Comment on the paper Eur. Phys. J. A (2019) 55:150

C. Gonzalez-Boquera¹, M. Centelles¹, X. Viñas¹ and L.M. Robledo²,³

¹ 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
² Departamento de Física Teórica and CIAFF, Universidad Autónoma de Madrid, E-28049 Madrid, Spain
³ Center for Computational Simulation, Universidad Politécnica de Madrid, Campus de Montegancedo, Boadilla del Monte, E-28660 Madrid, Spain

Received: date / Revised version: date

Abstract. The conclusions of the study published as Eur. Phys. J. A (2019) 55:150 questioning the adequacy of the recently proposed Gogny D1M* interaction for finite-nuclei calculations using harmonic oscillator (HO) basis are revised. The existence of an instability in finite nuclei for D1M* when coordinate-space methods are used to solve the HF equations (as shown in Eur. Phys. J. A (2019) 55:150) is independently confirmed using a computer code based on a quasilocal approximation (QLA) to the HF energy density with finite-range forces. We confirm that the most affected quantity in the coordinate-space calculation is the spatial density at the origin. Our study reveals that some findings concerning these instabilities are not easy to reconcile with the arguments used in Eur. Phys. J. A (2019) 55:150. For instance, some nuclei such as ⁴He and ⁴⁰Ca, which diverge in HF mesh-point calculations performed with D1M*, become perfectly stable when Coulomb force is switched off. We have also found instabilities in some nuclei when the D1M interaction is used. Finally, a connection between the occupancy of s-orbitals near the Fermi level and the appearance of instabilities is observed. Several convergence and stability studies are performed with HO basis of different sizes and oscillator parameters to demonstrate the robustness of the D1M* results for finite nuclei when the HO basis is used.

PACS.

In Ref. [1] 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⊙, in agreement with recent astrophysical observations [2,3]. We were motivated by the fact that this property is not achieved by any of the standard Gogny forces of the D1 family [4]. We also wanted to preserve the good description of the properties of spherical and deformed nuclei provided by the D1M force in Hartree-Fock-Bogoliubov (HFB) level [5]. In the fit of D1M* [1], 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 and the prediction for the maximum neutron star mass. Finally, the strength t₃ of the density-dependent term of the Gogny interaction was fine tuned to improve the quality of the computed binding energies. All of the finite-nuclei calculations in [1] were carried out with the HFBaxial code [6] using an approximate second-order gradient method to solve the HFB equations in a HO basis including up to 19 major oscillator shells and the oscillator lengths adapted to the characteristic A¹/⁶ length-scale dependence with mass number A. It is to be noted that all the HFB calculations of spherical and deformed nuclei with Gogny interactions have always been performed in a HO basis since the seminal paper of Dechargé and Gogny [7], including the calculations leading to the determination of the values of the parameters of the interaction. In particular, this is the case of the D1M interaction [5], to which we compare our results.

In a recent paper Eur. Phys. J. A (2019) 55:150 [8] and its preliminary version arXiv:1806.02080v1 [9], it is found that both the D1M* and D1N 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 RPA calculation of the nuclear matter response functions based on the continued fraction technique [10]. This procedure has already been applied in [10] 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 [11], it was concluded that the key quantity to
Bouyssy [18]. In the QLA the energy density functional for matter is approximated by a quasilocal functional obtained using the extended Thomas-Fermi (ETF) density matrix formalism [16]. As a consequence of finite-size instabilities, the neutron and proton densities, if \( \rho \) is reached in HF calculations of some nuclei, as for example \( ^{40} \text{Ca} \). The instabilities of D1M* and D1N were predicted in nuclear matter [9,8] and their appearance in coordinate-space calculations of spherical finite nuclei was confirmed in [9,8] using the FINRES4 code [12]. As a consequence of 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 non-linear HFB equations, without reaching convergence.

In our paper arXiv:1807.10159v1 [13] we commented on the results of Refs. [9,8] and provided additional (and in our opinion very relevant) information about the possible impact of the finite-size instability of the D1M* force on calculations of observables like binding energies, neutron and proton radii and density profiles of finite nuclei using a HO basis. As discussed in detail in [13], we have found several important facts that, in our opinion, cannot be easily explained with the arguments used in Refs. [9,8]. However, our paper [13]—available well before the submission date of Ref. [8] to European Physical Journal A—is never mentioned in Ref. [8] although it was early reported to the authors of [8].

In order to independently confirm the results of [9,8] we have performed HF calculations with Gogny forces on a spatial mesh. To this end we use the QLA described in Ref. [13]. In this approach the HF exchange energy density is approximated by a quasilocal functional obtained using the extended Thomas-Fermi (ETF) density matrix formalism [16], which is similar to the expansion for this quantity proposed by Negele and Vautherin [17] or by Campi and Bouyssy [18]. In the QLA the energy density functional for finite-range effective interactions becomes local and therefore the HF equations in coordinate-space take a similar form to those of Skyrme forces [19]. In Refs. [15,20,21] it has been shown that calculations in coordinate space using the QLA provide results that are very close to the full HF values obtained with the HO basis. It is also important to point out that the HF calculations performed using the QLA accurately agree with the results computed with the

detect spurious finite-size instabilities is the critical density \( \rho_c \). These instabilities develop unphysical results in some properties of the nuclei, as for example in the proton and neutron densities, if \( \rho_c \approx 1.2 \rho_0 \approx 0.20 \text{ fm}^{-3} \) for a momentum transfer of about 2.5 \text{ fm}^{-1}. This critical density may be reached in HF calculations of some nuclei, as for example \( ^{40} \text{Ca} \). The instabilities of D1M* and D1N were predicted in nuclear matter [9,8] and their appearance in coordinate-space calculations of spherical finite nuclei was confirmed in [9,8] using the FINRES4 code [12]. As a consequence of 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 non-linear HFB equations, without reaching convergence.

In our paper arXiv:1807.10159v1 [13] we commented on the results of Refs. [9,8] and provided additional (and in our opinion very relevant) information about the possible impact of the finite-size instability of the D1M* force on calculations of observables like binding energies, neutron and proton radii and density profiles of finite nuclei using a HO basis. As discussed in detail in [13], we have found several important facts that, in our opinion, cannot be easily explained with the arguments used in Refs. [9,8]. However, our paper arXiv:1807.10159v1 [13]—available well before the submission date of Ref. [8] to European Physical Journal A—is never mentioned in Ref. [8] although it was early reported to the authors of [9,8].

In order to independently confirm the results of [9,8] we have performed HF calculations with Gogny forces on a spatial mesh. To this end we use the QLA described in Ref. [13]. In this approach the HF exchange energy density is approximated by a quasilocal functional obtained using the extended Thomas-Fermi (ETF) density matrix formalism [16], which is similar to the expansion for this quantity proposed by Negele and Vautherin [17] or by Campi and Bouyssy [18]. In the QLA the energy density functional for finite-range effective interactions becomes local and therefore the HF equations in coordinate-space take a similar form to those of Skyrme forces [19]. In Refs. [15,20,21] it has been shown that calculations in coordinate space using the QLA provide results that are very close to the full HF values obtained with the HO basis. It is also important to point out that the HF calculations performed using the QLA accurately agree with the results computed with the

det
be noted that there exist nuclei with $D1M^*$, such as $^{16}O$, that seems to corroborate that the origin of the instabilities in spherical nuclei in coordinate-space calculations, as it reproduces all the instabilities of finite nuclei reported in [9,8]. As an example, Figs. 3 and 4 show the proton and neutron densities of $^{208}Pb$ calculated with the $D1M^*$ interaction and obtained after a given number of iterations using the QLA. Clearly, in this case the mesh-point density profiles display a divergent behaviour with increasing number of iterations.

Let us now turn our attention to several conclusions that can be extracted from the mesh calculation that are barely or not discussed at all in [9,8]. First, for spherical even-even symmetric nuclei from $N = Z = 2$ to $N = Z = 126$, the HF calculations on a mesh without Coulomb interaction performed with $D1M^*$ are perfectly stable and the corresponding densities are fully converged after a large number of iterations ($\sim 10000$ with a mixing factor 0.9 [13]). This seems to be in contradiction with, or unexplained by, the claim of [9,8] relating the instabilities to a critical density $\rho_c$ in nuclear matter. For instance, in the case of $^4$He and $^{40}$Ca including Coulomb effects, the HF results are unstable but turning the Coulomb force off makes the results completely stable in spite of the fact that the central proton and neutron densities are almost identical in the charged and uncharged cases. This fact seems to corroborate that the origin of the instabilities is more related to the isovector sector of the interaction than to the isoscalar sector. On the other hand, it is to be noted that there exist nuclei with $D1M^*$, such as $^{16}O$, $^{100}Sn$ or the very asymmetric $^{176}Sn$, that fully converge in the coordinate-space calculation, even with the Coulomb interaction switched on. This has been verified with both our QLA code and the FINRES$_4$ code [13]. It 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, as we shall discuss below, that also play a role.

We have also detected that when the $D1M$ interaction is applied in coordinate-space calculations some nuclei such as $^{52}$Ca, $^{54}$Ca, $^{56}$Ca, $^{54,56}$Ti, $^{56}$Fe, $^{60}$Fe, $^{62}$Fe, $^{60,62}$Ni and $^{62}$Ni are unstable at the HF level. As the critical density $\rho_c$ for $D1M$ is about 1.35$\rho_0$ [9,8], our finding seems to be in contradiction with the criterion proposed in Refs. [9,8] because $D1M$ should be stable according to it.

In the upper part of Table 1 we report the binding energies of the nuclei $^{16}$O, $^{132}$Sn and $^{208}$Pb calculated with the $D1M$ interaction using a HO basis [9], the FINRES$_4$ code [12] and the QLA used in this work. We can see that the HF binding energies computed with FINRES$_4$ are slightly larger than the ones 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$_4$ code, being the differences less than 1% for all considered nuclei. A similar situation is found for the nuclei $^{16}$O, $^{100}Sn$ and $^{176}Sn$ computed with the $D1M^*$ force, where the corresponding binding energies are given in the lower part of Table 1. These nuclei are found to be stable in coordinate space by independent calculations performed with the QLA and the FINRES$_4$ codes [13]. The agreement between the HO basis and mesh results is again excellent in $D1M^*$ when the mesh calculations converge, which further supports the reliability of using the HO basis approach with $D1M^*$. Regarding unstable nuclei in coordinate space, we have found, as discussed in [13], empirical evidence that the appearance of instabilities in finite nuclei is 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 (neutrons and protons) and $^{208}Pb$ (protons) computed with $D1M^*$. 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 $D1M^*$ force. A paradigmatic example is the case of the nuclei $^{22}$O and $^{24}$O. At HF level, the Fermi level of $^{22}$O is placed at the $1d_{5/2}$ orbital and this nucleus is stable, whereas the nucleus $^{24}$O has its Fermi level in the $2s_{1/2}$ orbital and it is unstable. Finally, let us point out that, in spite of the non-convergent behavior of the nucleon density profiles when the mesh-point calculation is unstable, there is an optimal number of iterations for which integrated quantities such as the total binding energies present a smooth plateau pattern, with values close to those obtained in the HO basis, that will diverge ultimately when the number of iterations grows [13].

As established in Refs. [11,9,8], RPA calculations of the nuclear matter response function allow one to detect in a rather efficient way instabilities that prevent obtaining fully converged self-consistent results in finite nuclei in the coordinate-space calculation (FINRES$_4$) [14]. The percentage deviation of the HO-basis energy from the coordinate-space energy is shown in brackets.

| $^A$X   | $B_{HO}$ (MeV) | $B_{QLA}$ (MeV) | $B_{FINRES}$ (MeV) |
|---------|---------------|-----------------|--------------------|
| $^{16}$O | 128.02        | 127.02 (0.79%)   | 128.07 (0.04%)     |
| $^{132}$Sn | 1102.57      | 1103.31 (0.07%)  | 1104.29 (0.16%)    |
| $^{208}$Pb | 1636.08      | 1637.96 (0.11%)  | 1639.31 (0.20%)    |
| $^{16}$O   | 128.32        | 127.29 (0.82%)   | 128.58 (0.21%)     |
| $^{100}$Sn | 827.98        | 824.71 (0.40%)   | 829.08 (0.13%)     |
| $^{176}$Sn | 1146.15       | 1146.26 (0.01%)  | 1147.54 (0.12%)    |

Table 1. For the $D1M$ and $D1M^*$ Gogny interactions, Hartree-Fock binding energies obtained from the HO-basis calculation, the coordinate-space quasilocal calculation (QLA) and the full coordinate-space calculation (FINRES$_4$) [14]. The percentage deviation of the HO-basis energy from the coordinate-space energy is shown in brackets.
coordinate space using some effective interactions, such as D1M* and D1N. However, our findings point out that the problem may be more involved and that additional investigations about the open questions suggested in this Comment are required.

In the paper where D1M* was proposed [1], we did finite-nuclei HFB calculations to fine-tune the density-dependent strength as to improve the agreement of binding energies with experimental data. For those calculations we used a HO basis with a maximum number of shells depending on the region of the nuclear chart. The calculation covered both deformed and spherical nuclei and we computed the properties of more than 600 even-even nuclei. In this calculations we did not observe any convergence issue. The stability of the HO basis calculations could be related to the ultraviolet cutoff in momentum space inherent to the HO basis. The ultraviolet cutoff serves as a regulator for problems related to high-momentum components in the wave function in a way that closely resembles other regulators in pairing calculations with zero range forces—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 prone to suffer the effect of those ultraviolet problems. This difference between HO basis and mesh calculations was already recognized in [25], where it was argued that the use of a HO basis “strongly renormalizes the interaction and inhibits the development of instabilities”. However, the authors of [25] conclude that “the D1M* interaction should only be used with the basis employed to fit its parameters”, a statement that, according to our experience, only applies to the binding energy of the nucleus and not to the rest of the observables. From the statement of [25] one should expect significant changes in the value of physical observables computed with D1M* as the HO basis size is changed. However, this is not 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* 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, 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 and D1M*, and even in the D1S case, as can be seen in Figs. [4,5]. It is to be pointed out that the central density does not enter significantly in most of the observables like radii or multipole moments as 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. [22] 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 [3]. In those calculations we used a HO basis very different from the one used in the D1N fit to ground-state properties and never observed any significant deviation in the shape and properties of the potential energy surfaces from the ones 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 $^{154}$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* (dotted) and we observe 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.

At this point it is worth to mention a difficulty of the HO basis connected with the evaluation of matrix elements of a two-body Gaussian interaction. The standard expressions [26,27] for those matrix elements are given in terms of quantities obtained as sums of very large terms which alternate in sign and therefore are prone to unwanted loss of accuracy. To understand the problem, let us imagine a calculation carried out with 64-bit floating point arithmetic with 13 digits 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. Sometimes, this numerical error turns a repulsive matrix element into an attractive one. This problem was first discussed in [27] and a partial solution was proposed there involving hypergeometric functions. Even using the proposal of [27], calculations with the Gogny force are usually restricted to at most 20-22 shells (although 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).

Taking the previous considerations into account, it is now possible to understand the results of Fig. 6 where the energy difference with respect to the reference 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 [8]. We show results for two oscillator lengths, one is $b = 1.65 \text{ fm}$ and corresponds to the minimum of the HFB energy with 16 shells (red curves). The other corresponds to $b = 1.9 \text{ fm}$. In this case the reference HFB energy at 16 shells is higher than the one for $b = 1.65 \text{ fm}$. This is the reason why, in the plot, the two set 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 at the level of a few keV. For $b = 1.65 \text{ fm}$ we observe a peculiar behaviour in the three parametrizations D1S, D1M and D1M* at $N_{\text{osc}} = 20$ that could be a consequence of the numerical error in the evaluation of matrix elements. At $N_{\text{osc}} = 22$ D1M* shows a dip and at $N_{\text{osc}} = 24$ the HFB calculation does not converge leading to wild numbers. This points to the above mentioned difficulty with the evaluation of the matrix elements that could eventually turn attractive matrix elements into repulsive ones and vice-versa. The $b = 1.9 \text{ fm}$ calculations seem much more stable and show in the three cases a good convergence rate with $N_{\text{osc}}$. In D1M* 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.

To finish, let us mention that a study of the convergence of calculations with the number of shells with Skyrme forces was carried out in [11]. In an spherical calculation and for contact forces they were able to reach 60 shells. As the HO basis is complete, in the limit of infinite number of shells the HO results should be equivalent to the ones on a mesh and therefore the appearance of difficulties with 50 or 60 shells is not surprising. For such a large number of shells the ultraviolet cutoff is increased and the regularization property of the HO basis is weakened. Comparing with the pairing case, if we increase the active window size the results will be unphysical. There is another difference with the present case: the expressions for the matrix elements of contact interactions in a HO basis differ from the ones obtained for Gaussian interactions and seem to be less likely to suffer from the numerical instabilities discussed above.

Acknowledgments

The authors are very grateful to K. Bennaceur for exchange of useful information. C.G., M.C., and X.V. were partially supported by Grant FIS2017-87534-P from MINECO and FEDER and Project MDM-2014-0369 of ICCUB (Unidad de Excelencia María de Maeztu) from MINECO. C.G. also acknowledges Grant BES-2015-074210 from MINECO. The work of LMR was partly supported by the Spanish MINECO Grant No. FPA2015-65929, No. FIS2015-63770 and No. PGC2018-094583-B-I00.

References

1. C. Gonzalez-Boquera, M. Centelles, X. Viñas and L.M. Robledo, Phys. Lett. B777 (2018) 195.
2. P.B. Demorest et al., Nature 467 (2010) 1081.
3. J. Antoniadis et al., Science 340 (2013) 448.
4. C. Gonzalez-Boquera, M. Centelles, X. Viñas and A. Rios, Phys. Rev. C96 (2017) 065806.
5. S. Goriely, S. Hilaire, M. Girod, and S. Péró, Phys. Rev. Lett. 102 (2009) 242501.
6. L.M. Robledo, HFBaxial computer code (2002).
7. J. Dechargé and D. Gogny, Phys. Rev. C21 (1980) 1568.
8. M. Martini, A. De Pace and K. Bennaceur, Eur. Phys. J. A55(2019) 150.
9. M. Martini, A. De Pace and K. Bennaceur, arXiv:1806.02080v1 (2018).
10. A. De Pace and M. Martini, Phys. Rev. C94 (2016) 024342.
11. V. Hellemans, A. Pastore, T. Duguet, K. Bennaceur, D. Davesne, J. Meyer, M. Bender and P.-H. Heenen, Phys. Rev. C88 (2013) 064323.
12. K. Bennaceur, FINRES4, (2018) unpublished.
13. C. Gonzalez-Boquera, M. Centelles, X. Viñas and L.M. Robledo, arXiv:1807.10159v1 (2018).
14. K. Bennaceur, private communication (2018).
15. V.B. Soubbotin, V.I. Tselyaev and X. Viñas, Phys. Rev. C67 (2003) 014324.
16. V.B. Soubbotin and X. Viñas, Nucl. Phys. A665 (2000) 291.
17. J.W. Negele and D. Vautherin, Phys. Rev. C5 (1972) 1472.
18. X. Campi and A. Bouyssy, Phys. Lett. B73 (1978) 273.
19. D. Vautherin and D.M. Brink, Phys. Rev. C5 (1972) 626.
20. S. Krewald, V.B. Soubbotin, V.I. Tselyaev and X. Viñas, Phys. Rev. C74 (2006) 064310.
21. B. Behera, X. Viñas, T.R. Routray, L.M. Robledo, M. Centelles and S.P. Pattnaik, J. Phys. G43 (2016) 045115.
22. R. Rodriguez-Guzman and L.M. Robledo, Phys. Rev. C89 (2014) 054310.
23. O. Bohigas, A.M. Lane and J. Martorell, Phys. Rep. 51 (1979) 267.
24. E. Merzbacher, Quantum Mechanics, Wiley & Sons 1961, p.168.
25. M. Girod and B. Grammaticos, Phys. Rev. C27 2317 (1983).
26. W. Younes, Computer Physics Communications, 180, 1013 (2009).
27. J. L. Egido, L. M. Robledo, and R. R. Chasman, Physics Letters B393, 13 (1997).