# **Finite-size instabilities in finite-range forces**

C. Gonzalez-Boquera,  $1, *M$ . Centelle[s](https://orcid.org/0000-0001-8508-604X)  $\bullet, 1, †X$ . Viñas  $\bullet, 1, †$  and L. M. Robledo  $\bullet^{2,3,§}$  $\bullet^{2,3,§}$  $\bullet^{2,3,§}$ 

<sup>1</sup>*Departament de Física Quàntica i Astrofísica and Institut de Ciències del Cosmos (ICCUB), Facultat de Física,*

*Universitat de Barcelona, Martí i Franquès 1, E-08028 Barcelona, Spain*

<sup>2</sup>*Departamento de Física Teórica and CIAFF, Universidad Autónoma de Madrid, E-28049 Madrid, Spain*

<sup>3</sup>*Center for Computational Simulation, Universidad Politécnica de Madrid,*

*Campus de Montegancedo, Boadilla del Monte, E-28660 Madrid, Spain*

(Received 17 February 2021; accepted 24 May 2021; published 14 June 2021)

It has been recently shown that some Gogny finite-range interactions suffer from finite-size instabilities in coordinate-space calculations [\[Eur. Phys. J. A](https://doi.org/10.1140/epja/i2019-12838-7) **55**, 150 (2019)]. We confirm this finding by using the Hartree-Fock (HF) method in the quasilocal approximation to finite-range forces. The use of the quasilocal approximation substantially simplifies the calculations as compared with those including the exact exchange contribution to the energy and HF fields. The quantity most affected by the finite-size instabilities in the coordinate-space calculations is the spatial density at the origin that wildly oscillates as the HF iterative process proceeds. In addition to the recent D1M<sup>∗</sup> parametrization of the Gogny force, we find that the D1M parametrization also shows this deficiency in several nuclei. We find that the harmonic-oscillator basis with its ultraviolet cutoff provides converged results in a wide and realistic range of basis sizes. This result serves as a justification of the numerous calculations with D1M and D1M<sup>∗</sup> in finite nuclei that show no trace of instability.

DOI: [10.1103/PhysRevC.103.064314](https://doi.org/10.1103/PhysRevC.103.064314)

### **I. INTRODUCTION**

In Ref. [\[1\]](#page-6-0) we proposed a new parametrization of the Gogny interaction, denoted D1M∗, aimed to obtain a stiffer equation of state (EoS) of neutron-star matter. The goal was to get maximum neutron-star masses of  $2M_{\odot}$ , in agreement with recent astrophysical observations [\[2,3\]](#page-6-0). We were motivated by the fact that this property is not achieved by any of the standard Gogny forces of the D1 family [\[4\]](#page-6-0). We also wanted to preserve the good description of binding energies [\[5\]](#page-6-0) and other observables [\[6\]](#page-6-0) provided by the D1M force in Hartree-Fock-Bogoliubov (HFB) and beyond-HFB calculations [\[6\]](#page-6-0). We recall that D1M was developed as an accurate Gogny HFB nuclear-mass model, achieving a rms deviation with respect to the known experimental masses below 800 keV [\[5,7\]](#page-6-0). In the fit of D1M<sup>∗</sup> [\[1\]](#page-6-0), we modified the eight finite-range strength parameters of the D1M force while keeping the other parameters at their nominal D1M values. Seven linear combinations of these strength parameters, related to different properties of symmetric nuclear matter, and the strength of the pairing interaction in the  $S = 0$ ,  $T = 1$  channel were constrained to maintain the same values as in D1M. The remaining combination was used to modify the slope of the symmetry energy and, therefore, the stiffness of the neutron matter EoS. In this way the prediction for the maximum neutron-star mass can

term of the Gogny interaction was fine tuned to improve the quality of the computed binding energies [\[1\]](#page-6-0). All of the finite-nuclei calculations in Ref. [\[1\]](#page-6-0) were carried out with the HFBAXIAL code  $[8]$  using an approximate second-order gradient method [\[9\]](#page-6-0) to solve the HFB equations in a harmonicoscillator (HO) basis including up to 19 major oscillator shells and the oscillator lengths adapted to the characteristic  $A^{1/6}$ length-scale dependence with mass number *A*. Actually, since the seminal paper of Dechargé and Gogny [\[10\]](#page-6-0), almost all of the HFB calculations of spherical and deformed nuclei with Gogny interactions have been performed in a HO basis, including the calculations involved in the determination of the parameters of the interactions. In particular, this is the case of the D1M interaction [\[5\]](#page-6-0), to which we compared our results. The HO basis, though, is not optimal to observe finite-size instabilities that may arise in coordinate-space calculations on a mesh.

be modified. Finally, the strength  $t_3$  of the density-dependent

# **II. FINITE-SIZE INSTABILITY IN COORDINATE-SPACE CALCULATIONS**

In Ref.  $[11]$  and its preliminary version  $[12]$ , it is found that both the D1M<sup>\*</sup> [\[1\]](#page-6-0) and D1N [\[13\]](#page-6-0) parametrizations of the Gogny force are affected by spurious finite-size instabilities in the  $S = 0$ ,  $T = 1$  channel. These instabilities are detected through a fully antisymmetrized random-phase approximation (RPA) calculation of the nuclear matter response functions based on the continued fraction technique [\[14\]](#page-6-0). This method produces results which are very similar to those of the

<sup>\*</sup>claugb@fqa.ub.edu

<sup>†</sup>mariocentelles@ub.edu

<sup>‡</sup>xavier@fqa.ub.edu

<sup>§</sup>luis.robledo@uam.es

<span id="page-1-0"></span>linear-response theory with the multipole decomposition method for the Gogny interaction [\[15\]](#page-6-0).

The procedure of Ref. [\[14\]](#page-6-0) has been applied to the search of instabilities in standard Gogny forces with or without tensor terms. In agreement with the results of previous analyses for Skyrme functionals [\[16,17\]](#page-6-0), it was concluded in Refs. [\[11,12\]](#page-6-0) that the key quantity to detect spurious finite-size instabilities is the nuclear matter critical density  $\rho_c$ , corresponding to the lowest density at which the nuclear response at zero transferred energy displays a pole. These finite-size instabilities may develop unphysical results in some properties of the nucleus, such as, for example, in the proton and neutron densities, if  $\rho_c \leq 1.2 \rho_0 \simeq 0.20 \text{ fm}^{-3}$  for a momentum transfer of about 2.5 fm<sup>-1</sup>. This critical density may be reached in HF calculations of some nuclei, such as, for example,  $^{40}$ Ca [\[16\]](#page-6-0). The instabilities of D1M<sup>\*</sup> and D1N were predicted in nuclear matter [\[11,12,14\]](#page-6-0) and their appearance in coordinate-space calculations of spherical finite nuclei was confirmed in Refs.  $[11,12]$  by using the FINRES<sub>4</sub> computer code [\[18\]](#page-6-0). As a consequence of the finite-size instabilities, the neutron and proton density profiles of nuclei largely vary from one iteration to the next in the iterative solution of the nonlinear HFB equations, without reaching convergence [\[16\]](#page-6-0).

The impact of finite-size instabilities in calculations with the Skyrme energy-density functional has been discussed thoroughly in the literature. In a recent review [\[19\]](#page-6-0), the link between finite-size instabilities and the existence of poles at finite-momentum transfer in the linear response of homogeneous nuclear matter has been extensively discussed. Instabilities also appear in certain Skyrme functionals in the  $S = 0$  channel in pure neutron matter and in heavy neutron droplets [\[20\]](#page-6-0) as well as in the spin channel when time-reversal invariance is broken in the calculation (such as in the case of odd-mass nuclei [\[21\]](#page-6-0), time-dependent HF calculations [\[22\]](#page-6-0), high-spin states [\[23\]](#page-6-0), or vibrational excited states [\[24\]](#page-6-0)).

In Ref. [\[25\]](#page-6-0) we commented on the main proposal of Ref. [\[12\]](#page-6-0) and provided initial information about the possible impact of the finite-size instability of the D1M<sup>∗</sup> force on HFB calculations of observables like binding energies, neutron and proton radii, and density profiles of finite nuclei using a HO basis.

To independently confirm the results of Refs. [\[11,12\]](#page-6-0) we have performed HF calculations with Gogny forces on a spatial mesh assuming spherical symmetry. To this end we use the quasi-local approximation (QLA) for finite-range forces described in Ref. [\[26\]](#page-6-0). In this approach the HF exchange energy density is approximated by a quasilocal functional obtained using the extended Thomas-Fermi (ETF) density matrix  $[27]$ , which is similar to the expansion for the density matrix proposed by Negele and Vautherin [\[28\]](#page-6-0) or by Campi and Bouyssy [\[29\]](#page-6-0). In the ETF method the density matrix is expanded in powers of  $\hbar$  with the  $\hbar^0$  term given by the density matrix in homogeneous matter (Slater approximation). To account for the inhomogeneities of the system we add a corrective  $\hbar^2$  contribution through second-order spatial gradients of densities and effective masses as well as their momentum derivatives computed at the Fermi surface [\[27\]](#page-6-0). Therefore, in the QLA, the energy density functional for finite-range effective interactions becomes local and therefore



FIG. 1. Solid lines show neutron density of <sup>208</sup>Pb computed with the D1M force with a HO basis with 12, 14, 16, 18, and 19 shells (yellow, red, green, blue, and black curves, respectively). Dashed lines show the same density obtained through a HF calculation on a mesh in the quasilocal approach. Dash-dotted lines show the same density extracted from Fig. 3 in Ref. [\[12\]](#page-6-0) (HF calculation on a mesh with the  $FINRES<sub>4</sub> code [18].$  $FINRES<sub>4</sub> code [18].$  $FINRES<sub>4</sub> code [18].$ 

the HF equations in coordinate space take a form similar to those of Skyrme forces  $[30]$ . In Refs.  $[26,31,32]$  it has been shown that calculations in coordinate space using the QLA provide results that are very close to the full HF values. To be more specific, our QLA results accurately agree with those obtained using the  $FINRES<sub>4</sub> code [18] used in$  $FINRES<sub>4</sub> code [18] used in$  $FINRES<sub>4</sub> code [18] used in$ Refs. [\[11,12\]](#page-6-0). As an example of the agreement, we show in Figs. 1 and 2 the <sup>208</sup>Pb neutron and proton density profiles calculated with the D1M interaction using both coordinate-space codes, where the close agreement between the two methods is clearly seen. From Figs. 1 and 2 we also learn that the mesh calculations produce density profiles with more pronounced oscillations near the center of the nucleus than the HO basis calculations (also shown in these figures for comparison). This is a first qualitative indication that spherical densities calculated in a mesh may be more affected by the finite-size



FIG. 2. The same as in Fig. 1 but for the proton density.

<span id="page-2-0"></span>

FIG. 3. The same as in Fig. [1](#page-1-0) but computed with the D1M<sup>∗</sup> force. The HF density is displayed for three different numbers of iterations.

instabilities than those computed with a HO basis. We also find that mesh calculations with the QLA are well suited for the analysis of instabilities in spherical nuclei in coordinatespace calculations because these calculations predict the same instabilities of finite nuclei reported in Refs. [\[11,12\]](#page-6-0). As an example, Figs. 3 and 4 show the proton and neutron densities of <sup>208</sup>Pb calculated with the D1M<sup>∗</sup> interaction and obtained after a given number of iterations using the QLA. Clearly, in this case the mesh-point density profiles display a divergent behavior with increasing number of iterations, while these densities are well behaved when computed in the HO basis.

As discussed in Refs. [\[11,12\]](#page-6-0) the instability is to be associated with the isovector channel of the interaction and its existence in finite nuclei is linked to central densities close to or in excess of a critical nuclear matter density  $\rho_c$ . However, our finite-nuclei calculations indicate that the situation is a bit more involved. For instance, we have found that there are examples of nuclei with D1M<sup>∗</sup>, such as  $16$ <sub>O</sub>,  $100$ <sub>Sn</sub>, or the very asymmetric  $176$ Sn, that fully converge in the coordinatespace calculation. This has been verified with both our QLA



FIG. 4. The same as in Fig. 3 but for the proton density.

code and the FINRES<sub>4</sub> code  $[33]$ . This result tells us that the asymmetry of the nucleus is not a sufficient condition for developing the finite-size instabilities and that there can be other factors, such as the structure of the nucleus, which may also play a role. This will be discussed below. On the other hand, in consonance with Refs. [\[11,12\]](#page-6-0), we find that all of our mesh-point calculations with  $D1M^*$  of  $N = Z$  nuclei with the Coulomb interaction switched off are always fully stable. This confirms the isovector nature of the instabilities since the asymmetry between protons and neutrons is lifted in these calculations. Nevertheless, it is a bit surprising that, in this case, rounding errors are unable to drive the system towards instability—see Ref. [\[16\]](#page-6-0) for a similar discussion with Skyrme functionals.

We have detected examples of finite-size instabilities in the HF-QLA coordinate-space calculations in other Gogny interactions, in addition to D1M<sup>∗</sup> and D1N. We have scanned on the order of 800 nuclei with the D1M parametrization at the QLA level assuming spherical symmetry and without including pairing correlations. We have found about 80 nuclei that become unstable (after a certain number of iterations), most of them with atomic number  $Z < 44$ . For example, the nuclei  ${}^{52}$ Ca,  ${}^{54}$ Ca,  ${}^{56}$ Ca,  ${}^{54}$ Ti,  ${}^{56}$ Ti,  ${}^{58}$ Fe,  ${}^{60}$ Fe,  ${}^{62}Fe$ ,  ${}^{60}Ni$ , and  ${}^{62}Ni$  diverge in the QLA-HF mesh calculations with D1M. When the pairing interaction is switched on, no significant changes are observed in this pattern. Instability seems to be associated with combinations of proton and/or neutron numbers around 34, 60, and 70 where  $s$  ( $l = 0$ ) and  $p$  ( $l = 1$ ) orbitals are expected near the Fermi level.<sup>1</sup> This is an unexpected finding because the critical density ρ*<sup>c</sup>* for D1M is about 1.35 $\rho_0$  and therefore this interaction, according to the nuclear matter criterion [\[11,12\]](#page-6-0), should not develop finite-size instabilities. These results clearly point out that the criterion of Refs.  $[11,12]$  should be complemented with finite-nuclei calculations for those interactions with  $\rho_c$  not too far from  $1.2\rho_0$ . Those finite-nuclei calculations would be of relevance especially in those regions where an *s* orbital is expected to lie close to the Fermi level. The results also point to the necessity to carry out calculations in a large set of nuclei in order to detect the finite-size instabilities. It is very common in the literature (see Ref. [\[17\]](#page-6-0) as an example) to consider just a handful of nuclei to assess the stability of a given functional and this might prove to be insufficient.

[I](#page-3-0)n the upper part of Table I we compare the binding energies of the nuclei  $^{16}O$ ,  $^{132}Sn$ , and  $^{208}Pb$  calculated with the D1M interaction using a HO basis [\[8\]](#page-6-0), our QLA mesh code and the FINRES<sub>4</sub> mesh code [\[18\]](#page-6-0). We can see that the HF binding energies computed with FINRES<sub>4</sub> are slightly more bound than those provided by the HO basis, as can be expected. On the other hand, the QLA results are in excellent agreement with those obtained in full HF calculations using the HO basis or the FINRES<sub>4</sub> code, with differences less than  $1\%$  for all considered nuclei. A similar situation is found for the nuclei

<sup>&</sup>lt;sup>1</sup>Please notice that the position of single-particle orbitals is determined by the self-consistent procedure and therefore it may change within a major shell.

<span id="page-3-0"></span>TABLE I. For the D1M and D1M<sup>∗</sup> Gogny interactions, Hartree-Fock binding energies obtained from the HO-basis calculation, the coordinate-space quasilocal calculation (QLA) and the full coordinate-space calculation (FINRES4) [\[33\]](#page-6-0). The percentage deviation of the HO-basis energy from the coordinate-space energy is shown in brackets. The Coulomb interaction is included in all the calculations.

	$B_{\text{HO}}$ (MeV)	$B_{\text{QLA}}$ (MeV)	$B_{\text{FINRES}_4}$ (MeV)
D <sub>1</sub> M			
$^{16}$ O	128.02	127.02 (0.79%)	128.07 (0.04%)
$132$ Sn	1102.57	1103.31 (0.07%)	1104.29 (0.16%)
208P <sub>b</sub>	1636.08	1637.96 (0.11%)	1639.31 (0.20%)
$DIM^*$			
$^{16}$ O	128.32	127.29 (0.81%)	128.58 (0.21%)
$100$ Sn	827.98	824.71 (0.40%)	829.08 (0.13%)
$176$ Sn	1146.15	1146.26 (0.01%)	1147.51 (0.12%)

 $16$ O,  $100$ Sn, and  $176$ Sn computed with the D1M<sup>\*</sup> force, where the corresponding binding energies are given in the lower part of Table I. As mentioned above, these nuclei are found to be stable with D1M<sup>∗</sup> in coordinate space by independent calculations performed with the QLA code and the FINRES4 code [\[33\]](#page-6-0). The agreement between the HO basis and mesh results is again excellent in D1M<sup>∗</sup> when the mesh calculations converge, which further supports the reliability of using the HO basis approach with D1M<sup>∗</sup>.

As we noticed in Ref.  $[25]$ , we have found empirical evidence that the appearance of the discussed instabilities in finite nuclei may be directly related to the presence of *s* orbitals in the neighborhood of the Fermi level. This is, for example, the case in the nuclei  ${}^{4}$ He and  ${}^{40}$ Ca (protons and neutrons) and 208Pb (protons) computed with D1M∗. The respective Fermi levels correspond to 1*s*, 2*s*, and 3*s* orbitals, and the three nuclei diverge in the mesh calculations. However, the nuclei  $^{16}$ O,  $^{100}$ Sn, or  $^{176}$ Sn, for which the *s* orbitals are far from the Fermi level, are stable with the same D1M<sup>∗</sup> force. A paradigmatic example is the case of the nuclei  $^{22}$ O and  $^{24}$ O. In the HF mesh calculation with D1M∗, the neutron Fermi level of <sup>22</sup>O is placed at the  $1d_{5/2}$  orbital and this nucleus is stable, whereas the nucleus  $24<sub>O</sub>$  has its neutron Fermi level in the  $2s_{1/2}$  orbital and the calculation of <sup>24</sup>O becomes quickly unstable after a few iterations. We have also considered the case where pairing correlations are taken into account through a HF + BCS mesh-point calculation within the QLA  $[31]$ (notice that this differs from the pairing calculation for open-shell nuclei of Ref. [\[11\]](#page-6-0) performed at the HFB level). Consistently with the previous discussion, the presence of *s* energy levels in the single-particle spectrum considered for the BCS space makes the calculation unstable when the *s* level is close to the Fermi level. If the occupation of the *s* level is small, i.e., this level is far from the Fermi level, the  $HF + BCS$ calculations may be stable. The number of iterations required for the instability to develop also seems to be correlated with the relative position of the *s* levels with respect to the Fermi energy [\[25\]](#page-6-0). Because only *s* wave functions do not vanish at the origin, the conspicuous role played by the *s* orbitals in the

divergence of the results may have to do with the fact that the instabilities in the nucleon densities develop at the center of the nucleus (see, for instance, Figs. [3](#page-2-0) and [4\)](#page-2-0).

Let us finish this section by pointing out that the criterion of Refs. [\[11,12,17\]](#page-6-0) based on the response function in infinite nuclear matter seems to require additional finite-nuclei calculations to pinpoint the deficiencies of effective nuclear interactions. In this respect, it would be worth extending the analysis of Ref. [\[24\]](#page-6-0), based on finding imaginary solutions of the RPA in finite nuclei, to the present case involving finite-range interactions. Finally, we would like to mention that we have computed the isovector effective mass [\[16\]](#page-6-0) for several parametrizations of the D1 family of the Gogny force. We have observed that these parametrizations appear to be more prone to develop instabilities in the coordinate-space calculations when the splitting of the neutron and proton effective masses becomes small or negative. In the future, we wish to explore further whether this and other signatures may help to single out the critical combinations of the coupling constants of the Gogny force that lead to the finitesize instabilities.

## **III. HARMONIC OSCILLATOR BASIS AS AN ULTRAVIOLET CUTOFF**

The use of the harmonic-oscillator basis is almost mandatory in order to handle, for all the different kinds of deformations one can find over the periodic table, the exchange and pairing fields present in finite-range forces. Hence, we used a HO oscillator basis in the paper where D1M<sup>∗</sup> was proposed [\[1\]](#page-6-0) to fine-tune the density-dependent strength so as to improve the agreement of binding energies with experimental data. For those calculations we used a basis with a number of shells depending on the region of the nuclear chart. We computed the properties of more than 600 eveneven nuclei covering both deformed and spherical systems. In these calculations with D1M<sup>∗</sup> we did not observe any convergence issue after the  $\approx$ 30 000 HFB calculations. The same stability has been confirmed in large-scale calculations of fission properties of very neutron-rich superheavy nuclei carried out recently [\[34\]](#page-6-0) with the D1M<sup>∗</sup> force. It has to be mentioned that finite-nuclei calculations with some Skyrme functionals show instabilities in the  $S = 1$  channel in spite of using a finite HO basis  $[21,24]$ . Whether this is the case with finite-range forces requires further studies. We remark that, at present, the conclusions of our work apply to the  $S = 0, T = 1$ channel.

The stability of the calculations performed with the HO basis could be related to its inherent ultraviolet (UV) cutoff. It serves as a pragmatic strategy for problems related to highmomentum components in the wave function in a way that closely resembles other cutoffs used in pairing calculations with zero-range forces—such as, for instance, the introduction of an active window. On the other hand, mesh calculations with the use of finite differences to evaluate derivatives are more prone to suffer from the effect of those high-momentum components. This difference between HO basis and mesh calculations was already recognized in Refs. [\[11,12\]](#page-6-0), where it was argued that the use of a HO basis "strongly renormalizes the interaction and inhibits the development of instabilities." It was concluded in Refs. [\[11,12\]](#page-6-0) that "the D1M<sup>∗</sup> interaction should only be used with the basis employed to fit its parameters." However, the latter statement, according to our experience, only applies to the binding energy of the nucleus (the variational quantity) and not to the rest of the observables. Actually, we have found no significant changes in the value of physical observables computed with D1M<sup>∗</sup> as the HO basis size is changed. This is the case for typical HO basis: we have carried out calculations including 11, 13, 15, 17, 19, and 20 full HO shells for some representative nuclei using both D1M<sup>∗</sup> and D1M. The range of nuclei considered includes deformed nuclei like  $^{224}Ra$ ,  $^{168}Er$ , or  $^{48}Cr$  and spherical nuclei like  ${}^{16}O$ ,  ${}^{40}Ca$ ,  ${}^{56}Ni$ ,  ${}^{100}Sn$ ,  ${}^{132}Sn$ , or  ${}^{208}Pb$ . Except for the binding energy (which is the variational magnitude and therefore always increases with increasing basis size), the changes in the other observables (radii, quadrupole deformation, octupole deformation, excitation energy of the lowest quasiparticle, etc.) are of the order of a few in a thousand when going from the smallest to the largest basis. Interestingly, as can be seen in Figs. [1–](#page-1-0)[4,](#page-2-0) we notice that the convergence rate with basis size of the density at the origin is rather slow and requires a large number of shells both in D1M<sup>∗</sup> and D1M, and even in the case of the D1S [\[35\]](#page-6-0) parametrization. It is to be pointed out that the central density does not enter significantly in most of the observables like radii or multipole moments because the corresponding operators go to zero at the origin. Also the energy, which should be more sensitive through the strongly repulsive density-dependent part of the interaction to the slow convergence rate of the central density, shows a smooth behavior. On the other hand, in Ref. [\[36\]](#page-6-0) we studied fission properties of the uranium isotopes including very-neutron-rich isotopes using, among others, the parametrization D1N, which is known to show instabilities in coordinate-space calculations  $[11,12]$ . In this case we used a HO basis very different from the one used in the fit of D1N to ground-state properties and never observed any significant deviation in the shape and properties of the potentialenergy surfaces from those obtained with the D1S and D1M parametrizations.

As additional evidence, we show in Fig. 5 the difference in HFB energies  $\Delta E$  when obtained with different number of HO shells  $[\Delta E = E_{\text{HFB}}(N) - E_{\text{HFB}}(N')]$ . The results are obtained and plotted as a function of the quadrupole deformation parameter  $\beta_2$  for the nucleus <sup>154</sup>Sm. To simplify the discussion, the same oscillator lengths are used in the whole deformation interval, and therefore the convergence of the relative energies is slower than in standard calculations. The two sets of curves correspond to D1M (full) and D1M<sup>∗</sup> (dotted) and we observe that they almost coincide in all the cases. All the results presented above constitute strong evidence that there is an ample range of valid HO basis where the results are converged and consistent.

Our approach is rather pragmatic because there is no formal justification of its validity in a regularizationrenormalization framework. It would be very illuminating to study the role of the HO basis from this perspective, but we feel that such a study lies well beyond the scope of the present paper. The UV and infrared properties of the HO basis have



FIG. 5. Energy difference  $\Delta E = E_{\text{HFB}}(N) - E_{\text{HFB}}(N')$  between the HFB energies computed with different number of HO shells and plotted as a function of the quadrupole deformation parameter  $\beta_2$ for the nucleus  $154$  Sm. The number of HO shells *N* and *N'* for each curve is indicated as labels. Full (dotted) lines correspond to the D1M (D1M∗) parametrizations.

been discussed recently in several studies, see, for instance, Refs. [\[37–41\]](#page-6-0).

At this point it is worth mentioning a difficulty of the HO basis connected with the evaluation of matrix elements of a two-body Gaussian interaction for large values of the HO quantum numbers. The standard expressions [\[42–44\]](#page-6-0) for those matrix elements are given in terms of finite alternating-in-sign sums. For large values of the HO quantum numbers, the terms in the sums become very large and their differences exceed the numerical accuracy of typical floating point numbers leading to an unwanted loss of accuracy<sup>2</sup> [\[44\]](#page-6-0). This effect starts to be relevant for 22–24 HO shells and can easily turn a repulsive matrix element into an attractive one. This is not a limiting problem for the HO basis because calculations with the Gogny force are in most of the applications well converged already with 22 shells. $3$ 

Taking the previous considerations into account, it is now possible to understand the results of Fig. [6](#page-5-0) where the energy difference with respect to a 16-shell calculation is shown as a function of the number of shells for the nucleus  $^{48}Ca$ . This figure is similar to Fig. 3 of Ref. [\[11\]](#page-6-0). We show results for two oscillator lengths, one is  $b = 1.65$  fm and corresponds to the minimum of the HFB energy with 16 shells (red curves). The other corresponds to  $b = 1.9$  fm. In this case the reference HFB energy at 16 shells is higher than the one for  $b = 1.65$  fm. This is the reason why, in the plot, the two sets of curves do not converge at the same value of the binding energy with 26 shells. We have tested that, with 26 shells, the binding energies with different oscillator lengths coincide

<sup>2</sup>To understand the problem, let us imagine a calculation carried out with 64-bit floating point arithmetic with 13 digit accuracy. If the alternating sign sum involves terms which are 13 orders of magnitude larger that the result of the sum, then the numerical error is of the order of the sum.

<sup>&</sup>lt;sup>3</sup>It is possible to reach 26 shells depending on the nucleus and the oscillator lengths—a typical example is fission where 26 shells are used in the *z* direction but with a large oscillator length.

<span id="page-5-0"></span>

FIG. 6. For the nucleus <sup>48</sup>Ca, difference in the total energy with respect to the 16 shell calculation as a function of the number of HO shells. Results for D1S (stars), D1M (bullets), and D1M<sup>∗</sup> (open circles) are shown for two different sets of oscillator lengths ( $b =$ 1.9 fm, black curves;  $b = 1.65$  fm, red curves). Note the small range of the vertical scale compared with the total energy of  $48$ Ca. The two sets of curves converge to different  $\Delta E$  values at 26 shells because the reference energy at 16 shells is higher for  $b = 1.9$  fm than for  $b = 1.65$  fm; we have verified that, at 26 shells, the energies from the two *b* values agree to within a few keV for each interaction.

at the level of a few keV for the three considered forces, namely, D1S, D1M, and D1M∗. We see in Fig. 6 that the D1S parametrization shows the fastest convergence of the energy with the number of HO shells, for either *b* value. For  $b = 1.65$  fm we observe a peculiar behavior in the three parametrizations at  $N_{\text{osc}} = 20$  that could be a consequence of the inaccurate evaluation of matrix elements. At  $N_{\text{osc}} = 22$ D1M<sup>\*</sup> shows a dip and at  $N_{\text{osc}} = 24$  the HFB calculation does not converge. We find that this lack of convergence should not be attributed to the finite-size instabilities as suggested in Ref. [\[11\]](#page-6-0), but rather to the inaccurate evaluation of matrix elements for large HO quantum numbers. The  $b = 1.9$  fm calculations seem much more stable and show in the three cases a good convergence rate with *N*osc. In D1M<sup>∗</sup> the convergence rate seems to be slower than for D1S and D1M. From the above results, it is clear that a stable and consistent solution to the problem of evaluating matrix elements of a finite-range Gaussian interaction for large oscillator quantum numbers is required.

In closing this section, we would like to mention also that a study of the convergence of calculations with the number of shells with Skyrme forces was carried out in Ref. [\[17\]](#page-6-0). In a spherical calculation and for contact forces they were able to reach 60 shells. Because the HO basis is complete, in the limit of an infinite number of shells, the HO results should be equivalent to those on a mesh and therefore the appearance of difficulties with 50 or 60 shells can be expected for interactions that present finite-size instabilities in mesh-point calculations. For such a large number of shells the ultraviolet cutoff is increased and the regularization property of the HO basis is weakened. Another difference of Skyrme calculations with the present case is that the expressions for

the matrix elements of contact interactions in a HO basis differ from those obtained for Gaussian interactions and seem to be less likely to suffer from the numerical instabilities discussed above.

#### **IV. SUMMARY AND CONCLUSIONS**

Let us summarize our main findings:

- (i) The QLA calculation for finite-range forces, with its local treatment of the exchange term [\[26\]](#page-6-0), represents an efficient alternative method to signal the existence of instabilities in discretized coordinate-space calculations.
- (ii) Our results independently confirm those of Refs. [\[11,12\]](#page-6-0) pointing to a finite-size instability in discretized coordinate-space calculations in the D1M<sup>∗</sup> and D1N Gogny interactions.
- (iii) We find that, also in the D1M Gogny interaction, there are several examples of nuclei that are unstable when computed in mesh-point calculations. Bcause the critical density  $\rho_c$  of D1M is 1.35 $\rho_0$ , this was *a priori* unexpected from the nuclear matter analysis [\[11,12\]](#page-6-0).
- (iv) When the discretized coordinate-space calculation converges, the numerical results obtained with FINRES4, QLA, and a HO basis are consistent.
- (v) The appearance of the instabilities seems to be connected with the presence and occupancy of *s* orbitals near the Fermi level.
- (vi) The HO basis with its inherent UV cutoff provides consistent results for the D1M<sup>∗</sup> interaction compatible with those obtained with D1S. There is an ample range of HO basis sizes (from 8 up to 24) that can be used in the calculations to accommodate different deformation regimes that produce essentially the same values of nonvariational observables.

We conclude that the criterion proposed in Ref. [\[11\]](#page-6-0) is not always sufficient to signal the existence of instabilities (D1M case) and finite-nuclei calculations in coordinate space may be required whenever the nuclear matter critical density ρ*<sup>c</sup>* of the interaction takes a value close to (and greater than) 1.2 $\rho_0$ . Finite-nuclei effects like the position of *s* orbitals relative to the Fermi level seem to be very relevant. The HO basis acts as a UV cutoff that allows consistent calculations, within the range of basis sizes considered, of finite nuclei with D1M<sup>∗</sup> and all the other interactions showing instabilities on a mesh like D1N or D1M. It would be highly desirable to extend the present analysis to a larger HO basis. It is also to be mentioned that the present analysis does not deal with instabilities in the spin channel. They will be addressed in subsequent work.

Finally, let us note that calculations with D1M<sup>∗</sup> are useful to elucidate the role played by the slope of the symmetry energy in determining nuclear structure properties.

#### **ACKNOWLEDGMENTS**

The authors are very grateful to K. Bennaceur for exchange of useful information. C.G.-B., M.C., and X.V. were partially <span id="page-6-0"></span>supported by Grants No. FIS2017-87534-P from MINECO and FEDER and No. CEX2019-000918-M from the State Agency for Research of the Spanish Ministry of Science and Innovation through the "Unit of Excellence María de Maeztu 2020-2023" award to ICCUB. C.G.-B. also acknowledges Grant No. BES-2015-074210 from MINECO. The work of L.M.R. was partly supported by the Spanish MINECO Grant No. PGC2018-094583-B-I00.

- [1] C. Gonzalez-Boquera, M. Centelles, X. Viñas, and L. M. Robledo, [Phys. Lett. B](https://doi.org/10.1016/j.physletb.2018.02.005) **779**, 195 (2018).
- [2] P. B. Demorest *et al.*, [Nature \(London\)](https://doi.org/10.1038/nature09466) **467**, 1081 (2010).
- [3] J. Antoniadis *et al.*, Science **340**[, 1233232 \(2013\).](https://doi.org/10.1126/science.1233232)
- [4] C. Gonzalez-Boquera, M. Centelles, X. Viñas, and A. Rios, Phys. Rev. C **96**[, 065806 \(2017\).](https://doi.org/10.1103/PhysRevC.96.065806)
- [5] [S. Goriely, S. Hilaire, M. Girod, and S. Péru,](https://doi.org/10.1103/PhysRevLett.102.242501) Phys. Rev. Lett. **102**, 242501 (2009).
- [6] L. M. Robledo, T. R. Rodríguez, and R. R. Rodríguez-Guzmán, J. Phys. G **46**[, 013001 \(2019\).](https://doi.org/10.1088/1361-6471/aadebd)
- [7] [S. Goriely, S. Hilaire, M. Girod, and S. Péru,](https://doi.org/10.1140/epja/i2016-16202-3) Eur. Phys. J. A **52**, 202 (2016).
- [8] L. M. Robledo, HFBaxial computer code (2002) (unpublished).
- [9] [L. M. Robledo and G. F. Bertsch,](https://doi.org/10.1103/PhysRevC.84.014312) Phys. Rev. C **84**, 014312 (2011).
- [10] J. Dechargé and D. Gogny, Phys. Rev. C **21**[, 1568 \(1980\).](https://doi.org/10.1103/PhysRevC.21.1568)
- [11] [M. Martini, A. De Pace, and K. Bennaceur,](https://doi.org/10.1140/epja/i2019-12838-7) Eur. Phys. J. A **55**, 150 (2019).
- [12] M. Martini, A. De Pace, and K. Bennaceur, [arXiv:1806.02080v1](http://arxiv.org/abs/arXiv:1806.02080v1) (2018).
- [13] [F. Chappert, M. Girod, and S. Hilaire,](https://doi.org/10.1016/j.physletb.2008.09.017) Phys. Lett. B **668**, 420 (2008).
- [14] [A. De Pace and M. Martini,](https://doi.org/10.1103/PhysRevC.94.024342) Phys. Rev. C **94**, 024342 (2016).
- [15] D. Davesne, J. Navarro, and A. Pastore, [arXiv:1811.02781.](http://arxiv.org/abs/arXiv:1811.02781)
- [16] [T. Lesinski, K. Bennaceur, T. Duguet, and J. Meyer,](https://doi.org/10.1103/PhysRevC.74.044315) Phys. Rev. C **74**, 044315 (2006).
- [17] V. Hellemans, A. Pastore, T. Duguet, K. Bennaceur, D. [Davesne, J. Meyer, M. Bender, and P.-H. Heenen,](https://doi.org/10.1103/PhysRevC.88.064323) Phys. Rev. C **88**, 064323 (2013).
- [18] K. Bennaceur, FINRES<sub>4</sub> code (unpublished).
- [19] [A. Pastore, D. Davesne, and J. Navarro,](https://doi.org/10.1016/j.physrep.2014.11.002) Phys. Rep. **563**, 1 (2015).
- [20] M. Kortelainen, J. McDonnell, W. Nazarewicz, E. Olsen, P.-G. Reinhard, J. Sarich, N. Schunck, S. M. Wild, D. Davesne, J. Erler, and A. Pastore, Phys. Rev. C **89**[, 054314 \(2014\).](https://doi.org/10.1103/PhysRevC.89.054314)
- [21] N. Schunck, J. Dobaczewski, J. McDonnell, J. Moré, W. [Nazarewicz, J. Sarich, and M. V. Stoitsov,](https://doi.org/10.1103/PhysRevC.81.024316) Phys. Rev. C **81**, 024316 (2010).
- [22] [S. Fracasso, E. B. Suckling, and P. D. Stevenson,](https://doi.org/10.1103/PhysRevC.86.044303) *Phys. Rev. C* **86**, 044303 (2012).
- [23] [V. Hellemans, P.-H. Heenen, and M. Bender,](https://doi.org/10.1103/PhysRevC.85.014326) Phys. Rev. C **85**, 014326 (2012).
- [24] [A. Pastore, D. Tarpanov, D. Davesne, and J. Navarro,](https://doi.org/10.1103/PhysRevC.92.024305) Phys. Rev. C **92**, 024305 (2015).
- [25] C. Gonzalez-Boquera, M. Centelles, X. Viñas, and L. M. Robledo, [arXiv:1807.10159.](http://arxiv.org/abs/arXiv:1807.10159)
- [26] [V. B. Soubbotin, V. I. Tselyaev, and X. Viñas,](https://doi.org/10.1103/PhysRevC.67.014324) Phys. Rev. C **67**, 014324 (2003).
- [27] V. B. Soubbotin and X. Viñas, [Nucl. Phys. A](https://doi.org/10.1016/S0375-9474(99)00558-8) **665**, 291 (2000).
- [28] J. W. Negele and D. Vautherin, Phys. Rev. C **5**[, 1472 \(1972\).](https://doi.org/10.1103/PhysRevC.5.1472)
- [29] X. Campi and A. Bouyssy, [Phys. Lett. B](https://doi.org/10.1016/0370-2693(78)90509-9) **73**, 263 (1978).
- [30] D. Vautherin and D. M. Brink, [Phys. Rev. C](https://doi.org/10.1103/PhysRevC.5.626) **5**, 626 (1972).
- [31] [S. Krewald, V. B. Soubbotin, V. I. Tselyaev, and X. Viñas,](https://doi.org/10.1103/PhysRevC.74.064310) *Phys.* Rev. C **74**, 064310 (2006).
- [32] B. Behera, X. Viñas, T. R. Routray, L. M. Robledo, M. Centelles, and S. P. Pattnaik, J. Phys. G **G43**[, 045115 \(2016\).](https://doi.org/10.1088/0954-3899/43/4/045115)
- [33] K. Bennaceur (private communication).
- [34] [R. Rodriguez-Guzman, Y. M. Humadi, and L. M. Robledo,](https://doi.org/10.1140/epja/s10050-020-00051-w) Eur. Phys. J. A **56**, 43 (2020).
- [35] [J. F. Berger, M. Girod, and D. Gogny,](https://doi.org/10.1016/0010-4655(91)90263-K) Comput. Phys. Commun. **63**, 365 (1991).
- [36] [R. Rodriguez-Guzman and L. M. Robledo,](https://doi.org/10.1103/PhysRevC.89.054310) Phys. Rev. C **89**, 054310 (2014).
- [37] [S. Kvaal, M. Hjorth-Jensen, and H. M. Nilsen,](https://doi.org/10.1103/PhysRevB.76.085421) Phys. Rev. B **76**, 085421 (2007).
- [38] S. A. Coon, M. I. Avetian, M. K. G. Kruse, U. van Kolck, P. Maris, and J. P. Vary, Phys. Rev. C **86**[, 054002 \(2012\).](https://doi.org/10.1103/PhysRevC.86.054002)
- [39] [R. J. Furnstahl, G. Hagen, and T. Papenbrock,](https://doi.org/10.1103/PhysRevC.86.031301) Phys. Rev. C **86**, 031301(R) (2012).
- [40] S. N. More, A. Ekström, R. J. Furnstahl, and G. Hagen, and T. Papenbrock, Phys. Rev. C **87**[, 044326 \(2013\).](https://doi.org/10.1103/PhysRevC.87.044326)
- [41] S. König, S. K. Bogner, R. J. Furnstahl, S. N. More, and T. Papenbrock, Phys. Rev. C **90**[, 064007 \(2014\).](https://doi.org/10.1103/PhysRevC.90.064007)
- [42] M. Girod and B. Grammaticos, Phys. Rev. C **27**[, 2317 \(1983\).](https://doi.org/10.1103/PhysRevC.27.2317)
- [43] W. Younes, [Comput. Phys. Commun.](https://doi.org/10.1016/j.cpc.2008.12.021) **180**, 1013 (2009).
- [44] [J. L. Egido, L. M. Robledo, and R. R. Chasman,](https://doi.org/10.1016/S0370-2693(96)01602-4) Phys. Lett. B **393**, 13 (1997).