

Beyond-mean-field corrections within the second random-phase approximation

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Abstract. A subtraction procedure, introduced to overcome double-counting problems in beyond-mean-field theories, is used in the second random-phase approximation (SRPA). Double-counting problems arise in the energy-density functional framework in all cases where effective interactions tailored at leading order are used for higher-order calculations, such as those done in the SRPA model. It was recently shown that this subtraction procedure also guarantees that the stability condition related to the Thouless theorem is verified in extended RPA models. We discuss applications of the subtraction procedure, introduced within the SRPA model, to the nucleus ^{16}O . The application of the subtraction procedure leads to: (i) stable results that are weakly cutoff dependent; (ii) a considerable upwards correction of the SRPA spectra (which were systematically shifted downwards by several MeV with respect to RPA spectra, in all previous calculations). With this important implementation of the model, many applications may be foreseen to analyze the genuine impact of 2 particle-2 hole configurations (without any cutoff dependences and anomalous shifts) on the excitation spectra of medium-mass and heavy nuclei.

1. Introduction

Several aspects of the nuclear many-body problem can be well described within the energy-density functional (EDF) theory at the mean-field level. However, a precise description of nuclear phenomena requires in some cases to go beyond this independent-particle picture. A special care has to be paid then to the fact that the starting point is not a bare many-body Hamiltonian but an energy functional of the density that is generated, in most cases, by a density-dependent effective interaction.

In general, mean-field-based models within the EDF theory correspond to the leading order of the many-body perturbative problem, that is described by the Dyson equation [1]. A way to go beyond this level of approximation is to truncate the perturbative expansion at the next



order, by including also the second-order contribution. By making this, however, an obvious risk of double counting exists. Since the parameters of the effective interaction are adjusted at the leading order, that is, with mean-field calculations, the strategy followed within the mean-field-based EDF is very similar to that governing the so-called density-functional theory, currently used in chemistry and solid-state physics: all the physics is supposed to be well described at the leading order and this is the reason why parameters are adjusted at this order in the EDF framework. When correlations are explicitly included in the theoretical model (for instance, when the computation is carried out at an higher order beyond the mean-field level), those correlations which are already implicitly contained in the numerical values of the parameters can then be obviously double counted. This problem may be however rigorously handled in the framework of the EDF and some solutions have been proposed. One of them is a subtraction procedure tailored for those beyond-mean-field cases where the mass operator acquires an energy dependence. This procedure was first introduced to cure double-counting problems in the framework of particle-vibration models [2] and then formulated so to be used in extended random-phase approximation (RPA) models, such as the second RPA (SRPA) [3].

2. SRPA and the subtraction method

2.1. Formalism of SRPA

The SRPA model is a natural extension of the RPA model, where the 2 particle-2 hole (2p2h) elementary configurations are added to the RPA 1 particle-1 hole (1p1h) excitations. The excitation operators are then written as linear superpositions of particle-hole, hole-particle, 2 particle-2 hole, and 2 hole-2 particle elementary excitations, where particle and hole single-particle states are defined with respect to the Hartree-Fock (HF) ground state.

The SRPA equations are very similar to the RPA equations and are written in a compact form as

$$\begin{pmatrix} \mathcal{A} & \mathcal{B} \\ -\mathcal{B}^* & -\mathcal{A}^* \end{pmatrix} \begin{pmatrix} \mathcal{X}^\nu \\ \mathcal{Y}^\nu \end{pmatrix} = \omega_\nu \begin{pmatrix} \mathcal{X}^\nu \\ \mathcal{Y}^\nu \end{pmatrix}, \quad (1)$$

where:

$$\mathcal{A} = \begin{pmatrix} A_{11'} & A_{12} \\ A_{21} & A_{22'} \end{pmatrix}, \mathcal{B} = \begin{pmatrix} B_{11'} & B_{12} \\ B_{21} & B_{22'} \end{pmatrix},$$

$$\mathcal{X}^\nu = \begin{pmatrix} X_1^\nu \\ X_2^\nu \end{pmatrix}, \quad \mathcal{Y}^\nu = \begin{pmatrix} Y_1^\nu \\ Y_2^\nu \end{pmatrix}.$$

The '11' part of the matrices represents the 1p1h sector, that corresponds to the RPA sub-matrices. New matrix elements enter into play in the '12' and '22' sectors and describe the 1p1h-2p2h and 2p2h-2p2h couplings, respectively. The 1p1h-2p2h coupling, in particular, is responsible for providing a physical description of the fragmentation and of the spreading width of the excitation modes, that cannot be done within a simple mean-field model.

The first large-scale SRPA calculations were performed only quite recently [4, 5, 6, 7, 8, 9], without any cut or simplification in the matrices to diagonalize and with large values of the energy cutoff. These calculations have allowed us to fully address for the first time some specific issues related to the SRPA model such as, for instance, the proper derivation of the new rearrangement terms generated by the density dependence of the force in the beyond-RPA matrix elements [7].

When traditional effective interactions are used for these calculations, the already mentioned double-counting problems arise and they should be handled. Moreover, an ultraviolet divergence occurs and has to be regularized when a zero-range force is used. This can be seen in all the calculations that were performed with effective interactions such as Skyrme or Gogny forces in Refs. [6, 7, 8, 9]. There are two types of results that have been obtained: (i) in the case of giant resonances and, in general, in those cases where the excitations are already well described by

the RPA, a strong downwards shift in energy of the response function was found with respect to the RPA. This strong and anomalous shift was a very surprising and unexpected result. In most cases, it produces strength distributions that are in less good agreement with the experimental data than the RPA. One would expect however that the SRPA, that contains the RPA as a simpler case, should provide similar results as the RPA in those cases where such model works well, that is, in those cases where the 1p1h configurations are the dominant configurations. (ii) For states that are mostly multiparticle–multihole states, the SRPA provides a better description than the standard RPA, which is very poor in describing such excitations.

In all cases, there is a strong cutoff dependence generated by the ultraviolet divergence associated to the zero–range of the used effective force.

Recently, it was pointed out that the standard SRPA does not satisfy the stability condition related to the Thouless theorem [10]. This was pointed out by Papakonstantinou in Ref. [11]. Such drawback of the SRPA and a procedure to overcome it will be discussed in the next Subsection.

2.2. Subtraction method

The formal properties of the SRPA model in its standard formulation, and all its advantages and drawbacks, were analyzed recently in Ref. [11]. In particular, a specific drawback of the model related to the stability condition (Thouless theorem) [10] was discussed. A possible direction to overcome this formal limitation of the standard SRPA model was suggested and consists in using a correlated ground state in the calculations instead of the HF state. This means that the so–called quasiboson approximation, also used in the RPA model, should be avoided in the SRPA model to ensure that the stability condition is satisfied. In a less recent work, Tselyaev suggested an alternative direction based on a subtraction procedure [3], that he had previously introduced to cure double–counting problems in models based on the particle–vibration coupling [2]. In Ref. [3], Tselyaev demonstrated that the use of such subtraction method ensures not only the cancelation of any double counting in extended RPA models such as the SRPA, but also the validity of the stability condition in those models.

The SRPA equations showed above may be written, after some manipulations, as RPA–type equations (that is, with only the '11' sector) where, however, the matrix elements acquire an explicit energy dependence. The cancelation of double counting is guaranteed when one imposes that the SRPA energy–dependent matrix calculated at zero energy is equal to the RPA matrix. This may be obtained by subtracting, to the energy–dependent contributions in the SRPA matrix elements, the same contributions calculated at zero energy. What Tselyaev calls the static correlations, that are already included in the model in the numerical values of the parameters of the effective interactions, are in this way counted only once. The genuine dynamic correlations, that this beyond–mean–field model introduces, are thus taken into account in a clean and proper way. As Tselyaev showed, it turns out that such procedure also allows one to demonstrate the validity of the Thouless theorem in the SRPA.

Recently, this subtraction method was applied within the SRPA and it was found that the anomalous huge downwards shift in energy that the standard SRPA produces with respect to the RPA is not obtained when the subtraction procedure is used [12]. This result indicates that such shift is not related to the enriched physical description of the excitation modes provided by the SRPA, but to the drawback of the model related to the violation of the stability condition. Moreover, the ultraviolet divergences are also canceled by the same subtraction. A very interesting remark on this method is the following: it appears clear that the subtraction acts mostly on the elementary 1p1h excitation energies by renormalizing them. This explains why the effects of the subtraction are mostly visible on those excitations that have a strong 1p1h nature and are very weakly mixed with multiparticle–multihole configurations. The subtraction actually acts as a corrective term that is added to the '11' part of the matrix. This corrective

term is calculated as a sum of terms with a cutoff in the 2p2h space. A coherent calculation is done if this cutoff is chosen equal to the 2p2h cutoff used to compute the matrix elements.

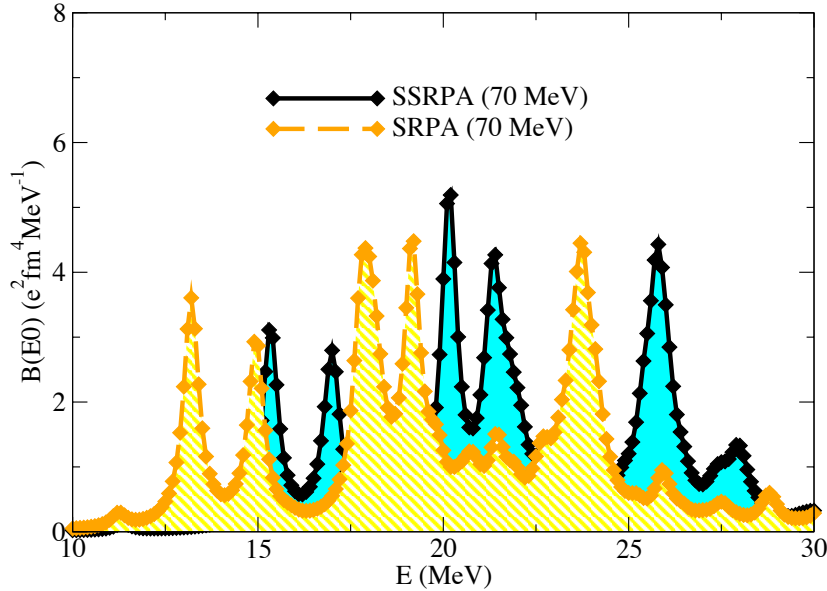


Figure 1. Isoscalar monopole response calculated for the nucleus ^{16}O with the Skyrme interaction SGII. The yellow area and orange dashed line refer to a standard SRPA calculation with a cutoff of 70 MeV in the 2p2h configurations. The cyan area and solid black line correspond to a subtracted SRPA calculation with the same cutoff of 70 MeV both in the matrices and in the corrective term for the 2p2h configurations.

On the other side, multiparticle–multihole excitations (that were already well described by the standard SRPA model) are practically not affected by the subtraction.

An illustration of the found results is shown in Fig. 1, where the isoscalar monopole response calculated for the nucleus ^{16}O with the Skyrme interaction SGII is presented. The yellow area and orange line refer to a standard SRPA calculation with a cutoff of 70 MeV in the 2p2h configurations. The cyan area and black solid line correspond to subtracted SRPA (SSRPA) calculations with the same cutoff of 70 MeV in the matrices and in the subtractive term for the 2p2h configurations.

One observes that the subtraction produces an upwards shift of the energies that goes in the good direction to cure the anomalous downwards shift generated by the standard SRPA. This goes in the correct direction also to provide a better comparison with the experimental results. The agreement is improved with respect to both the standard SRPA and the RPA. For example, for the isoscalar quadrupole response of the nucleus ^{16}O , the subtracted SRPA model provides a centroid energy and a width of 20.21 and 4.05 MeV, respectively. The RPA model leads to 20.73 and 2.42 MeV, respectively. The corresponding experimental values [13] are 19.76 and 5.11 MeV, respectively. One observes that the energy of the centroid is slightly decreased by the subtracted SRPA with respect to the RPA and is closer to the experimental value. The width is remarkably increased by the SRPA and this is indeed the most relevant improvement expected from the SRPA model, with respect to the RPA model, in the description of giant resonances.

3. Conclusions

A subtraction procedure proposed by Tselyaev for extended RPA models [3] was recently applied to the SRPA model to remove double-counting problems, to ensure the validity of the stability condition, and to cancel all the ultraviolet divergences associated to the zero range of the used effective interaction.

An application to the nucleus ^{16}O was discussed and a comparison with the RPA spectrum and the experimental measurements was shown for the isoscalar quadrupole resonance. The subtracted SRPA model leads to a centroid energy which is in better agreement with the experimental value compared to the RPA centroid. The most important improvement provided by the SRPA is found however in the description of the spreading width of the excitation mode, which is remarkably increased by the SRPA with respect to the RPA. The great advantage of the subtracted SRPA, with respect to the standard SRPA, is not only the suppression of the anomalous downwards shift of the energies that the standard SRPA produces with respect to the RPA, but also the fact that the predictions are fully cutoff independent because all the ultraviolet divergences are removed by the subtraction.

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