Second RPA with Skyrme Interaction

D Gambacurta,1,2  M Grasso3 and F Catara1,2

1 Dipartimento di Fisica e Astronomia dell’Università di Catania, Via S.Sofia 64, I-95123 Catania, Italy
2 Istituto Nazionale di Fisica Nucleare, Sezione di Catania, Via S.Sofia 64, I-95123 Catania, Italy
3 Institut de Physique Nucléaire, Université Paris-Sud, IN2P3-CNRS, F-91406 Orsay Cedex, France

E-mail: danilo.gambacurta@ct.infn.it

Abstract.

The Second Random Phase Approximation (RPA) is a natural extension of RPA obtained by introducing more general excitation operators where two particle-two hole configurations, in addition to the one particle-one hole ones, are considered. Some Second RPA results with Skyrme force in 16O are presented. Different levels of approximation are compared and in particular the quality of the diagonal approximation is tested. The issue of the rearrangement terms to be used in the matrix elements beyond the standard RPA ones, when density-dependent force are used, is briefly discussed. Two approximated, and generally used, schemes are used: the rearrangement terms are neglected in the matrix elements beyond RPA or evaluated with the RPA prescription. As a general feature of Second RPA results, a several-MeV shift of the strength distribution to lower energies is systematically found with respect to RPA distributions.

1. Introduction

The Hartree-Fock (HF) plus the random phase approximation (RPA) is a widely used microscopic approach for the study of collective excitations in many-body systems. The HF method allows to obtain the self-consistent mean field in which the particles are assumed to move independently, their energies and wave functions, and thus the HF ground state. The solution of the RPA equations gives the energies and the wave functions of the collective excitations that are assumed to be superpositions of particle-hole and hole-particle configurations built on top of a correlated ground defined as the vacuum of the phonon operators describing the excited states.

In the nuclear context, the HF + RPA framework with Skyrme interaction has been extensively applied for the description of the Giant Resonances and, in general, a quite good reproduction of the energies and transition probabilities associated to these excitations is found. On the other hand, in several works (see for example [1, 2, 3]) it has been underlined that the coupling of one particle-one hole configurations with more complex states has to be taken into account in order to describe some important effects, as for example the spreading width of the excitations. In such a direction, a natural extension of RPA is the so-called Second RPA (SRPA) [4] where two particle-two hole (2p2h) excitations, in addition to the one particle-one hole (1p1h) ones, are introduced. To our knowledge, current versions of SRPA are based on non-interacting 2p2h configurations and only the interaction between 2p2h and 1p1h has
been generally taken into account, in the so-called diagonal approximation. In this work, we present full Skyrme-SRPA results obtained for the doubly magic nucleus $^{16}$O. The diagonal approximation is employed here just to analyze its quality.

It is well known that, when density-dependent forces are used, the residual interaction used in the RPA matrices contains the so-called rearrangement terms coming from second derivative of the energy density functional with respect to the density (for more details see [6]). When dealing with the SRPA problem with density-dependent forces, a first formal aspect to consider is the determination of the residual interaction that has to be used in the new matrix elements with respect to RPA (see [5] and [6]). For the results shown here, we have explored two possibilities, often used in extensions of RPA, that we will discuss in the following.

In Section 2 the formal scheme of SRPA is briefly summarized, while in Section 3 some results for the monopole and quadrupole nuclear response obtained within SRPA are shown and compared with the RPA ones. A comparison of the full SRPA results with those obtained in the diagonal approximation is also presented. Moreover, the transition densities for the giant monopole resonances are analyzed and the radial distributions related to the main peaks are shown for RPA and SRPA. Conclusions and perspectives are finally discussed in Section 4.

2. Formal scheme

We briefly recall the main formal aspects of SRPA that may be found in several articles (see, for instance, Ref. [4]). SRPA is a natural extension of RPA where the excitation operators $Q^+\nu$ are a superposition of $1p1h$ and $2p2h$ configurations:

$$Q^\nu = \sum_{ph} (X^\nu \rho \delta_{ph} a_h - Y^\nu \rho a_h^{\dagger} a_p) + \sum_{p<p',h<h'} (X^\nu_{ph'p'h} a_h^{\dagger} a_{h'}^{\dagger} a_{p'} a_{p'}) - Y^\nu_{ph'p'h} a_h^{\dagger} a_{h'}^{\dagger} a_{p'} a_{p'}).$$ (1)

The $X$’s and $Y$’s are solutions of the equations,

$$\begin{pmatrix} A & B \\ -B^* & -A^* \end{pmatrix} \begin{pmatrix} X^\nu \\ Y^\nu \end{pmatrix} = \omega \nu \begin{pmatrix} X^\nu \\ Y^\nu \end{pmatrix},$$ (2)

where:

$$A = \begin{pmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{pmatrix}, B = \begin{pmatrix} B_{11} & B_{12} \\ B_{21} & B_{22} \end{pmatrix}, X^\nu = \begin{pmatrix} X^\nu_1 \\ X^\nu_2 \end{pmatrix}, Y^\nu = \begin{pmatrix} Y^\nu_1 \\ Y^\nu_2 \end{pmatrix}.$$

The indices 1 and 2 are a short-hand notation for the $1p1h$ and $2p2h$ configurations, respectively. $A_{11}$ and $B_{11}$ are the usual RPA matrices, $A_{12}$ and $B_{12}$ are the matrices coupling $1p1h$ with $2p2h$ configurations and $A_{22}$ and $B_{22}$ are the matrices coupling $2p2h$ configurations among themselves. Both in RPA and SRPA, resort to the quasi boson approximation (QBA) is made, which consists in the use of the HF ground state in the evaluation of the matrix elements appearing in the equations of motion. The matrix elements of the $B_{12}$, $B_{21}$ and $B_{22}$ matrices are found to be zero within QBA [4]. The other matrix elements are:

$$A_{12} = A_{ph,p1p2,h1,h2} = \langle HF | [a_{h1}^{\dagger}, a_{p1}^{\dagger}, a_{p2}^{\dagger}, a_{h2} a_{h1}] | HF \rangle =$$

$$= \chi(h_1,h_2)\tilde{V}_{h1,p1,p2}\delta_{hh_2} - \chi(p1,p2)\tilde{V}_{h1,h1p1,h}\delta_{pp2}$$ (3)

$$A_{22} = A_{p1h1p2h2,p1'p2'h1'h2'} = \langle HF | [a_{h1}^{\dagger}, a_{h2}^{\dagger}, a_{p1}^{\dagger}, a_{p2}^{\dagger}, [H, a_{p1}^{\dagger}, a_{p2}^{\dagger}, a_{h1'}^{\dagger} a_{h1}^{\dagger}] | HF \rangle =$$
\[ (\epsilon_{p_1} + \epsilon_{p_2} - \epsilon_{h_1} - \epsilon_{h_2})\chi(h_1, h_2)\delta_{h_1 h_1'}\delta_{h_2 h_2'} + \chi(h_1, h_2)\tilde{V}_{p_1 p_1' p_2 p_2'}\delta_{h_1 h_1'}\delta_{h_2 h_2'} + \chi(p_1, p_2)\chi(h_1, h_2)\chi(p_1', p_2')\chi(h_1', h_2')\tilde{V}_{p_1 p_1' h_1 h_1'}\delta_{h_2 h_2'}\delta_{p_2 p_2'} \] 

where the \(\epsilon\)'s are the HF single particle energies, \(\tilde{V}\) is the residual interaction and \(\chi(ij)\) is the antisymmetrizer for the indices \(i, j\).

It can be shown [7, 8], that the SRPA problem can be reduced to an energy-dependent, RPA-like, eigenvalue problem but where the \(A_{11}\) RPA matrix depends on the excitation energies

\[ A_{1,1'}(\omega) = A_{1,1'} + \sum_{2,2'} A_{1,2}(\omega + i\eta - A_{2,2'})^{-1} A_{2,1'}. \]  

In order to calculate this energy-dependent part one has to invert the \(A_{22}\) matrix defined in Eq. (4), whose dimensions are generally very large, requiring thus a strong numerical effort. However, if only the diagonal terms of the matrix (4) are considered, resorting to the so-called diagonal approximation, the inversion is algebraic. This approximation, often used in SRPA calculations, amounts to treat the \(2p2h\) configurations as unperturbed since the residual interaction is neglected. The quality of this approximation will be analyzed in Section 3.

Expressions (3) and (4) are valid in cases where the interaction is not density dependent. Rearrangement terms should be included in the case of density-dependent forces. The results hereafter discussed have been obtained by using two approximated choices, often used in beyond RPA calculations: i) we have calculated the matrix elements (3)-(4) without any rearrangement terms, ii) we have evaluated them by adding the usual RPA rearrangement contributions also in the \(A_{12}\) and \(A_{22}\) matrices.

3. Results in \(^{16}\text{O}\)

In this Section we present the nuclear strength distributions in \(^{16}\text{O}\) obtained in SRPA for the monopole and quadrupole multipolarities and we compare them with the RPA ones. The SGII [9] parametrization of the effective interaction has been used in the present calculations. At SRPA level different levels of approximation will be considered. As discussed above, in the case of density-dependent interactions it is not fully clear how to define the residual interaction appearing in the matrix elements beyond RPA, in particular as far as the rearrangement terms are concerned. By following a variational approach, SRPA equations in the case of density-dependent forces can be derived [5]. It is found that rearrangement terms are also present in matrix elements beyond RPA. In the \(A_{22}\) matrix we have only the ones giving the correct HF single particle energies while in \(A_{12}\), \(B_{12}\) matrices they appear in residual interaction but they have a different expression from the standard RPA prescription. The numerical implementation of these results is still in progress. In this work two different choices, very often used in beyond RPA-like calculations, are tested: (i) the interaction is used without rearrangement terms in matrix elements beyond RPA; (ii) rearrangement terms are included also in matrix elements beyond RPA, calculated with the usual RPA prescription. Furthermore, the full SRPA calculations are compared with the ones obtained when the diagonal approximation is used.

In order to make simpler the comparison between different results, we have folded the discrete spectra coming out from our calculations with a Lorentzian with a width of 1 MeV. The continuous strength distributions shown in this work are thus obtained by using this smoothing procedure.

In RPA calculations, \(1p1h\) configurations with unperturbed energy up to 100 MeV are considered, while in the SRPA ones, we have considered all the \(2p2h\) configurations with an unperturbed energy lower than an energy cutoff \(E_{\text{cut}}\). In Figs. 1 and 2 we show the monopole
and quadrupole strength distributions, respectively, for different choices of $E_{\text{cut}}$ (indicated in MeV in parenthesis in the figures). From the figures we see that a cutoff equal to 120 MeV gives stable results. Similar stability checks have been systematically made for all the results shown in the following.

The multipole transition operators used are

\begin{align}
  F^{IS}_S &= \sum r_i^2 Y_{\lambda_0}(\hat{r}_i) \\
  F^{IV}_S &= \sum r_i^2 Y_{\lambda_0}(\hat{r}_i) \tau_z(i)
\end{align}

in the isoscalar and isovector channel, respectively.

In Fig. 3 we show the RPA (dashed black lines) and SRPA (full red lines) results for the isoscalar (upper panel) and isovector (lower panel) monopole strength distributions. In both isoscalar and isovector cases the strongest effect in SRPA is a several-MeV shift of the strength distribution to lower energies with respect to RPA. This result seems to be a general feature of SRPA and has been found also in different SRPA calculations [10, 11, 12]. Looking at the figures, however, one sees that the profiles of the strength distributions are not very much changed, except for the above mentioned shift.

In the same figure we show also the SRPA results obtained with rearrangement terms in matrix elements beyond RPA (dot-dashed blue lines) are presented in order to evaluate their effect. We remark that these rearrangement terms have been calculated with the usual RPA procedure for all the matrix elements. For the isoscalar monopole case (top panel of Fig. 3) the residual interaction seems to be more repulsive when rearrangement terms are added providing a smaller energy shift to lower energies with respect to RPA. The strength distribution appears very strongly fragmented when rearrangement terms are included in all matrix elements. We know that the adopted way to evaluate the rearrangement terms in beyond RPA matrix elements is not the correct one even if it is currently used. Work is in progress to obtain the correct expressions: the fact that the SRPA($^*$) results are so different from the SRPA ones underlines that this is a very delicate point and indicates that the proper expressions are needed.
In Fig. 4 the full SRPA results, full (red) lines, are compared with the ones obtained in the diagonal approximation, dot-dashed (blue) lines. The results are quite different and this suggests that the residual interaction should not be neglected in the matrix $A_{22}$ in Skyrme-SRP A calculations. In particular, the strength distributions are pushed down towards even lower energies with respect to the complete calculations.

In Fig. 5 we show, for the monopole isoscalar case, the SRPA transition density referring to the peak at $\sim 17$ MeV while the RPA transition density is evaluated for the peak at $\sim 21$ MeV in top panel of Fig. 3. The profiles are not very different meaning that the nature of these RPA and SRPA excited states is not very different in terms of the spatial distributions of wave functions contributing to them.

Different is the case for the isovector responses. In Fig. 6 the RPA (SRPA) transition density, for the monopole response, is calculated for the peak at $\sim 29$ MeV (25 MeV) shown in the bottom panel of Fig. 3. Important differences are visible between RPA and SRPA suggesting that the nature of SRPA and RPA excited states in terms of radial distribution of wave functions contributing to the excitation is quite different.

4. Conclusions and perspectives

We have performed Skyrme-SRP A calculations for describing collective states in $^{16}$O. The SRPA scheme is fully treated without resorting to a general used approximated scheme, i.e. the diagonal approximations. The rearrangement terms of the residual interaction are treated in this work (i) by neglecting them in the matrix elements beyond RPA; (ii) by calculating them with the usual RPA procedure for all the matrix elements. Work is in progress to calculate the proper expressions to be used in beyond RPA matrix elements [5].

A shift towards lower energies of the strength distributions for giant resonances is generally found in SRPA with respect to RPA case. This shift being very strong, Skyrme-SRP A energies of giant resonances are typically too low with respect to the experimental response (Skyrme-RPA results are in general in good agreement with the experimental data for these excitations). This
Figure 5. (Color online) Comparison between RPA (full lines) and SRPA (dotted lines) transition densities for the monopole isoscalar states (see text): in the panel (a) neutron (thin lines) and proton (bold lines) parts, while in panel (b) the isoscalar (thin lines) and isovector (bold lines) ones. See text for more details.

Figure 6. (Color online) Comparison between RPA (full lines) and SRPA (dotted lines) transition densities for the monopole isovector states (see text): in the panel (a) neutron (thin lines) and proton (bold lines) parts, while in panel (b) the isoscalar (thin lines) and isovector (bold lines) ones. See text for more details.

A strong shift could be, at least partially, ascribed to the use of QBA. Some comments about the use of QBA in SRPA can be found in the literature [10, 13, 14]: it is said that its use in SRPA is a more drastic and severe approximation than in RPA. Extensions to cure this problem in the context of SRPA have been proposed and applied to a simple model [14] and to metal clusters [10]. Future applications to nuclei are in progress.

Finally, we plan in future works to explore with SRPA heavier or more exotic nuclei and to check the model dependence of the results by employing also other Skyrme parametrizations.

References
[1] Chomaz Ph and Frascaria N, Phys. Rep. 252, 275 (1995).
[2] Bortignon PF Nucl. Phys. A 687, 329c (2001).
[3] Colo G, Van Giai N, Bortignon PF and Broglia RA, Phys. Rev. C 50, 1496 (1994).
[4] Yannouleas C, Phys. Rev. C 35, 1159 (1986).
[5] Grasso M, Gambacura D and Catara F, arXiv:1003.2021v1 [nucl-th]
[6] Gambacura F, Grasso M and Catara F, Phys. Rev. C 81, 054312 (2010).
[7] da Providencia J, Nucl. Phys. 61, 87 (1965).
[8] Drozd S, Klent V, Speth J, and Wambach J, Nucl. Phys. A 451, 11 (1986).
[9] Van Giai N and Sagawa H, Phys. Lett. B 106 379 (1981); Nucl. Phys. A 371 1 (1981).
[10] Gambacura D and Catara F, Phys. Rev. B 79, 085403 (2009).
[11] Papakonstantinou P and Roth R, Phys. Lett. B 671, 356 (2009).
[12] Papakonstantinou P and Roth R, Phys. Rev. C 81, 024317 (2010).
[13] Lauritsch G and Reinhard PG, Nucl. Phys. A 509, 287 (1990); Takayanagi K, Shimizu K and Arima A, Nucl. Phys. A 477, 205 (1988).
[14] Gambacura D, Grasso M, Catara F, and Sambataro M, Phys. Rev. C 73, 024319 (2006).
[15] Gambacura D and Catara F, Phys. Rev. B 81, 085418 (2010).