Skyrme second random-phase approximation
description of low-lying dipole states in $^{48}$Ca isotope

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Abstract. We apply the second random phase approximation (RPA) with Skyrme interaction to the study of low-lying dipole strength distributions of $^{48}$Ca, in the energy region of the excitation spectrum between 5 and 10 MeV. RPA models do not usually predict any presence of strength in this energy region, while experimentally a significant amount of strength is found. The inclusion of the two particle - two hole configurations within the second RPA is found to be very important. Several states are obtained and many of them, despite being essentially two particle - two hole states, show quite large B(E1) values. These results are in reasonable agreement with other beyond mean-field predictions and with the corresponding experimental measurements. A detailed analysis of the properties of the most collective state is done in terms of its one particle - one hole nature and its transition densities.

1. Introduction
In the last years the properties of the low-lying dipole response in neutron rich nuclei have been studied with particular attention to the appearance of the so-called Pygmy Dipole Resonance. A recent review about the main theoretical results and experimental measurements can be found in Ref. [1]. In very light nuclei, the development of a strong dipole response at low energies is usually related to the extremely small value of the separation energies. These low-energy states are not collective excitations and have mainly a single-particle character [2]. Low-energy dipole excitations have been observed also for the isotopes $^{16-22}$O [3]. From the experimental point of view, the character of these excitations (collective or single-particle) has not yet been clearly elucidated.

For heavier stable and unstable nuclei, the development of a pygmy dipole response in neutron-rich systems is currently related to the formation of a thick neutron skin at the surface of the nucleus: the low-lying dipole modes are interpreted in terms of oscillations of the skin against the core composed by both neutrons and protons. From the theoretical point of view, pygmy resonances have been analyzed with several models. Some examples are the relativistic and non-relativistic (Q)RPA approach (see, for instance, Ref. [1] and references therein, and Refs. [4]-[8]), the particle-phonon-coupling models (Ref. [1] and references therein), a semiclassical coupled-channels approach for Sn isotopes [9, 10], hydrodynamical models [11], the phonondamping model [12], and the so-called Extended Theory of Finite Fermi Systems (ETFFS) [13].
Discrepancies among the different theoretical predictions are found concerning in particular the collective character and the fragmentation of the low-lying modes. It is well known that each excitation mode is characterized by an escape ($\Gamma^\uparrow$) and a spreading ($\Gamma^\downarrow$) width as well as by a Landau damping. The latter can already be described by a standard discrete RPA calculation. The spreading width cannot be described by the standard RPA since more complex configurations (collective coordinates or multiparticle-multihole configurations) have to be included within a beyond mean-field model. Among the different beyond mean-field models that allow one to describe, at least partially, the width and the fragmentation of the excitation modes, the second random-phase approximation (SRPA) is a powerful theoretical tool where the coupling with 2 particle–2 hole ($2p2h$) configurations is included within an RPA-like formalism. In this way, the so-called spreading widths can be described together with the Landau damping. Escape widths are missing if the coupling to the continuum is not included. To include higher multiparticle-multihole configurations different directions may be followed [14, 15].

Due to the heavy numerical effort required, the SRPA equations have been usually solved resorting to some approximations. Recently, full SRPA calculations have been performed for some O and Ca isotopes [16, 17]. In particular, in Ref. [17] calculations with the density-dependent Skyrme interaction have been performed adopting two currently used approximations for treating the rearrangement terms of the residual interaction appearing in beyond-RPA matrix elements. The two approximations consist in either neglecting these rearrangement terms or treating them with the standard RPA procedure. Important differences have been found between the corresponding two sets of results. The same authors of Ref. [17] have addressed this point in a more recent work [18] where a procedure to derive the expressions of all the rearrangement terms within the SRPA framework has been presented and applied to calculations for the nucleus $^{16}$O. In this first application, the importance of the proper treatment of the rearrangement terms in SRPA for the description of the fragmentation of the excited modes has been shown. In this work, the low-lying excitation spectrum of the stable isotopes $^{48}$Ca is analyzed within the Skyrme-SRPA model.

The paper is organized as follows. In section 2 the main formal aspects of the SRPA model are briefly recalled. In section 3 the low-lying strength distributions are analyzed for the $^{48}$Ca and the transition densities associated to some states are displayed. We draw our conclusions in section 4.

2. Formalism
The excited states in SRPA are superpositions of 1 particle-1 hole ($1p1h$) and $2p2h$ configurations. The SRPA equations can be written in the compact form

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

(1)

where:

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

$$X^\nu = \begin{pmatrix}
X_1^\nu \\
X_2^\nu
\end{pmatrix}, \quad Y^\nu = \begin{pmatrix}
Y_1^\nu \\
Y_2^\nu
\end{pmatrix}.$$
Table 1. Total $B(E1)$ ($e^2 f m^2$) and EWSRs ($e^2 f m^2 MeV$) integrated up to 10 MeV as a function of the energy cutoff $ECUT$ (MeV) on the $2p2h$ configurations for $^{48}$Ca.

| $ECUT$ (MeV) | $\sum B(E_1)$ | EWSRs |
|-------------|----------------|-------|
| 40          | 0.184          | 1.623 |
| 45          | 0.218          | 1.895 |
| 50          | 0.226          | 1.944 |
| 55          | 0.240          | 2.049 |
| 60          | 0.230          | 1.964 |

New types of rearrangement terms have been obtained for the other matrix elements in Ref. [18] within a variational derivation of the SRPA equations. The expressions of these rearrangement terms are reported in Ref. [18] and are used in this work.

3. Results

The experimental low-lying dipole response of the $^{48}$Ca isotope has been recently analyzed [19] and the development of a low-energy strength, between 5 and 10 MeV, has been observed. From the theoretical point of view, it has been found that relativistic and non-relativistic (Q)RPA models are not able to well describe the low-lying response in $^{48}$Ca because they either do not provide the good excitation energies (too high energies) or do not predict the experimental fragmentation of the peaks. For example, in recent calculations performed with the relativistic RPA model no strength has been found in the response below the excitation energy of 10 MeV [20]. The same kind of results is obtained in our Skyrme SGII-RPA calculations. On the other hand, a reasonable agreement (energies and fragmentation) with the experimental results has been found within the ETFFS model [13, 21] where a quasiparticle-phonon coupling is included.

We perform SRPA calculations with the Skyrme interaction SGII. More details about the calculations can be found in Ref. [22]. Because of the zero-range of the Skyrme interaction, a natural energy cutoff is not provided. Different procedures to treat this problem may be envisaged for future studies (see, for instance, the exploratory work presented in Ref. [23]). In this work, we have introduced an energy cutoff ($ECUT$) on the $2p2h$ configurations. By varying it from 40 to 60 MeV we have verified that a reasonable stability of the results is achieved around a cutoff of 50-55 MeV. The total $B(E1)$ and EWSRs values, integrated up to an energy of 10 MeV, are shown in table 1 as a function of the energy cutoff $ECUT$ on the $2p2h$ configurations.

The $B(E1)$ distributions for different choices of the energy cutoff are plotted in figure 1 up to an excitation energy of 10 MeV. The employed transition operator is

$$F_{10} = e_p \sum_{i=1}^{Z} r_i Y_{10}(\Omega_i) - e_n \sum_{i=1}^{N} r_i Y_{10}(\Omega_i)$$  \hspace{1cm} (2)

where $e_p$ and $e_n$ are the kinematic charges, $e_p = Ne/A$ and $e_n = Ze/A$, respectively. One can observe that the results do not change strongly starting from a cutoff of 45 MeV. In what follows, we will analyze the results obtained with a cutoff of 60 MeV (bottom panel of figure 1).

These results are qualitatively of the same type as those found in Ref. [21] with the ETFFS approach which is also a beyond-mean-field model where the coupling is done with collective phonons instead of $2p2h$ configurations (as is done in SRPA). We can compare the location of the theoretical peaks with the experimental distribution (see, for instance, figure 2 of Ref. [21]). We can distinguish two regions: from 6 to 8 MeV and from 8 to 10 MeV. Experimentally, the highest peak in the first region is found at $\sim 7$ MeV whereas in our case we have several small peaks

3
between 6 and 8 MeV and the highest peak is located around 6.2 MeV. In the interval between 8 and 10 MeV, our response is more fragmented than the experimental one. Experimentally, peaks are found around 8.5, 9 and 9.5 MeV. Our highest peak is located at \( \sim 9.1 \) MeV. We have also evaluated the response in the nucleus \(^{40}\)Ca. Experimentally, a negligible strength has been found for this nucleus between 5 and 10 MeV (figure 2 of Ref. [21]). Some peaks are actually found at low energy but the corresponding strength is much lower than in \(^{48}\)Ca (almost a factor 10).

An interesting information that can be analyzed 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 SRPA normalization condition,

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

we plot in figure 2 the \(B(E1)\) values corresponding to a cutoff of 60 MeV (upper panel, same as in bottom panel of figure 1) and the quantity \(N_1\) (lower panel) for each excitation. One observes that all the excitations present a mixing of \(1p1h\) and \(2p2h\) configurations. Those which have the highest \(1p1h\) content (around 50\%) may be interpreted as excitations that already exist in the RPA spectrum at higher energies (the first excitations in RPA are located around 11 MeV) and that are shifted down to lower energies due to the coupling with \(2p2h\) configurations. In the SRPA spectrum we also see several states which present a dominant \(2p2h\) nature and show a relatively large \(B(E1)\) despite their very low content of \(1p1h\) configurations (see for instance the energy region around 9 MeV).

In the following we focus our attention to the most collective state located at about 9.09 MeV. In figure 3 we show the transition densities corresponding to this peak. We show separately the

\[48\text{Ca}\]
For each state the $B(E1)$ value corresponding to a cutoff of 60 MeV (upper panel) and the total $1p1h$ contribution $N_1$ to the norm of the state defined in Eq. (3) (lower panel), are shown for $^{48}$Ca.

We see that the neutron transition density dominates over the proton one that is almost vanishing in the external part of the nucleus while in the interior the two densities oscillate out of phase. This leads to a strong mixing of isoscalar and isovector components.

In SRPA as well as in RPA the reduced transition probability for a one-body operator describing the excitation from the ground state to a state $\nu$ can be written as

$$B(E\lambda) = \left| \sum_{ph} b_{ph}(E\lambda) \right|^2 = \left| \sum_{ph} (X_{ph}^{\nu} - Y_{ph}^{\nu}) F_{ph}^{\lambda} \right|^2$$

where $F_{ph}^{\lambda}$ are the multipole transition amplitudes associated to a $1p1h$ configuration. We remark that also in the case of SRPA only $1p1h$ amplitudes appear in the expression of the transition probability.
Table 2. Particle-hole configurations which give the major contributions to the dipole low-lying state located at 9.09 MeV. For each \( ph \) configuration, the energy, the contribution to the norm of the state \( A_{ph} \), the partial contribution to the reduced transition amplitude \( b_{ph} \) (\( \text{e fm} \)) and the matrix element of the transition operator \( F^\lambda_{ph} \) are reported. The superscripts \( \pi \), \( \nu \) refer to proton and neutron states, respectively.

| \( ph \) conf. | \( E \) (MeV) | \( A_{ph} \) | \( b_{ph}(E1) \) | \( F^\lambda_{ph} \) |
|--------------|-------------|------------|----------------|----------------|
| \( (2p_{3/2},1d_{5/2})^\pi \) | 17.499 | 0.002 | -0.039 | 1.343 |
| \( (1f_{7/2},1d_{5/2})^\pi \) | 11.732 | 0.001 | -0.098 | 3.304 |
| \( (1f_{5/2},1d_{5/2})^\pi \) | 19.246 | 0.006 | -0.032 | -0.734 |
| \( (2p_{1/2},2s_{1/2})^\pi \) | 14.133 | 0.005 | 0.045 | -1.233 |
| \( (2p_{3/2},1d_{3/2})^\pi \) | 12.120 | 0.007 | -0.023 | 0.451 |
| \( (2p_{1/2},1d_{3/2})^\pi \) | 13.809 | 0.000 | -0.014 | 1.053 |
| \( (1f_{5/2},1d_{3/2})^\pi \) | 13.867 | 0.017 | 0.197 | 2.756 |
| \( (2p_{3/2},1d_{5/2})^\nu \) | 15.683 | 0.006 | -0.044 | 1.410 |
| \( (2p_{3/2},2s_{1/2})^\nu \) | 11.773 | 0.006 | -0.055 | 1.737 |
| \( (2p_{1/2},2s_{1/2})^\nu \) | 13.556 | 0.001 | -0.015 | -1.248 |
| \( (2p_{3/2},1d_{3/2})^\nu \) | 10.329 | 0.011 | -0.020 | 0.456 |
| \( (2p_{1/2},1d_{3/2})^\nu \) | 12.112 | 0.001 | 0.018 | 1.084 |
| \( (1f_{5/2},1d_{3/2})^\nu \) | 14.072 | 0.009 | 0.105 | 2.675 |
| \( (2d_{5/2},1f_{7/2})^\nu \) | 12.698 | 0.001 | 0.014 | 1.212 |
| \( (1g_{9/2},1f_{7/2})^\nu \) | 11.364 | 0.008 | 0.149 | 4.171 |

In table 2 we report the particle-hole configurations which provide the major contributions to the dipole peak. For each configuration we report the unperturbed energy, the contribution \( A_{ph} \) to the norm of the state, the partial contribution \( b_{ph} \) to the reduced transition amplitude (see Eq. (4)) and the matrix element \( F^\lambda_{ph} \) of the transition operator. By looking at the the partial contribution \( b_{ph} \) to the reduced transitions we can see that strong cancellations of the proton contributions are present while a quite coherent behavior is exhibited by the neutron \( 1p1h \) configurations. In particular, we observe strong contributions coming from the outermost neutrons. This result, together with the profile of the corresponding transition density indicates that this state shows some features usually associated to pygmy resonances.

In table 3 we compare the total \( B(E1) \) and EWSRs integrated up to 10 MeV and the corresponding centroid energies with the experimental values [21] for the \( ^{48}\text{Ca} \). We see that the SRPA total \( B(E1) \) is much larger, almost by a factor 4, than the experimental value. This is due to the larger number of states obtained in SRPA with respect to the experimental spectrum and, at the same time, to their higher strength (figure 4). The same kind of discrepancies is found for the EWSRs while the SRPA centroid energy is very close to the experimental value. Regarding these large differences some comments are in order. First we recall that, because of the non-local terms of the Skyrme interaction, the double commutator sum rule is
Table 3. Total $B(E1)$ and EWSRs integrated up to 10 MeV and corresponding centroid energies obtained in SRPA compared with the experimental values [21] for the $^{48}$Ca isotope.

|                  | $^{48}$Ca |
|------------------|----------|
| $\sum B(E1)$ ($10^{-3} \ e^2 \ fm^2$) | SRPA 230 |
|                  | Exp 68.7 ± 7.5 |
| $\sum E_i B_i (E1)$ ($10^{-3} \ e^2 \ fm^2 \ MeV$) | SRPA 1964 |
|                  | Exp 570 ± 62 |
| $E_{centroid}$ MeV | SRPA 8.54 |
|                  | Exp 8.40 |

Figure 4. Comparison of the experimental $B(E1)$ strength distribution [21] (upper panel) with the SRPA calculations (lower panel) for $^{48}$Ca.

enhanced with respect to the classical sum rule by a factor 1.35 for SGII. However, this is not enough to explain the strong deviation with respect to the experimental values. It could be also interesting to analyze whether or not this kind of discrepancy may depend on the choice of the Skyrme interaction. As a check, we have performed SRPA calculations by using the parametrization SLy4 and the same kind of deviations has been found. In a recent work [24] it has been suggested that the low-lying dipole strength distribution could be be eventually related to the slope of the symmetry energy. This kind of analysis is however beyond our present scopes and it will be performed in future investigations. Finally, we recall that theoretical $B(E1)$ values much larger than the corresponding experimental results have also been found within the ETFFS model for the nucleus $^{44}$Ca; it has been shown that this discrepancy is related to the use of some approximations in the treatment of pairing and continuum coupling [13]. We also mention that in previous experimental measurements a much larger strength had been found in the energy region from 5 to 10 MeV [25]. Finally, as mentioned above, since the low-lying dipole states obtained in SRPA have a strong $2p2h$ nature, it could more appropriate the use of a transition operator containing both one-body and two-body terms. Of course, the use of such a more general operator would affect the total strength associated to this energy region. This investigation is however left as a subject for a future work.
4. Conclusions
In this work, we have analyzed the low-energy dipole spectrum (from 5 to 10 MeV) of the $^{48}\text{Ca}$ isotope in the framework of the Skyrme-SRPA model. The Skyrme interaction SGII is used. The distribution and the fragmentation of the peaks is in reasonable agreement with the corresponding experimental measurements. This kind of results cannot be provided by the standard RPA model: SGII-RPA calculations do not lead to any strength in the energy region from 5 to 10 MeV. However, we have found a $B(E1)$ value integrated up to 10 MeV which is quite larger than the corresponding experimental result.

The inclusion of $2p2h$ configurations and their coupling with the $1p1h$ ones and among themselves within SRPA has a two-fold effect on the low-lying dipole strength. From one side the states that already exist in RPA are shifted to lower energies. These states maintain a quite strong $1p1h$ nature. On the other side several other states of almost pure $2p2h$ character appear. They are excited by the one-body dipole operator through their $1p1h$ components.

A detailed analysis of the most collective peak is done, by looking in particular to the corresponding transition densities. A strong mixing of its isoscalar and isovector components has been found showing thus some features generally associated with a dipole pygmy resonance.

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