_{\text{OS}}) - E_{\text{min}}(11)$ for (a) cadmium and (b) oxygen nuclei.

dimension of the working basis beyond our current maximum of $N_{\text{OS}} = 21$.

We generalize these results to the study of g.s. energies in two isotopic chains, namely, oxygen and cadmium isotopes. In Fig. 3 we show the energy gained by increasing the number of major harmonic oscillator shells with respect to the energy obtained with $N_{\text{OS}} = 11$. Additionally, these values are calculated with the optimal choice of the oscillator length for each N_{OS} ,

$$E_{\text{min}}(N_{\text{OS}}) = \min\{E(N_{\text{OS}}, b)\}; \quad (8)$$

i.e., they correspond to the minima of the curves shown in Fig. 2. First of all, a flat behavior in the HFB energies with respect to N_{OS} means a converged calculation. However, we see in Fig. 3 that a strict convergence is reached only for the nucleus ^{16}O . In the rest of the oxygen and cadmium nuclei we observe an increase in energy gain when we include more harmonic oscillator states in the working basis. Such an increase is larger for heavier isotopes. For example, performing calculations in a basis with $N_{\text{OS}} = 21$ for ^{16}O yields only ~ 0.06 MeV of extra g.s. energy compared to a calculation with $N_{\text{OS}} = 11$, and such gains gradually grow, reaching ~ 0.36 MeV for the ^{24}O nucleus. The situation with cadmium nuclei is similar, but the lack of convergence in the $N_{\text{OS}} = 11$ basis is much more profound for these heavier systems. Hence, the calculation with $N_{\text{OS}} = 11$ is underconverged by 1.70 MeV for ^{90}Cd compared to the calculation with $N_{\text{OS}} = 21$, and this value reaches 6.94 MeV for the nucleus ^{152}Cd . In Fig. 3 we also observe that the energy gain obtained by increasing the basis with two units of N_{OS} is not always monotonic. To get

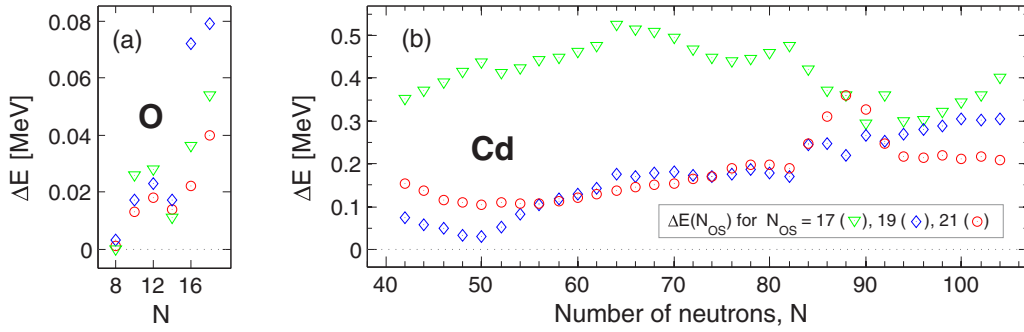


FIG. 4. Obtained HFB energy gains by including two more major oscillator shells in the working basis, $\Delta E(N_{OS}) = E_{\min}(N_{OS} - 2) - E_{\min}(N_{OS})$, for (a) oxygen and (b) cadmium isotopes.

more insight into this matter, we define such an energy gain as

$$\Delta E(N_{OS}) = E_{\min}(N_{OS} - 2) - E_{\min}(N_{OS}), \quad (9)$$

Figure 4 shows $\Delta E(N_{OS})$ for $N_{OS} = 17, 19, 21$ in oxygen and cadmium isotopic chains. First, we see once again a fully converged calculation for ^{16}O with $\Delta E(N_{OS})$ effectively being equal to zero. Second, we notice irregularities in the convergence pattern for the majority of nuclei. This is particularly well seen for the cadmium isotopes, where the convergence pattern $\Delta E(21) < \Delta E(19) < \Delta E(17)$ does not generally hold. In addition, we can also notice a clear disturbance of the slowly varying $\Delta E(N_{OS})$ patterns in the isotopic region around the magic ^{130}Cd nucleus. Therefore, any extrapolation method that assumes a continuous and smooth reduction of the energy gain obtained by adding two major shells is not supported by the present calculations [8,20,21,27].

IV. EXTRAPOLATIONS TO AN INFINITE BASIS

The evident incomplete convergence in practical HFB calculations of ground-state energies prompts us to search for a systematic and reliable method to extrapolate the results obtained in a truncated harmonic oscillator basis to the limit of an infinite basis. One of the early attempts to quantify for the numerical error due to the basis truncation is based on the assumption that the g.s. energy follows a law $\Delta E(N_{OS}) \approx \Delta E(N_{OS} - 2)/2$, which by summing the arithmetic series would imply an estimate $E_{\infty} \approx E_{\min}(N_{OS}) - \Delta E(N_{OS})$ [8,20,21,27]. According to our previous discussion of Fig. 4, this ansatz is too crude and not general enough to give a reliable estimation of E_{∞} . A number of more elaborate phenomenological extrapolation schemes have also been used in nuclear structure calculations [31–34], but most of them include some arbitrary which prevent their use in global calculations.

The rest of the paper is devoted to the performance analysis of a more general theoretically justified extrapolation scheme that was first introduced by Furnstahl, Hagen, and Papenbrock in Ref. [22], and subsequently developed in Refs. [23–25]. The underlying idea behind this approach is on a par with assertions of quantum field theories, where the energy of a particle enclosed in a finite volume is shifted by the imposed boundary conditions. For example, it was shown in Refs. [35,36] that the mass of a trapped particle exhibits an exponential convergence

to the infinite volume value at a certain theoretically predicted rate. In our case, the corresponding spatial confinement is present by virtue of the localized nature of the SHO basis. The effective dimensions of the enclosing volume are deduced from the spatial extensions of the oscillator functions. By truncating our working basis, we effectively impose a spherical hard-wall boundary condition in coordinate space and an analogous intrinsic sharp boundary in momentum space. These induced infrared (IR) and ultraviolet (UV) cutoffs of the basis, Λ_{IR} and Λ_{UV} , are modulated by the actual nucleus in consideration and the model space parameters N_{OS} and b , but are independent of the particular potential used. With the cutoffs explicitly considered, it is possible to derive the finite volume corrections to various nuclear structure observables, such as g.s. energies and radii, hence effectively extending the dimensions of the working basis to infinity.

As a proof of theoretical concept, a row of successful tests for the suggested extrapolation were performed on a number of model potentials, as well as an example of the deuteron with a realistic chiral effective field theory (χEFT) potential [22]. Although derived at first only for systems that could be reduced to single-particle degrees of freedom, the extrapolations showed a good reliability and robustness even in many-body calculations. Hence, the extrapolation method was used in the nuclei ^6He and ^{16}O computed with a no-core shell model and a couple-cluster method respectively [22]. Since then, the extrapolation for the binding energy has also been applied to several other nuclei [37–41], but without a particular analysis of its reliability.

Based on the previous insights, in Ref. [25], Furnstahl *et al.* have enhanced the theoretical basis of the derived IR correction formula to extend its applicability to many-body fermionic systems. The tests performed in three oxygen isotopes, $^{16,22,24}\text{O}$, generally confirmed the anticipated improvement of such IR extrapolations for atomic nuclei and brought us closer to the question of error quantification of the extrapolation.

Despite the demonstrated success of the method for these individual nuclei, the proposed scheme has not yet been put to a systematic test with widely used EDFs, exploring its precision, accuracy, and reliability throughout the whole isotopic chains, particularly in the neutron-rich extremes of heavier nuclear systems where the lack of convergence is largest. It is the purpose of this section to systematically test the performance of the suggested energy correction procedure within the HFB

framework with the Gogny D1S EDF. We start by introducing the relevant tools for the energy extrapolation on an example of ^{16}O . Later, we check the performance of the method in the nucleus ^{120}Cd . Finally, we perform a systematic study of the IR extrapolation scheme in the cadmium isotopic chain from proton to neutron drip lines.

A. Characteristic cutoffs of the basis

Following the arguments addressed in Refs. [22,42], there are two momentum cutoffs imposed by the truncation of the model space for a given finite single-particle basis of harmonic oscillator functions. One of the cutoffs is associated with the highest excitation energy of the chosen basis, $E_{\text{max}} = \hbar\omega(N_{\text{OS}} + 3/2)$ (see Fig. 1). In a semiclassical approximation, the maximum momentum a particle in such a basis can reach is $\Lambda_0 \equiv \sqrt{2mE_{\text{max}}}$ or in terms of basis parameters

$$\Lambda_0 = \sqrt{2(N_{\text{OS}} + 3/2)} \times \hbar/b. \quad (10)$$

We take this as a leading-order estimate of the corresponding UV momentum cutoff of the basis, i.e., $\Lambda_{\text{UV}} \approx \Lambda_0$.

The second cutoff is induced in the opposite energy limit of the finite SHO basis, which at low energies is shown to be effectively equivalent to a spherical cavity with a sharp boundary radius L_{IR} [24]. Choosing the classical turning point of a harmonic oscillator $L_0 \equiv \sqrt{2E_{\text{max}}/m\omega^2}$, or

$$L_0 = \sqrt{2(N_{\text{OS}} + 3/2)} \times b, \quad (11)$$

as a first-order approximation for this radius suggests $L_{\text{IR}} \approx L_0$. The associated IR cutoff is then defined as $\Lambda_{\text{IR}} \equiv \pi/L_{\text{IR}}$.

The complete convergence in a finite SHO basis can now be attained by the fulfillment of both UV and IR conditions imposing constraints on the choice of the basis. The first requirement is to select the basis in such a way that the highest momentum scale λ of the employed interaction is smaller than the maximum momentum in the working basis, i.e., $\lambda < \Lambda_{\text{UV}}$. This will ensure that all the ultraviolet physics set by the interaction has been captured in the working basis, which would provide a UV-converged result of the calculation. The second condition requires that the effective spatial radial extent L_{IR} of the chosen basis is large enough to encompass the many-body wave function, i.e., $r < L_{\text{IR}}$. It is this second condition that can usually never be fully achieved in practice for neutron-rich nuclei due to the different asymptotic behavior of the nuclear wave function (exponential falloff) and the SHO basis (Gaussian falloff) in coordinate space. Thus, in order to obtain the greatest degree of convergence in a truncated model space, one usually performs calculations in the largest accessible N_{OS} and seeks an optimal compromise between the IR and UV conditions by finding the binding energy minimum through variation of the intrinsic oscillator length b (see Fig. 2). However, selecting calculations performed only with sufficiently small oscillator lengths, one can strive to ensure the UV condition and thereby effectively isolate the systematic error coming from the lack of IR convergence.

While this is easily achievable in many-body calculations with interactions where the cutoff is set using an UV regulator, the situation is different in the current EDF approaches. Since the Gogny interaction has contact terms in the spin-orbit and

density-dependent part of the functional, it does not have an intrinsic momentum cutoff. Rios and Sellahewa [43] have recently shown that the D1S parametrization, once decomposed in partial waves, contains significant matrix elements connecting high and low momenta in some channels of the interaction. Nonetheless, it still remains to be investigated whether these two-body matrix elements have noticeable impact on the whole HFB calculation for a particular nucleus under consideration. However, in many cases we are able, *a posteriori*, to determine the parameters of the working basis in order to effectively ensure the UV criterion $\lambda < \Lambda_{\text{UV}}$, whereupon the IR extrapolation scheme could be applied to account for the IR corrections.

B. The first-order IR extrapolation

One of the actual challenges in accounting for the boundary effects enacted by the IR cutoff was the determination of the effective impenetrable extend of the chosen set of SHO basis functions in a most accurate and universal way. The choice of the maximum displacement, L_0 , can qualitatively explain the concept of extrapolation, but it is only a leading-order estimate for the extent of the oscillator wave function. As it was recently shown, the correct box size of the SHO basis for a many-body system is deduced by matching the smallest eigenvalue of total squared momentum operator for a particular nucleus in a given SHO basis to the analogous smallest value in the spherical cavity [25]. The resulting effective radius L_{eff} is then

$$L_{\text{eff}} = \left(\frac{\sum_{nl} v_{nl} a_{ln}^2}{\sum_{nl} v_{nl} \kappa_{ln}^2} \right)^{1/2}, \quad (12)$$

where the κ_{ln}^2 are the eigenvalues of the momentum squared operator diagonalized in the SHO basis, v_{nl} are the occupation numbers of nucleons giving the lowest kinetic energy in SHO basis, and a_{ln} are the $(n+1)$ th zeros of the spherical Bessel function j_l .

With the effective hard-wall boundary of the SHO basis properly identified, one can now recast the initial problem of having the given many-body system enclosed by a harmonic oscillator soft cavity into the one with a sharp infinite potential with an effective radius L_{eff} . Such problems of confined quantum systems have been studied already (e.g., [44] and citations therein) with various techniques available for the energy corrections. One can proceed by making a linear energy approximation of the many-body wave function and impose a vanishing Dirichlet boundary condition at L_{eff} . Whereas the details of the derivation can be found in Ref. [25], the resulting analytical expression of the first-order IR correction is then of the form

$$E_L(L_{\text{IR}}) = A_{\infty} \exp(-2k_{\infty}L_{\text{IR}}) + E_{\infty}, \quad (13)$$

where for the atomic nucleus the proper radius is $L_{\text{IR}} = L_{\text{eff}}$ that depends both on the basis and the particular isotope, while A_{∞} , k_{∞} , and E_{∞} are taken as fit parameters. This derived exponential pattern of the IR correction was shown to be independent of the particular potential and validated in the examples mentioned above [23–25].

C. Playground test with ^{16}O

We now illustrate the suggested extrapolation concept and introduce the relevant benchmarking tools for this method using the nucleus ^{16}O as an example. The commencing test with this nucleus is prompted by the well-converged HFB results starting already with a basis of $N_{\text{OS}} = 15$, as is evident from Figs. 2 and 3. In Figs. 5(a) and 5(c) we show the HFB energy as a function of the effective radial extent L_{eff} . In order to apply the IR corrections, we start by selecting only those calculations for which the UV cutoff of the basis is sufficiently large, so that the results are considered to be UV converged. This is done by taking into account only those g.s. energies that are computed in a basis with the UV cutoff above a certain threshold value; that is, $\Lambda_{\text{UV}} > \Lambda_{\text{thr}}$. For this illustration we take $\Lambda_{\text{thr}} = 750 \text{ MeV}/c$, and justify this choice later. The selected HFB energies are represented by the filled symbols in Fig. 5(a). We find that all of them almost perfectly fall on an exponential curve, consistent with the theoretical predictions for UV-converged results. The observed rise of the g.s. energies at larger values of L_{eff} [Fig. 5(a), hollow symbols] is due to an insufficient UV convergence. Those calculations are excluded from the fit to the form of Eq. (13). The solid lines in Fig. 5(a) represent the separate fits to the HFB energies calculated in different combinations of the basis dimensions, N_{OS} . The inset, Fig. 5(b), shows the corresponding extrapolated values E_{∞} together with a reference value of a virtually converged calculation $E_{\text{min}}(21)$. We see in this figure that differences around 60 keV are obtained. Although we do not directly attribute such a spread in the extrapolated values to the uncertainty of the method, it is nevertheless representative of the precision and accuracy level of the extrapolation scheme.

Nevertheless, we have to mention that some of the points used in the extrapolation given in Figs. 5(a) and 5(b) are already close to the converged value. In order to imitate a typical situation (common to heavy and neutron-rich nuclear systems) of having access only to an insufficiently large working basis for complete convergence, we limit ourselves now to a SHO basis with $N_{\text{OS}} = 13$. In this case the calculations for ^{16}O are not fully converged. Furthermore, an accurate, precise, and reliable extrapolation should also be largely insensitive to the choice of the threshold momentum Λ_{thr} , as long as the UV convergence is ensured. We verify this criterion for ^{16}O by fitting to different sets of HFB calculations, defined by the choice of a threshold value $\Lambda_{\text{thr}} = 850, 950, 1050 \text{ MeV}/c$. The illustration of this benchmark can be seen in Fig. 5(c), where fits for different threshold values are provided by the colored lines. All HFB points are found to be on an exponential curve and the quality of the exponential convergence pattern is particularly well seen in Fig. 5(d). The corresponding E_{∞} estimates of the fits, shown in Fig. 5(e), yield a narrow spread of their values, falling very close to the converged energy value $E_{\text{min}}(21)$ even in cases where the closest points used in the fit are a few MeV above this value. This indicates good stability, accuracy, and precision of the method in this specific example.

We now perform a systematic analysis to estimate the dependence of the extrapolated values on the choice of Λ_{thr} . It is expected that, below a certain value of Λ_{thr} , the computed HFB energies values could be affected by a lack of UV convergence (or ‘‘UV contamination’’). The knowledge of a lower limit of Λ_{thr} will allow us to include as many computed HFB data points into our extrapolation as possible. To this end, we perform a series of extrapolations obtained in bases with various sets of N_{OS} and b parameters, and vary the threshold momentum across a wide range of $450 \leq \Lambda_{\text{thr}} \leq$

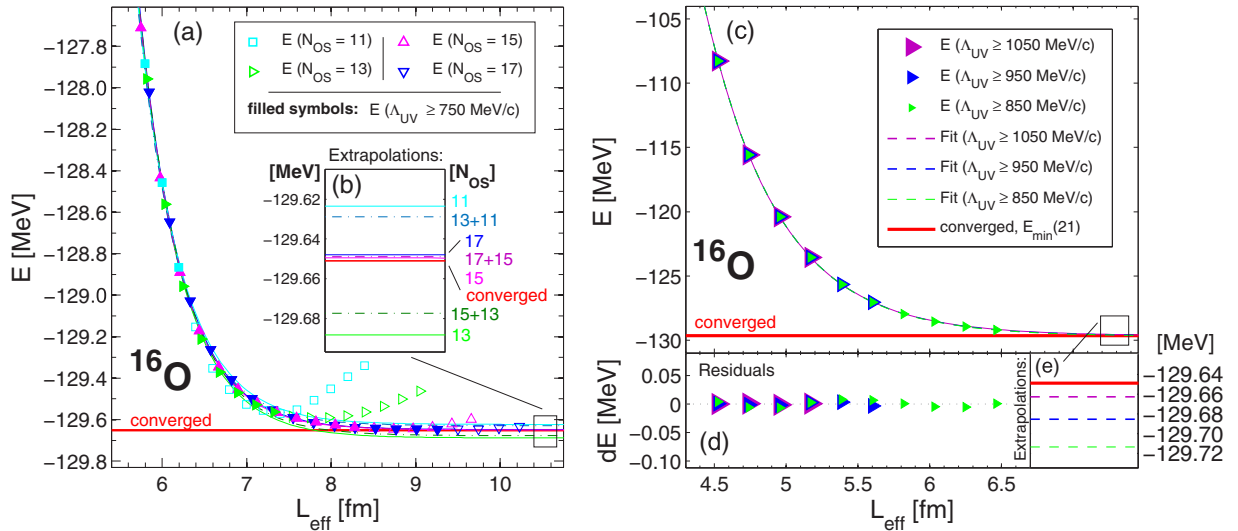


FIG. 5. (a) calculated HFB energies for the nucleus ^{16}O using SHO bases with $N_{\text{OS}} = 11, \dots, 17$ as a function of L_{eff} . Filled symbols indicate g.s. energies having $\Lambda_{\text{UV}} > 750 \text{ MeV}/c$, the red line shows the converged result, and other continuous and dot-dashed lines are the corresponding fits to Eq. (13); (b) the inset shows E_{∞} values for different extrapolations; (c) HFB energies calculated in a basis having $N_{\text{OS}} = 13$ and filtered out by conditions $\Lambda_{\text{thr}} = 850, 950, \text{ and } 1050 \text{ MeV}/c$. The corresponding fits are shown with dashed lines; (d) residuals defined as $dE = E(L_{\text{eff}}) - E_L(L_{\text{eff}})$; and (e) the corresponding extrapolations. See figure labels.

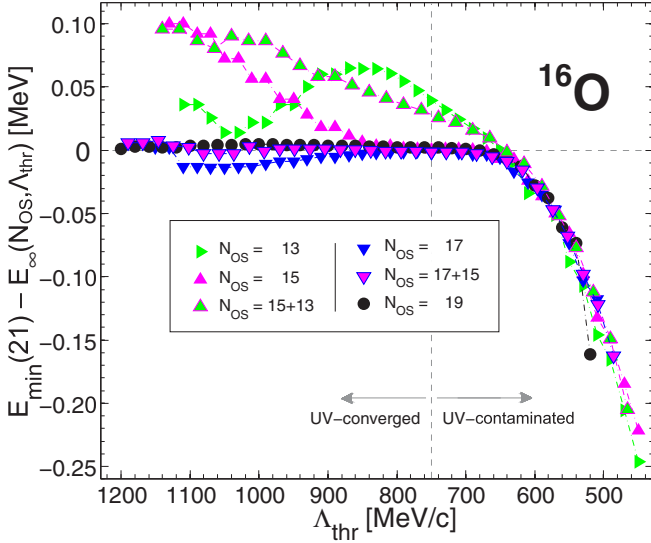


FIG. 6. Difference of the calculated $E_{\min}(21)$ and the energy obtained with IR extrapolations from different combinations of basis dimension N_{OS} and Λ_{thr} values.

1250 MeV/c. In Fig. 6 we plot the difference between $E_{\min}(21)$ and the extrapolated values. Hence, positive (negative) values give extrapolated g.s. energies below (above) $E_{\min}(21)$, which is considered to be the converged g.s. energy. We observe first that lowering Λ_{thr} below a certain limit, namely, 620 MeV/c, we start to incorporate into our extrapolation an increasing amount of points which are not sufficiently UV converged. Therefore, the inclusion of these points deteriorates the quality of the fit and should be eliminated from the IR extrapolating data set. Resting upon the results of these calculations, we estimate the threshold for a significant UV contamination lies around $\Lambda_{thr} \approx 750$ MeV/c in ^{16}O . We also observe a slight dependence of the extrapolated g.s. energies on Λ_{thr} of about 0.1 MeV if HFB results with $N_{OS} \leq 15$ are considered, even in the regions well above the estimated onset of the UV contamination. Consequently, the extrapolated results are not completely free of Λ_{thr} dependencies unless a sufficiently large value of N_{OS} is chosen.

To conclude this section, we summarize the necessary criteria for the IR extrapolation to be robust and reliable. Assuming that the set of parameters (N_{OS}, b) defining the basis of HFB calculations ensures the UV convergence of the g.s. energies, the following properties must hold for the E_{∞} estimates:

- (i) Independence of the chosen threshold value Λ_{thr} that defines the set of HFB energies used in the fits according to criterion $\Lambda_{UV} > \Lambda_{thr}$.
- (ii) Insensitivity to the basis dimensionality used to compute the HFB energies chosen in the fit dataset. That is, the E_{∞} values should be independent of whether we pick a calculation performed with $N_{OS} = 17$, with $N_{OS} = 19$, or even if we combine the two sets.
- (iii) Finally, given that the fully converged value of the HFB g.s. energy is generally unknown, extrapolations should be able to at least reproduce the best converged

HFB calculation available, i.e., $E_{\min}(21)$ in this work, or yield E_{∞} estimates that are below that value.

D. Cadmium isotopic chain

In the previous section we studied the nucleus ^{16}O to benchmark the IR extrapolation scheme and establish the main properties that the extrapolated energy should fulfill. We now apply the same method to extract the E_{∞} estimates first in the nucleus ^{120}Cd , and then for the whole cadmium isotopic chain. As we showed in Figs. 2(b) and 3(a), none of these nuclei are fully converged. The HFB energy as a function of the effective spatial radial extent L_{eff} and the corresponding fits to Eq. (13) for the nucleus ^{120}Cd are plotted in Fig. 7. Following the prescription found in the previous section, we impose a cutoff of $\Lambda_{UV} > 750$ MeV/c to select SHO bases with sufficiently high momentum cutoff. We observe in Fig. 7(a) a qualitative exponential decay with respect to L_{eff} . However, the extrapolated values show a larger spread in absolute energy than in the case of ^{16}O , as can be seen in Fig. 7(b). For example, the E_{∞} estimate is about 1.7 MeV lower with the extrapolation from the $N_{OS} = 15$ basis than from the one with $N_{OS} = 17$. In addition, the minimal g.s. HFB energy attained in the $N_{OS} = 21$ basis, i.e., the $E_{\min}(21)$ value, lies between the two extrapolated energies mentioned above. Similarly to Fig. 6, we plot the dependence of the extrapolated energies on the Λ_{thr} value in Fig. 8 for the nucleus ^{120}Cd . In this case the situation is far from fulfilling the requirements for a robust and reliable extrapolation given in the previous section. We found rather unstable results for extrapolations from $N_{OS} = 13, 15$, and 17 bases for large values of Λ_{thr} that are precisely the ones that should be better UV converged. In those cases, the spread in the extrapolated energies produced by the particular choice of Λ_{thr} can be as large as 7 MeV. In

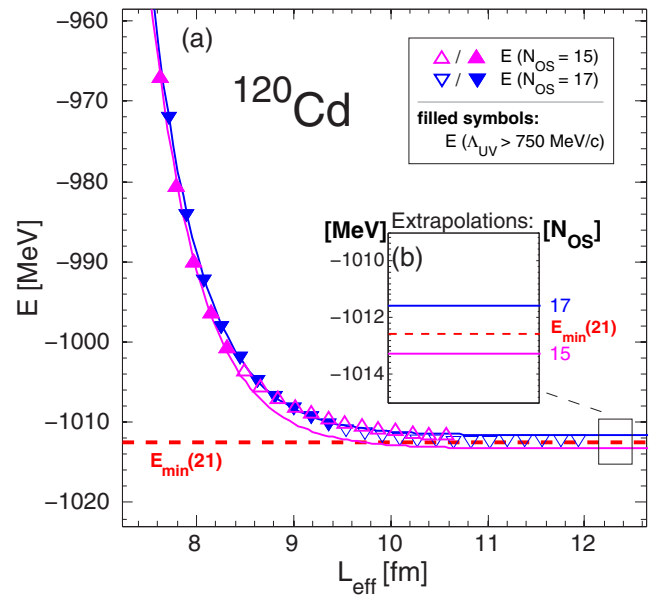
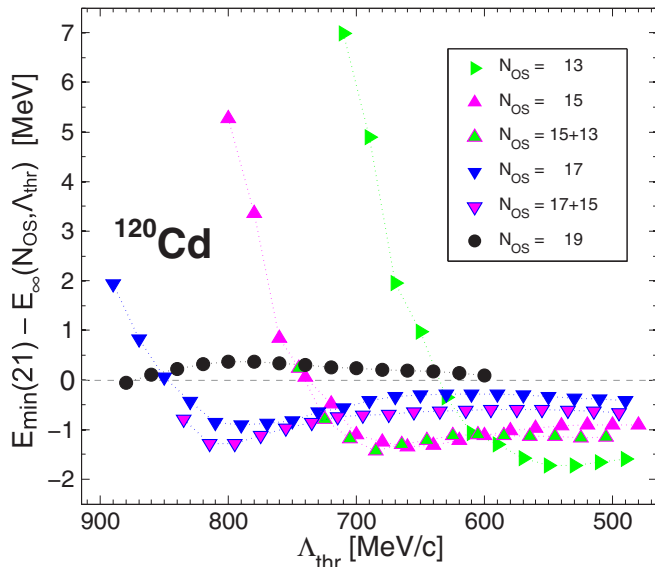


FIG. 7. Similar to Figs. 5(a) and 5(b), but for ^{120}Cd nucleus for $N_{OS} = 15$ and 17 bases. The E_{\min} values is indicated by the dashed red line.

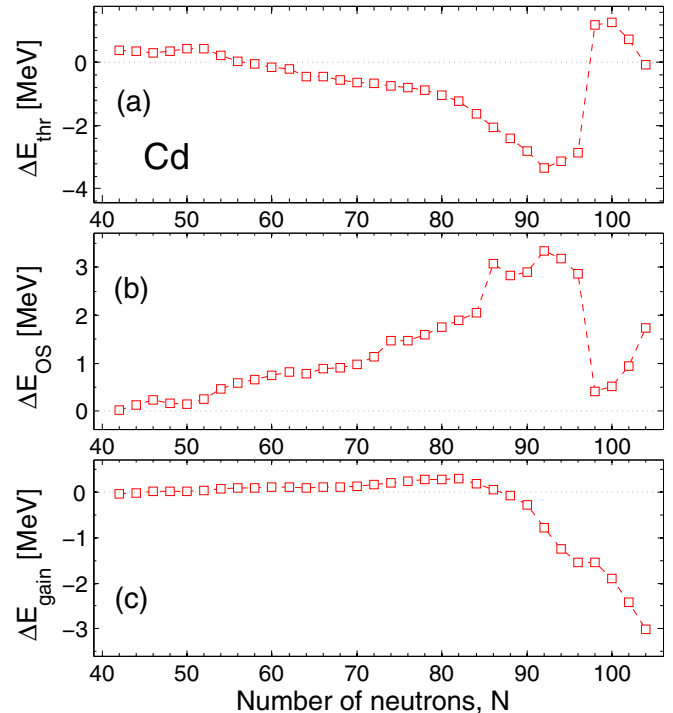
FIG. 8. Similar to Fig. 6 but for ^{120}Cd .

addition, when the fits are performed for the $N_{\text{OS}} = 13, 15,$ and 17 results separately, as well as combinations thereof, the extrapolated energies are systematically less bound than the best value reached with the $N_{\text{OS}} = 21$ basis in the range of Λ_{thr} where a flatter behavior is found. Since the extrapolation method is intended to estimate the remaining energy missed by the truncation of the working basis, these results are not acceptable. However, the only exception are the extrapolations from HFB energies obtained with $N_{\text{OS}} = 19$ basis, which seem to be most reliable.

So far we have discussed the performance of the IR extrapolation method for individual nuclei. For the sake of completeness, we analyze the reliability and stability of the method in the whole cadmium isotopic chain. According to the points raised in the previous section to define the quality of the extrapolated energies, let us define the following quantities for each nucleus in the chain:

- (i) $\Delta E_{\text{thr}} \equiv E_{\infty}(\Lambda_{\text{thr}} = 750 \text{ MeV}/c) - E_{\infty}(\Lambda_{\text{thr}} = 900 \text{ MeV}/c)$ with $N_{\text{OS}} = 19$ fixed to check the dependence on the chosen threshold value Λ_{thr} . Hence, $\Delta E_{\text{thr}} \approx 0$ would mean good performance.
- (ii) $\Delta E_{\text{OS}} \equiv E_{\infty}(N_{\text{OS}} = 17) - E_{\infty}(N_{\text{OS}} = 19)$ with $\Lambda_{\text{thr}} = 750 \text{ MeV}/c$ fixed to check the dependence on N_{OS} . As in the previous point, $\Delta E_{\text{OS}} \approx 0$ would mean good performance.
- (iii) $\Delta E_{\text{gain}} \equiv E_{\text{min}}(21) - E_{\infty}(N_{\text{OS}} = 19, \Lambda_{\text{thr}} = 750 \text{ MeV}/c)$ to check the quality of the extrapolation with respect to the lowest HFB energy computed in this work. Thus, ΔE_{gain} should be equal to zero for converged cases and slightly positive for those HFB calculations which are not converged.

In Fig. 9 we show these three quantities as a function of the number of neutrons in the nuclei $^{90-152}\text{Cd}$. We observe first that the three conditions given above are not completely fulfilled simultaneously throughout the whole cadmium isotopic chain.

FIG. 9. ΔE_{thr} , ΔE_{OS} , and ΔE_{gain} for $^{90-152}\text{Cd}$ isotopes as a function of the neutron number.

Nevertheless, in many nuclei the dependencies on Λ_{thr} and N_{OS} are rather mild, with $|\Delta E_{\text{OS}}| \approx |\Delta E_{\text{thr}}| \leq 2 \text{ MeV}$ in the range of $N = 42-84$. In this region, the differences of the extrapolated energies with respect to the best values obtained with $N_{\text{OS}} = 21$ basis are close to zero or slightly above, providing a physically sound extrapolation. However, the situation is different in the neutron rich region above $N \geq 86$, where the extrapolations are remarkably dependent on the choice of both Λ_{thr} and N_{OS} , and they lie above the best HFB energies directly computed, i.e., $\Delta E_{\text{gain}} < 0$. Therefore, whereas in the first region some systematic error bars could be extracted from the extrapolation, that is not the case in the neutron-rich region.

We now represent in Fig. 10 the same quantities but as a function of the two-neutron separation energy $S_{2n}(N) \equiv E(Z, N-2) - E(Z, N)$, where the shell gaps, corresponding to $N = 50$ and 82 magic numbers, are well seen. From the astrophysical point of view, the most interesting aspect is that the ill behavior of the extrapolation method with the present EDF is significantly larger for isotopes beyond $N = 82$ when the two-neutron separation energy is less than 5 MeV approximately, which is precisely the relevant range in r -process calculations.

A similar result is obtained in the magnesium isotopic chain (not shown) where such an erratic behavior of the extrapolated energy is also found in the neutron rich part of the chain ($S_{2n} \leq 5 \text{ MeV}$). Therefore, the present extrapolation scheme with Gogny EDF is not able to provide reliable estimations of E_{∞} values in those loosely bound regions, where the lack of convergence is also the largest. One possible explanation is that the momentum threshold chosen to select the set of

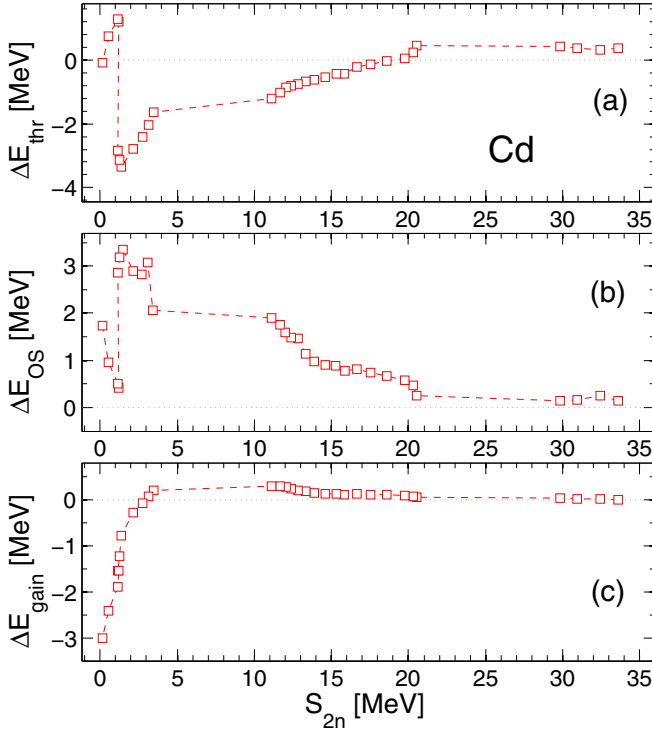


FIG. 10. Similar to Fig. 9 but as a function of the S_{2n} , which were obtained directly from HFB calculations in the $N_{OS} = 21$ basis *without* extrapolations.

points used for the extrapolations, though in some case as large as $\Lambda_{thr} = 1200$ MeV/ c , is not large enough to ensure the UV convergence. This could be justified by the absence of an explicit regulator in momentum space in the Gogny EDF. Another, complementary option could be the fact that a simple exponential extrapolation cannot fully capture the IR physics of the present EDF. By the same arguments, the considered extrapolation scheme cannot be used to extract the two-neutron separation energies from the E_∞ values. Despite this, being energy differences of the neighboring nuclei, the particle separation energies are expected to be better converged. Indeed, this is the case as can be seen in Fig. 11, where calculated S_{2n} values are shown without any extrapolations. The obtained energies are distributed among the shaded column bins according to the basis dimensions of the calculations. Moreover, in order to see the convergence patterns more clear, the separation energies for each isotope are shifted down by a constant that equals the S_{2n} value obtained in the $N_{OS} = 11$ [Fig. 11(a)] or $N_{OS} = 13$ [Fig. 11(b)] basis. Furthermore, for better readability, the two-neutron separation energies are also displaced within each column bin so that the lower absolute S_{2n} values are shifted closer to the left edge of each shaded region, while the higher ones are closer to the right edge (by analogy to Fig. 10). We see that for isotopes having $S_{2n} > 5$ MeV, the enlargement of the basis beyond $N_{OS} = 11$ affects their values up to 0.3 MeV at most, Fig. 11(a). For nuclei which have $S_{2n} < 5$ MeV the spread around zero reference value is about double twice as high, reaching as much as 0.6 MeV for the dripline isotope

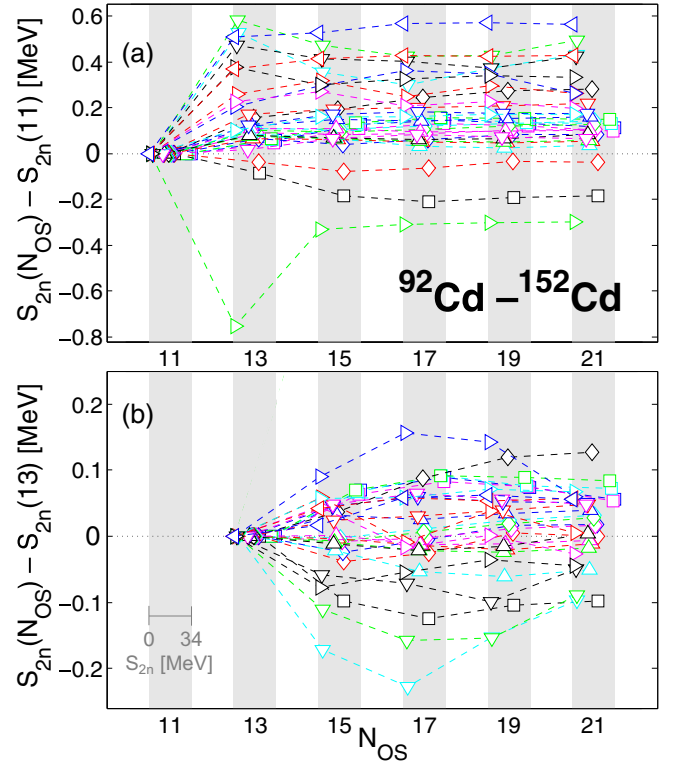


FIG. 11. S_{2n} energies of cadmium isotopes calculated in different basis dimensions (shaded bins). Color code and symbols are same as in Fig. 3.

^{152}Cd predicted by the Gogny D1S EDF. By the same token, Fig. 11(b) shows the convergence patterns zeroed out for a somewhat larger $N_{OS} = 13$ basis. Here we see that almost all of the S_{2n} values in $N_{OS} = 21$ basis fall within a 0.1 MeV spread. However, we observe a somewhat larger spread for nuclei having $S_{2n} < 5$ MeV in the $N_{OS} = 15, 17, 19$ bases. All in all, despite the fact that two-neutron separation energies do not exhibit any noticeable convergence pattern when the basis size is increased, these quantities reach a much better degree of convergence already in relatively small bases.

V. SUMMARY AND DISCUSSION

We have studied the convergence pattern of the HFB energies as a function of the maximum number of SHO shells included in the working basis, N_{OS} , as well as a function of the oscillator length, b . The calculations were performed with the Gogny D1S EDF. Generally, one has to include a prohibitively large number of N_{OS} in practical calculations to ensure convergence. In order to circumvent this shortcoming, one can opt to use various extrapolation techniques to obtain an estimate of the converged observables. While the ansatz $\Delta E(N_{OS}) \approx \Delta E(N_{OS} - 2)/2$, that is central in a purely phenomenological energy correction scheme [8,21], proved generally *not* to hold, we have turned to and studied one of the most promising extrapolation schemes recently proposed, namely the IR extrapolation [25].

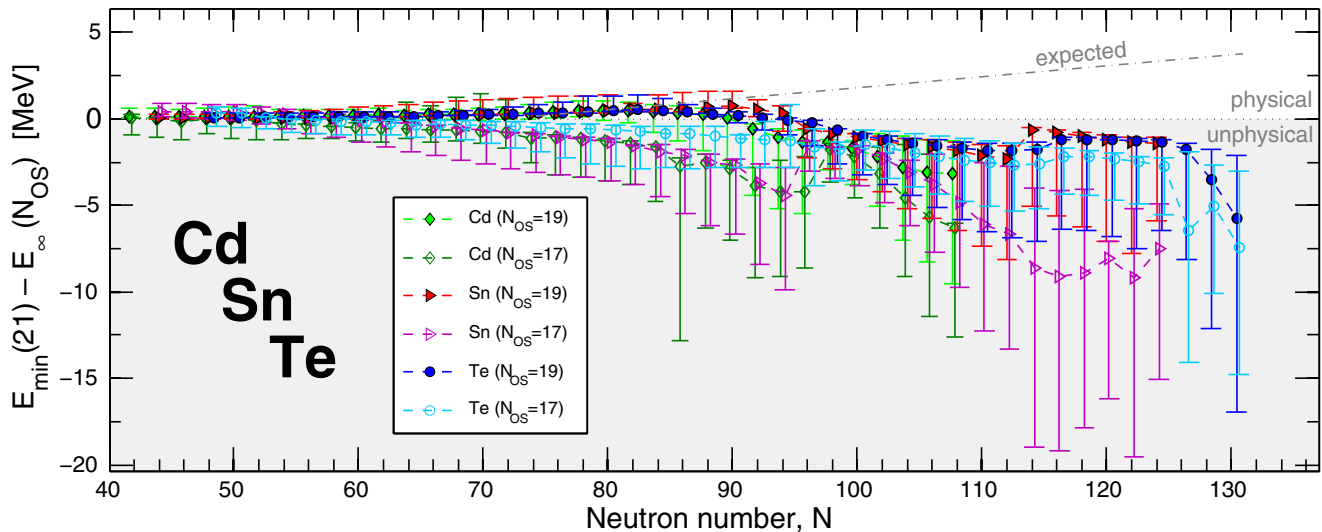


FIG. 12. The plot shows the results of IR extrapolation for nuclei in cadmium, tin, and tellurium isotopic chains as a function of neutron number in form of the differences $E_{\min}(21) - E_{\infty}(N_{OS})$ with momentum threshold $\Lambda_{\text{thr}} = 750$ MeV/ c . Two dimensions of model space are considered: $N_{OS} = 17$ (hollow symbols) and $N_{OS} = 19$ (filled symbols), separately. The associated error bars represent the spread in corresponding E_{∞} values from the variation of the threshold parameter in the interval $700 < \Lambda_{\text{thr}} < 900$ MeV/ c .

We have seen that the application of the considered IR extrapolation to a test case of ^{16}O seems to work nearly perfectly, providing reliable results that are both threshold independent and consistent with the fully converged reference value. A more serious benchmark, first by application to the nucleus ^{120}Cd , and then to the whole set of nuclei in the cadmium isotopic chain, revealed, however, some limitations of the proposed scheme for the HFB energy obtained with the Gogny D1S EDF.

Figure 12 summarizes the conducted analysis of the IR extrapolation scheme for cadmium isotopes, as well as extends the scope of the study to tin and tellurium nuclei. As is the case with all considered isotopic chains, the most robust extrapolations are obtained for isotopes in the direct vicinity of the stability region. Nevertheless, in this region the extrapolations are least relevant due to the larger degree of convergence of the HFB calculations in comparison to the neutron-rich isotopes. However, as one moves away, towards the neutron drip line, the IR extrapolations fail to yield reliable results. In particular, the discrepancy of the extrapolations from $N_{OS} = 17$ and $N_{OS} = 19$ values (with $\Lambda_{\text{thr}} = 750$ MeV/ c) reach easily up to 5–8 MeV. Besides that, varying Λ_{thr} for neutron-rich nuclei has a much greater impact on the estimated E_{∞} values (spanning energies of 10–15 MeV for $A \sim 115$). Finally, we also notice that the IR corrections can no longer even reproduce the most converged HFB calculations at hand [i.e., the $E_{\min}(21)$ values] in the neutron-rich tail of the isotopic chain, which is evident by the negative unphysical estimates for $N \gtrsim 96$ in Fig. 12. These results have been supported

by similar findings for other isotopic chains throughout the nuclear chart [45].

To summarize, our HFB calculations with Gogny EDF show that the investigated extrapolation schemes are so far applicable only in the regions of well-bound nuclei. The origin of these behavior could be the lack of UV convergence even in harmonic oscillator basis with a momentum cutoff of ≈ 1 GeV/ c due to the presence of contact terms in the Gogny EDF (and in most of the EDFs used nowadays). In such a case, the IR extrapolation should not be applied unless an ultraviolet regulator is explicitly included in the EDF. Additionally, it is also possible that even though the calculations are UV converged, the simple exponential extrapolation is not enough to produce physically sound extrapolated HFB energies with the present functional. Disentangling these two aspects requires one to either explicitly include a regulator in the definition of the functional or to consider all terms of the EDF as finite range.

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