Second random-phase approximation with the Gogny force. First applications.

D. Gambacurta,[1] M. Grasso,[2] V. De Donno,[3] G. Co',[3] and F. Catara[4]

[1] *Grand Accélérateur National d'Ions Lourds (GANIL), CEA/DSM-CNRS/IN2P3, Bvd Henri Becquerel, F-14076, Caen, France*

[2] *Institut de Physique Nucléaire, Université Paris-Sud, IN2P3-CNRS, F-91406 Orsay Cedex, France*

[3] *Dipartimento di Matematica e Fisica "E. De Giorgi", Università del Salento and INFN, Sezione di Lecce, I-73100 Lecce, Italy*

[4] *Dipartimento di Fisica e Astronomia and INFN, Via Santa Sofia 64, I-95123 Catania, Italy*

We present the first applications of the second random-phase-approximation model with the finite-range Gogny interaction. We discuss the advantages of using such an interaction in this type of calculations where 2 particle-2 hole configurations are included. The results found in the present work confirm the well known general features of the second random-phase approximation spectra: we find a large shift, several MeV, of the response centroids to lower energies with respect to the corresponding random-phase-approximation values. As known, these results indicate that the effects of the 1 particle-1 hole/2 particle-2 hole and 2 particle-2 hole/2 particle-2 hole couplings are important. It has been found that the changes of the strength distributions with respect to the standard random-phase-approximation results are particularly large in the present case. This important effect is due to some large neutron-proton matrix elements of the interaction and indicates that these matrix elements (which do not contribute in the mean-field calculations employed in the conventional fit procedures of the force parameters) should be carefully constrained to perform calculations beyond mean-field approach.

PACS numbers: 21.10.Re,21.60.Jz

The new and complex phenomenology associated to exotic neutron-rich and neutron-deficient isotopes is enriching the experimental landscape in nuclear physics. In the perspective of improving the theoretical description of exotic nuclei, efforts are concentrated on the refinement of the existing many-body theories, as well as on the microscopic derivation of the nuclear interaction. Both aspects are fundamental and complementary to improve our description of the nucleus as a many-body interacting system. In the context of the Energy Density Functional theories, complex configurations and correlations are included nowadays within several theoretical frameworks beyond the conventional mean-field models based on both the Skyrme and the Gogny effective interactions as well as on relativistic formulations (e.g. in Refs. [1–6]).

Within the scheme of the standard random-phase approximation (RPA) the excited states are described as superpositions of 1 particle-1 hole ($1ph$) and 1 hole-1 particle ($1hp$) configurations. Evidently, those excited states containing non negligible multiparticle-multihole components are not well described by this theory. Furthermore, the width of the excited states cannot be reproduced except for the single-particle Landau damping. A well known extension of the RPA scheme is the second RPA (SRPA) model which is obtained with the inclusion of the 2 particle-2 hole ($2ph$) configurations. This leads to a richer treatment of the excitation modes. The spreading width can also be described owing to the coupling with the $2ph$ configurations.

After having presented in previous works some applications of the SRPA theory with the Skyrme zero-range interaction [7–9] we present here the first applications of the SRPA theory with the Gogny force. Although the use of a finite-range interaction turns out to be numerically more demanding with respect to the zero-range case, it presents some advantages. The first one is related to the fact that the Gogny force has been introduced and adjusted to be used in both the Hartree-Fock and the pairing channels. Since in the SRPA theory not only the standard RPA-type particle-hole (ph) matrix elements of the interaction are present, it seems to us that the use of a force tailored to handle also other kinds of terms, such as the particle-particle matrix elements, is more appropriate. A second, non negligible, advantage is the finite range of the four central terms of the Gogny force. We expect that this feature provides, in a natural way, convergent results with respect to the increase of the energy cutoff in the $2ph$ space of the SRPA calculations. We do not expect a full convergence because the Gogny interaction contains also density-dependent and spin-orbit terms which are of zero-range type. We remark that our SRPA calculations are not fully self-consistent because we neglect the Coulomb and the spin-orbit terms in the residual interaction. This means that the dependence of the results on the numerical cutoff is related in this work only to the zero-range density-dependent part of the interaction. The cutoff-dependence of the Skyrme-SRPA results has been addressed and discussed in Ref. [7].

The details of the SRPA formalism may be found in the literature. The derivations of the SRPA secular equations carried out by using the method of the equations of motion [10] or by considering the small-amplitude limit of the time-dependent density-matrix theory [11, 12] provide expressions of the matrices A and B which are valid in cases where the interaction does not depend on the density. The case of a density-dependent force in extended RPA theories has been discussed in some early works [13, 14]. The specific case of the SRPA model has been considered in Ref. [8], where a prescription to treat the rearrangement terms of the residual interaction in matrix elements beyond RPA has been derived. This prescription has been applied also in the present work. In Ref. [10] it is demonstrated that the energy-weighted sum rules (EWSR's) are satisfied in the SRPA model.

To present the first applications where the Gogny interaction is employed in SRPA calculations we have chosen the nucleus ^{16}O. This allows us to better control the heavy numerical problem associated with the diagonalization of the SRPA matrix. Furthermore, the study of this nucleus allows us a direct comparison of our SRPA results with previous Skyrme-SRPA results [7]. In our calculations we used the D1S parametrization of the Gogny interaction [15, 16].

As an illustration, in the present article we show only results regarding the monopole isoscalar response. The calculations are performed in spherical symmetry in the harmonic oscillator basis. As anticipated, the Coulomb and the spin-orbit contributions are not taken into account in the residual interaction. The single-particle and the $1ph$ spaces have been chosen large enough to ensure that the values of the EWSR's are stable. All the single-particle states with an unperturbed energy lower than 60 MeV (that is, all the $1ph$ configurations with an unperturbed excitation energy up to 100 MeV) are included in the calculations. In the $2ph$ space, we have considered all the configurations with an unperturbed energy lower than an energy cutoff E_{cut} and we have studied the numerical stability of the results with respect to the choice of the cutoff.

In these first applications of the Gogny-SRPA model we have found that some neutron-proton ($\nu\pi$) matrix elements of the interaction, appearing in the beyond-RPA block matrices, are very large, some of them being from 5 to 10 times larger than all the other matrix elements. These matrix elements, that are absent in the standard RPA calculations, have a strong impact on the stability of the results, in particular on the peak structure of the response. As we shall show below, their effects are especially strong in the matrix elements coupling $1ph$ and $2ph$ configurations (that is, 3 particle-1 hole or 3 hole-1 particle matrix elements). To analyze and single out these effects we have performed two different kinds of calculations: (a) a full SRPA calculation where all the $2ph$ configurations are included; (b) a calculation performed by considering only the $2ph$ configurations that are composed by pure neutron and proton excitations. This means that in the case (b) we do not include the $2ph$ configurations where the two particles and the corresponding two holes have a different isospin nature, that is $\nu\pi$ or $\pi\nu$ configurations. As a consequence, no $\nu\pi$ matrix elements of the interaction are present in the SRPA matrices in the case (b). In the following we will indicate the two calculations (a) and (b) as SRPA and SRPA*, respectively. The strong impact of the $\nu\pi$ matrix elements of the interaction can be seen in Fig. 1 where the isoscalar monopole response for the operator

$$F^{IS} = \sum r_i^2 Y_{00}(\hat{r}_i), \tag{1}$$

calculated in the SRPA (a) and in the SRPA* (b) scheme is displayed for two values of the cutoff energy, E_{cut} = 60 and 80 MeV. The corresponding Gogny-RPA results are also plotted in the two panels of the figure. folded

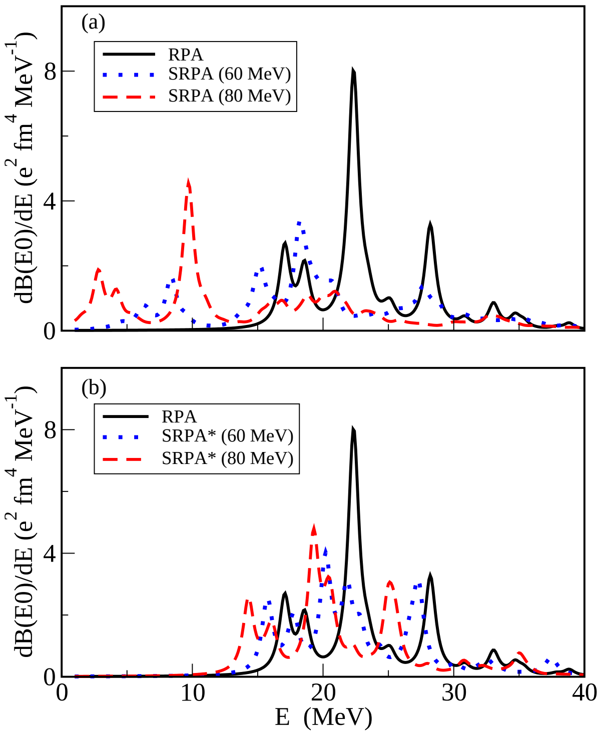

FIG. 1. (Color online) (a) Isoscalar monopole response for the nucleus ^{16}O calculated with the Gogny-RPA model (full line) and with the SRPA approach with an energy cutoff on the $2ph$ configurations of 60 (dotted line) and 80 (dashed line) MeV. (b) Same as in (a) but in the SRPA* scheme. See the text for more details.

the discrete spectra with a Lorentzian function with a width of 1 MeV. We see that in the SRPA scheme the responses associated with the different cutoff values are appreciably different and, for E_{cut} = 80 MeV, the main peak of the response is pushed at energies more than 10 MeV lower than in the RPA case (a). The SRPA* results of panel (b) are much more stable with respect to the change of the cutoff energy. This can also be seen by considering the centroid energies of the strength distributions. When the energy cutoff is increased from 60 to 80 MeV the centroid goes from 20.37 to 15.30 MeV (deviation of 25%) in the full SRPA calculations whereas it is much less shifted, from 23.97 to 22.37 MeV (7%), in the SRPA* case. *It is also worth noticing that in the latter case the difference between the spectra corresponding to the two Ecut is essentially just a shift, while when the (nu pi) matrix elements are not neglected, the SRPA strength distribution is very much different from the RPA one.* To check more in detail the stability of the results in the SRPA* case, we have performed also calculations with cutoff values of 100 and 120 MeV (Fig. 2). When the cutoff is changed from 80 to 100 MeV the centroid is shifted from 22.37 to 21.32 MeV (5%) and when the cutoff is changed from 100 to 120 MeV the centroid moves from 21.32 to 20.49 MeV (4%). We conclude that the stability that is expected when the Gogny interaction is employed seems to be achieved in the SRPA* case where, by construction, all the large $\nu\pi$ matrix elements of the residual interaction in the beyond RPA blocks of the matrices are neglected. The strong impact of these matrix elements can also be seen in Fig. 3 where we plot the discrete spectra in a logarithmic scale to emphasize the fragmentation of the response. The SRPA and SRPA* spectra (full lines) correspond to a cutoff of 80 MeV. In the two panels of this figure, as a comparison, also the corresponding RPA results are plotted (dashed lines). We observe that not only the energies but also the fragmentation of the peaks is strongly affected in the SRPA response that is shown in (a). The monopole case is presented here as an illustration, however, we have verified that also in the dipole and quadrupole cases the spectra (energies and fragmentation) are strongly modified in the full SRPA scheme where all the $\nu\pi$ matrix elements of the residual interaction are included.

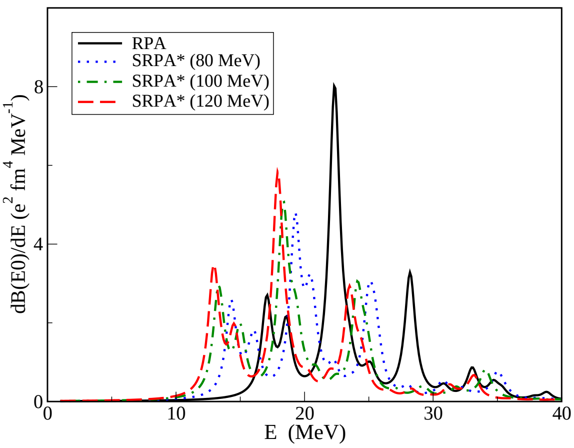

FIG. 2. (Color online) Isoscalar monopole response for the nucleus ^{16}O calculated in the SRPA* case with cutoff energies of 80 (dotted line), 100 (dot-dashed line) and 120 (dashed line) MeV. The Gogny-RPA results are also plotted (full line).

The effect we have just pointed out, related to the presence of some very large $\nu\pi$ matrix elements, is not so surprising. These matrix elements do not contribute at the mean-field level where the fit procedures are commonly performed to select the values of the parameters of the effective interactions such as the Skyrme and Gogny forces. For this reason, we cannot exclude that their inclusion in actual calculations may have an unexpected and strong impact. It is also interesting to remark that analogous important effects related to large $\nu\pi$ matrix elements have been found in the Gogny case also in recent applications of the variational multiparticle-multihole configuration interaction theory to the low-lying spectroscopy of the nucleus ^{30}Si [17]. These findings are coherent with our results and suggest that these matrix elements of the interaction should be carefully tuned in the fit procedures.

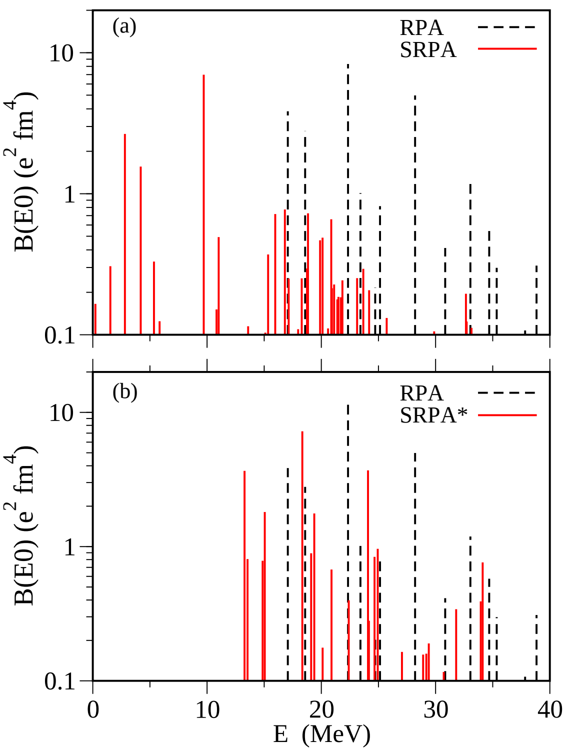

FIG. 3. (Color online) Isoscalar monopole discrete strength distributions for the nucleus ^{16}O calculated within the SRPA model (full line) with a cutoff energy of 80 MeV (a). (b) Same as in (a) but in the SRPA* scheme. *In both panels* , the Gogny-RPA results are also plotted (dashed lines) as a reference.

By comparing the present results with the corresponding Skyrme results of Ref. [7] we observe that also in that case a similar behaviour is found, although less pronounced. This effect of the SRPA theory is found not only in nuclear physics when phenomenological interactions like the Skyrme and Gogny forces are used. This effect is present also in nuclear calculations which employ forces derived from realistic interactions [18, 19], as well as in a completely different domain, that is, in calculations carried out for metallic clusters (where the interparticle interaction is the Coulomb force) [20]. It is important to underline that the shift found in the Gogny case is comparable to the corresponding Skyrme result only when all the large $\nu\pi$ matrix elements are omitted in the Gogny case (SRPA* scheme). Otherwise, their effect is too strong in pushing the centroid energies to lower values.

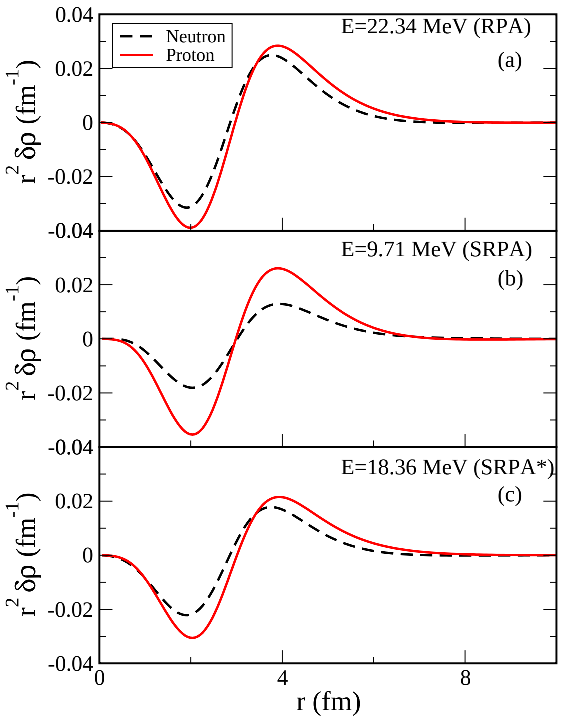

FIG. 4. (Color online) Neutron (dashed lines) and proton (full lines) transition densities for the main peaks of the RPA (a), SRPA (b) and SRPA* (c) strength distributions.

We have studied the effects of these matrix elements on the transition densities which are shown in Fig. 4 for the energies of the main peaks of RPA, SRPA and SRPA* strength distributions. In this figure, the neutron and proton transition densities are indicated by the dashed and full lines, respectively. In the upper panel (a) the neutron and proton RPA transition densities are plotted for the state located at $\sim$ 22.34 MeV. In the middle (b) and lower (c) panels we show the transition densities for the states located at 9.71 and 18.36 MeV, corresponding to the states obtained in the SRPA (b) and SRPA* (c) cases. We observe that the shapes of the profiles are rather similar. This indicates that the nature of these

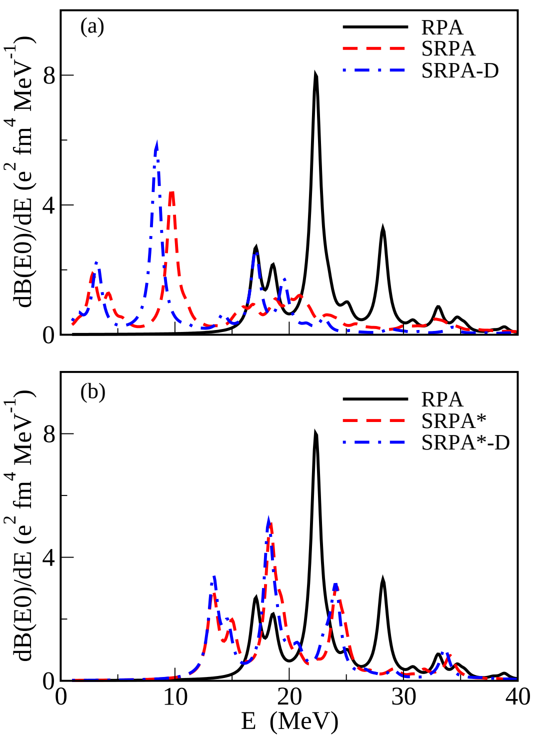

FIG. 5. (Color online) Isoscalar monopole distributions for the nucleus ^{16}O calculated within the SRPA (a) and SRPA* (b) model (dashed lines) with a cutoff of 80 MeV. The comparison with the corresponding spectra obtained in the diagonal approximation (dot-dashed lines) is shown. The Gogny-RPA results are also plotted (full lines).

RPA and SRPA excited states does not change very much in terms of the spatial distributions of the contributing wave functions. We conclude that, at least in this case, the $\nu\pi$ matrix elements affect the energy and the strength distributions while the shapes of the radial distributions of the contributing nucleons are not appreciably modified.

Finally, in the framework of the Gogny-SRPA model we have checked the validity of the so-called diagonal approximation, which amounts to neglect the coupling of the 2ph configurations among themselves. The results obtained by adopting this approximation will be identified as SRPA-D. The validity of this approximation has been tested in Ref. [7] by using the Skyrme interaction. In this case, large differences with respect to the complete calculations have been found. In Fig. 5 we compare the results obtained in the full SRPA (a) and SRPA* (b) models with the corresponding results obtained in the diagonal approximation. All the calculations have been carried out by using an energy cutoff of 80 MeV. We observe that in both cases the shifts and the shapes of the strength distributions do not strongly change when the residual interaction in the $2ph$ space is neglected, the differences being larger in the SRPA case than in the SRPA* one. The relatively small differences that have been found between the SRPA* and the SRPA*-D cases indicate that the effect of the $\nu\pi$ matrix elements is mainly related to the coupling of the $1ph$ configurations with the $2ph$ ones. In the SRPA* case, panel (b), we see that the results obtained within the diagonal approximation are extremely close to the full ones and the same behavior is found also for larger energy cutoff. By comparing these results with those obtained by using the Skyrme interaction [panel (a) of Fig. 8 of Ref. [7]] we deduce that in the Gogny case the diagonal approximation provides results which are much closer to the full results, at least in the monopole case.

In summary, we have found that in the Gogny-SRPA calculations the responses are very strongly affected by some $\nu\pi$ matrix elements of the residual interaction, particularly in the channels which couple the $1ph$ with the $2ph$ configurations. These matrix elements do not contribute in Hartree-Fock and standard RPA calculations. Therefore, they do not contribute in the calculations where the parameters of the effective forces are fixed by the usual fitting procedures. To check and constrain their effects, it is thus necessary to go beyond the conventional procedures. We suggest some different possible directions that may be followed to constrain these matrix elements. First, it is evident that the $\nu\pi$ matrix elements of the residual interaction play an important role in charge-exchange RPA calculations. This means that charge-exchange Gogny-RPA calculations could in principle provide important indications to better constrain in general this type of matrix elements. It is also interesting to notice that the same $\nu\pi$ matrix elements of the residual interaction entering in the SRPA formalism are also present in the variational multiparticle-multihole model of Ref. [3]. The two models could thus be used in a complementary way to analyze the impact of these terms and to guide toward a better control of their contributions in beyond mean-field theories.

---

[1] M. Bender and P.-H. Heenen, Phys. Rev. C 78, 024309 (2008).
[2] G. Colò, H. Sagawa, and P. F. Bortignon, Phys. Rev. C 82, 064307 (2010).
[3] N. Pillet, J.-F. Berger, and E. Caurier, Phys. Rev. C 78, 024305 (2008).
[4] J.-P. Delaroche, M. Girod, J. Libert, H. Goutte, S. Hilaire, S. Péru, N. Pillet, and G. F. Bertsch, Phys. Rev. C 81, 014303 (2010).
[5] E. Litvinova, P. Ring, and V. Tselyaev, Phys. Rev. C 75, 064308 (2007).
[6] T. R. Rodriguez and J. L. Egido, Phys. Rev. C 81, 064323 (2010).
[7] D. Gambacurta, M. Grasso, and F. Catara, Phys. Rev. C 81, 054312 (2010).
[8] D. Gambacurta, M. Grasso, and F. Catara, J. Phys. G 38, 035103(2011).
[9] D. Gambacurta, M. Grasso, and F. Catara, Phys. Rev. C 84, 034301 (2011).
[10] C. Yannouleas, Phys. Rev. C 35, 1159 (1987).
[11] M. Tohyama and M. Gong, Z. Phys. A 332, 269 (1989).
[12] D. Lacroix, S. Ayik, and Ph. Chomaz, Prog. Part. Nucl. Phys. 52, 497 (2004).
[13] M. Waroquier, J. Ryckebusch, J. Moreau, K. Heyde,N. Blasi, S.Y. van der Werf, and G. Wenes, Phys. Rep. 148, 249 (1987).
[14] S. Adachi and S. Yoshida, Phys. Lett. B 81, 98 (1979).
[15] J. Dechargé and D. Gogny, Phys. Rev. C 21, 1568 (1980).
[16] J. F. Berger, M. Girod, and D. Gogny, Comput. Phys. Commun. 63, 365 (1991).
[17] N. Pillet, V.G. Zelewinski, M. Dupuis, J.F. Berger, and J.M. Daugas, Phys. Rev. C 85, 044315 (2012).
[18] P. Papakonstantinou and R. Roth, Phys. Lett. B 671, 356 (2009).
[19] P. Papakonstantinou and R. Roth, Phys. Rev. C 81, 024317 (2010).
[20] D. Gambacurta and F. Catara, Phys. Rev. B 79, 085403 (2009); D. Gambacurta and F. Catara, Phys. Rev. B 81, 085418 (2010)