Subtraction method in the Second Random Phase Approximation

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Abstract. We discuss the subtraction method applied to the Second Random Phase Approximation (SRPA). This method has been proposed to overcome double counting and stability issues appearing in beyond mean-field calculations. We show that the subtraction procedure leads to a considerable reduction of the SRPA downwards shift with respect to the random phase approximation (RPA) spectra and to results that are weakly cutoff dependent. Applications to the isoscalar monopole and quadrupole response in $^{16}$O and to the low-lying dipole response in $^{48}$Ca are shown and discussed.

1. Introduction

The random-phase approximation (RPA) is a microscopic theory applied very successful for the study of the main properties of collective states. In RPA, collective excitations are described as a superposition of 1 particle-1 hole (1p1h). This method, especially when applied within the Energy Density Functional (EDF) framework, allows to describe fairly good global properties of giant resonances, such as the centroid energy and the total strength distribution.

On the other hand, the RPA model has some very well known limits. Among them we recall that the width and fine structure of the nuclear excitations cannot be reproduced except for the single-particle Landau damping and for the escape width (if continuum states are taken into account). A well-known extension of the RPA scheme is the second RPA (SRPA) model which amounts to enlarge the space of basic elementary excitations by including 2 particle-2 hole (2p2h) configurations. This leads to a richer treatment of the excitation modes.

Only in the last years, large-scale SRPA calculations have been performed, showing merits and limits of this approach. Performing such calculations has allowed to show some features of the SRPA that could not be seen in previous applications, because of strong truncations in the model space or approximations. In particular, the SRPA spectrum is systematically lowered by several MeV with respect to that obtained in the ordinary RPA.

The origin of this SRPA can be traced back to the implicit inclusion of correlations in the ground state that have been already taken into account at mean-field level [1, 2]. This issue leads also to a violation of the Thouless theorem within the SRPA and to stability problems [3]. A solution to both drawbacks was recently applied [4, 5], based on a subtraction procedure [1, 2] suited for beyond RPA approaches.
In this paper, we first briefly discuss the subtraction method in the SRPA framework and then some applications are presented. In particular, the case of the monopole and quadrupole response in the nucleus $^{16}$O and of the low-lying dipole response in $^{48}$Ca, will be shown and discussed.

2. The subtraction procedure in SRPA

In the RPA approximation the excitations operators are assumed to be a linear superposition of 1p1h operators:

$$ Q^\dagger_{\nu} = \sum_{ph} X^{\nu}_{ph} a_p^\dagger a_h - \sum_{ph} Y^{\nu}_{ph} a_h^\dagger a_p. $$

(1)

where for notation simplicity, the coupling to total quantum numbers is not indicated.

In the case of the SRPA, the 2p2h configurations are explicitly considered in the description of the excitations operators, having the following structure:

$$ Q^\dagger_{\nu} = \sum_{ph} X^{\nu}_{ph} a_p^\dagger a_h - \sum_{ph} Y^{\nu}_{ph} a_h^\dagger a_p + \sum_{p<p',h<h'} (X^{\nu}_{php'h'} a_p^\dagger a_h^\dagger a_{p'} a_{h'}) - (Y^{\nu}_{php'h'} a_h^\dagger a_p^\dagger a_{p'} a_{h'}). $$

(2)

In both cases, the energies $\omega_{\nu}$ of the excited states and their wave function (e.g. the $X's$ and $Y's$ amplitudes) are obtained by solving an eigenvalue problem of this form:

$$ \begin{pmatrix} A & B \\ -B^* & -A^* \end{pmatrix} \begin{pmatrix} X^{\nu} \\ Y^{\nu} \end{pmatrix} = \omega_{\nu} \begin{pmatrix} X^{\nu} \\ Y^{\nu} \end{pmatrix}. $$

(3)

In the RPA case the $A$ and $B$ matrices describe the coupling among the 1p1h configurations, while in SRPA, more general block matrices appear, describing the coupling of the 1p1h configurations with the 2p2h configurations and of the 2p2h configurations among themselves, (see for example Ref. [6]).

The subtraction procedure consists in subtracting in the $A_{11}$ block of the SRPA matrix the quantity

$$ E_{11'} = - \sum_{2,2'} A_{12}(A_{22'})^{-1} A_{2',1'} - \sum_{2,2'} B_{12}(A_{22'})^{-1} B_{2',1'}. $$

(4)

where the indices 1 and 2 stand for the 1p1h and 2p2h configurations, respectively. This subtraction guarantees that the subtracted SRPA (SSRPA) response reduces to the RPA one in the zero–frequency limit. When density-dependent interactions are employed, the subtraction procedure requires also the modification of the $B_{11}$ matrix [4].

As discussed above, large scale SRPA calculations [6, 7, 8, 9] show that the SRPA spectrum is systematically lowered by several MeV with respect to that obtained in RPA. On the other hand, RPA results based on the EDF framework are typically in very good agreement with experimental data, at least concerning the centroid energies and total strength of the giant resonances. Therefore, the inclusion of the 2p2h configurations often worsens the RPA description. In the next section, we show the effect of the subtraction procedure in strongly reducing this strong shift.

From a numerical point of view, the main cost in calculating the correction (4) consists in inverting the $A_{22}$ matrix. This inversion becomes trivial if the matrix is assumed to be diagonal. Therefore the correction can be calculated with a reasonable extra–numerical effort. Hereafter, we will use the acronyms SSRPA$_F$ to denote the subtracted SRPA in the full scheme, e.g. full inversion of the $A_{22}$ matrix, and SSRPA$_D$ to denote the subtracted SRPA assuming diagonal the $A_{22}$ matrix in the correction term (4).
3. Subtracted SRPA results

3.1. Results in $^{16}$O: isoscalar monopole and quadrupole response

In this section we show the effect of the subtraction method, in the case of the isoscalar monopole and quadrupole response in $^{16}$O. We perform Hartree-Fock plus RPA calculations. The SGII [10] interaction is used. We include all the 1p1h configurations with energy less than 100 MeV. For the 2p2h space in the SRPA calculations, we take the cutoff to be at 70 MeV and 50 MeV for the monopole and the quadrupole cases, respectively. Those values lead to about 5000 2p2h configurations in each of the two cases. This number is small enough so that we can still fully invert the matrix $A_{22}'$ to perform the subtraction without approximation. In all the figures that follow, we fold the calculated response with a Lorentzian of width 0.5 MeV.

Fig. 1 shows the isoscalar monopole strength distribution, calculated with the unmodified SRPA and with the SSRPA$_F$, using a cutoff on the 2p2h configurations in the correction term of Eq. (4) equal to 50, 60, and 70 MeV. In the last of these cases, all the SRPA 2p2h configurations are included in the correction. The effect of the subtraction, as we expected, is to shift the SRPA spectrum upwards, by amounts that increase with the cutoff in the correction terms. The important differences between the three subtracted strength functions indicate that it is crucial to include all the 2p2h states in the correction terms containing $(A_{22}')^{-1}$ in Eq. (4). Figs. 2 displays the same results as Fig. 1 but in the isoscalar quadrupole channel (where the 2p2h cutoff is at 50 MeV in the SRPA calculation). The cutoffs in the correction terms are at 40, 45, and 50 MeV. The remarks made about the first figure apply here as well.

Figs 3 and 4 compare the full and diagonal subtracted SRPA results with the 70 MeV and 50 MeV cutoff in the correction terms, respectively. We observe that the SSRPA$_F$ and SSRPA$_D$ results are very similar, the difference being a small shift to larger excitation energies in the SSRPA$_D$.

Another very positive feature of the SSRPA results is the very weakly dependence on the 2p2h cutoff. This can been seen in Fig. 5, where we show the isoscalar monopole responses, with cutoffs for the correction terms at 70, 80, and 90 MeV. The three strength functions are
very similar showing that the subtraction procedure provides much more robust, e.g. cutoff–insensitive, results. A similar behaviour has been found also for the quadrupole case.

3.2. Results in $^{48}$Ca: low-lying dipole response
The dipole response below the neutron threshold in $^{48}$Ca has been measured with the ($\gamma, \gamma'$) reaction [11]. Systematic future studies of the nuclear dipole response are planned at ELI-NP in Bucharest, both below [12] and above [13] the neutron separation threshold.

A cutoff of 100 MeV is used in building the 1p1h configurations, ensuring a full preservation of the isoscalar and isovector Energy Weighted Sum Rules (EWSRs). Deviations of less than 1\% are found in both cases in RPA. In the SRPA calculations, a cutoff of 60 MeV in the 2p2h configurations is used. The EWSRs are satisfied as in RPA, with deviations less than 1\%. On the other side, the SSRPA model provides by construction the same inverse moment $m_{-1}$ as in RPA, but not the same moment $m_1$ and deviations of $\approx 5 – 7 \%$ are found for the EWSRs.

We recall that RPA predictions fail in reproducing such a low-lying strength either because the lowest RPA energies are larger than 10 MeV or because the RPA model cannot provide the observed fragmentation. Only beyond mean-field models including correlations, such as the SRPA or the extended theory of finite Fermi systems (ETFFS) [11, 14], based on the quasiparticle–phonon coupling, could account for this low–lying strength in $^{48}$Ca. A fragmented SRPA dipole strength below 10 MeV was indeed illustrated in Ref. [8] for $^{48}$Ca. However, the SRPA $B(E1)$ transition probability, integrated up to 10 MeV, was found to be definitely much larger than the experimental value. By using the implemented SRPA model augmented via the subtraction method, we show here that problem of overestimation of the transition probability is strongly reduced, providing thus a rather good description of the experimental data. Some states having strong 1p1h components, which are too much shifted downwards by the standard SRPA, are pushed to higher energies by the subtraction, reducing in this way the $B(E1)$ value below 10 MeV. Moreover, previous applications of the SRPA and SSRPA were done without including the spin-orbit and Coulomb terms in the residual interaction. In this work, all the terms of the interaction consistently with the mean-field Hartree-Fock description are included. Due to the inclusion of all terms of the residual interaction, the present SRPA results are different.
compared to those illustrated in Ref. [8], where the spin–orbit and the Coulomb contributions were not taken into account. In Fig. 6(a) we show the experimental transition probabilities $B(E0)$ 

\[
B(E0) \propto \frac{1}{E} \frac{d^2 \sigma}{dE d\Omega}
\]

and the theoretical predictions calculated with the standard SRPA (dashed red bars; the values have been divided by 2) and with the SSRPA (blue thick bars). The fragmentation of the states follows quite well the experimental distribution in the energy position of the main peaks. The total strength integrated between 5 and 10 MeV is shown in Table I. The first column shows the experimental result and the second and third columns the corresponding values obtained with the SRPA and the SSRPA models, respectively. Whereas the SRPA value is eight times larger than the experimental result, the SSRPA summed $B(E1)$ is very close to the measured value. A similar behaviour is found also for the EWSR integrated up to 10 MeV, shown in the second line of Table I.

An interesting information that can be analysed in connection with the strength distribution is the composition of the excitation modes in terms of 1p1h and 2p2h configurations. By extracting the expression of $N_1$ from the normalization condition,

\[
\sum_{ph} (|X_{ph'}|^2 - |Y_{ph'}|^2) + \sum_{p'h' > h'} (|X_{p'h'h'}|^2 - |Y_{p'h'h'}|^2) = N_1 + N_2 = 1,
\]

we plot in Figs 7 and 8 the $B(E1)$ values corresponding and the quantity $N_1$ (lower panel) for each excited state in SRPA and SSRPA, respectively. One observes that, in the SRPA case, a strong mixing of 1p1h and 2p2h components is present. On the contrary, in the SSRPA case, states having mainly a 2p2h nature remain as a consequence of the subtraction procedure, pushing up state with a strong 1p1h component.

4. Conclusions

In this paper we have shown and discussed recent applications of the SRPA framework where the subtraction method has been employed. The implemented subtraction method is able to
Figure 7. (Color online) For each state the SRPA $B(E1)$ value and the total 1p1h contribution $N_1$ to the norm of the state defined in Eq. (5) (lower panel), are shown.

Figure 8. (Color online) For each state the SSRPA $B(E1)$ value and the total 1p1h contribution $N_1$ to the norm of the state defined in Eq. (5) (lower panel), are shown.

|                  | Exp | SRPA | SSRPA |
|------------------|-----|------|-------|
| $\sum B(E1)$    | 0.068 | 0.563 | 0.078 |
| $\pm 0.008$     |      |      |       |
| $\sum_i E_i B_i(E1)$ | 0.570 | 4.618 | 0.621 |
| $\pm 0.062$     |      |      |       |

Table 1. Experimental [11] and theoretical $\sum B(E1)$ in (e² fm²) and $\sum_i E_i B_i(E1)$ in (MeV e² fm²) summed between 5 and 10 MeV.

strongly reduce the shift of the strength found in SRPA. and to provide robust and weakly cutoff dependent predictions. Applications for the description of the monopole and quadrupole response in $^{16}$O are shown. After that, the low-lying dipole response in $^{48}$Ca, is studied, showing that the subtracted SRPA results improve to a great extent the agreement with experimental data.

References
[1] Tselyaev V I 2007 Phys. Rev. C 75 024306
[2] Tselyaev V I 2013 Phys. Rev. C 88 054301
[3] Papakonstantinou P 2014, Phys. Rev. C 90, 024305
[4] Gambacurta D, Grasso M and Engel J 2015 Phys. Rev. C 92 034303
[5] Gambacurta D and Grasso M 2016 Eur. Phys. J. A 52 198
[6] Gambacurta D, Grasso M, and Catara F 2010 Phys. Rev. C 81 054312
[7] Gambacurta D, Grasso M, and Catara F 2011 J. Phys. G 38 035103
[8] Gambacurta D, Grasso M, and Catara F 2011 Phys. Rev. C 84 034301
[9] Gambacurta D, Grasso M, De Donno V, Co G and Catara F 2012 Phys. Rev. C 86 021304(R)
[10] Giai N V and Sagawa H 1981, Phys. Lett. B 106, 379
[11] Hartmann T et al. 2004, Phys. Rev. Lett. 93 192501
[12] Ur C A et al. 2016 Romanian Reports in Physics, Vol. 68, Supplement, P. S483S538,
[13] Camera F et al. 2016 Romanian Reports in Physics, Vol. 68, Supplement, P. S539S619
[14] Tertychny G 2007 et al. Nucl. Phys. A 788, 159c