



# Isoscalar and isovector giant resonances in a self-consistent phonon coupling approach



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## ARTICLE INFO

### Article history:

Received 11 February 2015

Received in revised form 13 July 2015

Accepted 1 August 2015

Available online 5 August 2015

Editor: J.-P. Blaizot

### Keywords:

Giant resonances

Random-phase approximation

Phonon coupling

## ABSTRACT

We present fully self-consistent calculations of isoscalar giant monopole and quadrupole as well as isovector giant dipole resonances in heavy and light nuclei. The description is based on Skyrme energy-density functionals determining the static Hartree–Fock ground state and the excitation spectra within random-phase approximation (RPA) and RPA extended by including the quasiparticle-phonon coupling at the level of the time-blocking approximation (TBA). All matrix elements were derived consistently from the given energy-density functional and calculated without any approximation. As a new feature in these calculations, the single-particle continuum was included thus avoiding the artificial discretization usually implied in RPA and TBA. The step to include phonon coupling in TBA leads to small, but systematic, down shifts of the centroid energies of the giant resonances. These shifts are similar in size for all Skyrme parametrizations investigated here. After all, we demonstrate that one can find Skyrme parametrizations which deliver a good simultaneous reproduction of all three giant resonances within TBA.

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The method of choice for the description of resonance spectra in many-body systems is the long established random-phase approximation (RPA) [1]. First quantitative modeling for nuclei worked on the basis of shell-model potentials and the Landau–Migdal theory for the residual interaction [2,3] and has since then found widespread applications, for reviews see [4,5]. Almost in parallel, one worked on a fully self-consistent description of nuclear ground-states and RPA excitations. First attempts have been plagued by deficiencies of the early forms of the Skyrme force [6]. Meanwhile, self-consistent nuclear models have been developed much further such that giant resonances can be well described by appropriate choice of the parametrization [7]. However, RPA is confined to one-particle-one-hole ( $1p1h$ ) configurations and it is known that complex configurations play a role for a correct description of damping mechanisms (spreading width) [8]. A convenient way to augment RPA by complex configurations is provided by the phonon coupling model [9–13]. Over the last decade the self-consistent versions of this approach were developed both in relativistic [14] and in non-relativistic [15,16] frameworks. Here we will consider the implementation of the non-relativistic RPA ex-

tended by including the quasiparticle-phonon coupling at the level of the time-blocking approximation (TBA) [17–19]. It was found for the example of the giant dipole resonance (GDR) that the step from RPA to TBA may require a readjustment of the Skyrme parametrization [20]. It is the aim of this letter to put the considerations on a broader basis and to check simultaneously the three most important giant resonances, isovector dipole, isoscalar monopole, and isoscalar quadrupole. We will do that for a further developed TBA which includes full RPA self-consistency and treats the continuum states exactly. The present letter focuses on the physics content. The technical details of this extension will be discussed elsewhere [21].

In a self-consistent approach to nuclei, one defines a density functional, or an effective Lagrangian, with a number of free parameters which are adjusted to ground-state properties as well as to properties of excited states. Such effective theories are able to reproduce in mean field approximation nuclear observables all over the periodic table [22–24] with possible extensions to astrophysical applications [25,26]. Excited states are described at mean field level by RPA (with which we mean throughout the paper a description of excitation on a basis of  $1p1h$  states). One might assume that self-consistent mean-field theories which describe rather well bulk properties of nuclei, such as the Thomas–Reiche-

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Kuhn (TRK) sum rule and the nuclear symmetry energy [27] should have no problem in systematically reproducing the centroid energies of the giant dipole resonance (GDR) as a function of the nucleon number  $A$ . This is not the case, however, as has been discussed in detail in several recent reviews on mean-field theories which include strength functions obtained within the quasiparticle RPA (QRPA) [7,28,29]. It was impossible to describe ground-state properties and the centroid energy of the GDR both in light and heavy nuclei with the same effective interaction.

Recently we have suggested a possible solution for this problem. In [20], we have shown that the explicit inclusion of quasiparticle-phonon coupling within TBA combined with proper readjustment of the Skyrme parametrization may solve the problem of mean-field theories in reproducing the trends of centroid energies of the GDR.

In our first publication on this topic [20], we have investigated only the isovector GDR in these nuclei but not isoscalar resonances. The main topic in this short note concerns the isoscalar monopole (GMR) and quadrupole (GQR) resonances, which we have ignored previously. Here we present briefly the most important results for the GDR, GMR and GQR in  $^{16}\text{O}$ ,  $^{40}\text{Ca}$  and  $^{208}\text{Pb}$ . A more detailed discussion of varied parametrizations and of the details of our new method for handling continuum RPA and TBA (see below) will be included in a forthcoming publication [21].

Our approach is based on the response function formalism developed within the Green function method (see [2,3]). The aim is to compute the strength function  $S_Q(E)$  which represents the distribution of the transitions strengths induced by an external excitation with the single-particle operator  $Q$ . It is defined in terms of the response function  $R(\omega)$  by

$$S_Q(E) = \frac{1}{\pi} \text{Im} \langle Q | R(E + i\Delta) | Q \rangle, \quad (1)$$

where  $E$  is the excitation energy and  $\Delta$  is an artificial width parameter which is taken to be  $\Delta = 400$  keV throughout this paper. This parameter serves two purposes: from a mathematical side, it is introduced to circumvent possible singularities in  $R(\omega)$ , and from a physical side, it mimics some remaining contributions to the spectral spreading not included in the model. (Mind that pure RPA models in discrete representation need  $\Delta = 1\text{--}2$  MeV for that while the TBA model in continuum representation covers already a large deal of the width.) The response function is a solution of the Bethe–Salpeter equation

$$R(\omega) = R^{(0)}(\omega) - R^{(0)}(\omega) (V + W(\omega)) R(\omega), \quad (2)$$

where  $R^{(0)}(\omega)$  is the uncorrelated particle-hole ( $ph$ ) propagator,  $V$  is the amplitude of the static residual  $ph$  interaction, and  $W(\omega)$  is the amplitude of the dynamic interaction that includes coupling to  $1p1h \otimes$  phonon configurations. In RPA, the amplitude  $W$  is omitted. In TBA, both  $V$  and  $W(\omega)$  are included. A detailed description of  $W$  is given in Ref. [30], Eqs. (41), (44)–(46).

In detail, the TBA as a model that incorporates quasiparticle-phonon coupling on top of the ordinary RPA correlations is described in Refs. [17–19]. As TBA accounts for correlation effects in excitations one should also include such correlations in the ground state. This is done, e.g., in the formulation of [17–19], where both dynamic and static ground-state correlations (GSC) induced by  $1p1h \otimes$  phonon configurations are taken into account. Here, we suppose that a dominant fraction of GSC is already incorporated in density functional theory (DFT) and develop RPA about the DFT ground state. It is then necessary for a consistent description to remove that part in the dynamical interaction  $W(\omega)$  which would induce GSC from the  $W$  terms. This is just the static part  $W(\omega = 0)$ . Ground state stability is thus achieved by the subtraction  $W(\omega) \rightarrow W(\omega) - W(0)$  [31]. In the present TBA study, we

apply such a subtraction scheme to the amplitude  $W(\omega)$  in Eq. (2), for details see [30]. The subtraction scheme allows us (i) to avoid double counting in the model based on the energy functional with phenomenologically adjusted parameters, (ii) to ensure stability of solutions of the TBA eigenvalue equations, (iii) to accelerate the convergence in the TBA when the model configuration space is enlarged, and (iv) to keep zero energies of the spurious states in the self-consistent TBA [30,32].

We solve Eq. (2) both in RPA and TBA. In the self-consistent RPA based on DFT the  $ph$  interaction  $V$  is given as second derivative of the energy functional  $E[\rho]$  and the single-particle properties are derived from the self-consistent potential, which is determined by the first derivative of  $E[\rho]$  [33,34]. In what follows we assume that  $E[\rho]$  is the Skyrme energy functional [22]. The input data for the TBA are, as in RPA, the  $ph$  interaction  $V$ , single-particle energies and the corresponding single-particle wave functions. Beyond these one also needs phonons. In our approach, the characteristics of the phonons (excitation energies and transition amplitudes) are calculated within the fully self-consistent RPA. The amplitudes of the quasiparticle-phonon interaction  $g$  are determined as a convolution of the interaction  $V$  with the RPA transition amplitudes (see, e.g., [30]). In agreement with the general equations of the Green-function method [2,35], the interaction  $V$  in this convolution is defined by the same formula (including all the velocity-dependent, spin-orbit, Coulomb and rearrangement terms) as the interaction  $V$  in the RPA equations. Thus, no new parameters for the TBA are introduced. A word is in order for this choice of particle-phonon coupling. Density functionals are usually not designed to derive the particle-phonon interaction (or equivalently a particle-particle interaction). The present identification with the  $ph$  interaction is motivated by an exact representation [2,35]. The application to the effective Skyrme interaction is a working prescription and, we hope, an acceptable approximation.

In our previous calculations [20], we have employed approximations for the matrix elements of the amplitude  $V$ . First, we have neglected the spin-spin, spin-orbit, and Coulomb terms of the interaction. Second, the velocity-dependent exchange terms of  $V$  were included in the local-exchange approximation (LXA) only (see [36]). In the present investigations, we use fully self-consistent scheme and calculate the matrix elements of  $V$  exactly. (Note that the spin-spin terms of  $V$  are omitted as in [20]; this does not break self-consistency because these were not active in the ground state.) For that reason, we had to change the treatment of the continuum. So far we used the method of Shlomo and Bertsch [37] in which Eq. (2) is solved in coordinate space. This method of accounting for the continuum is very efficient in the case of zero-range interactions. However, its implementation in the fully self-consistent RPA calculations in which the residual interaction is deduced from the full Skyrme functionals leads to serious difficulties. These difficulties increase in TBA due to appearance of complex configurations. We thus include the continuum in a step-wise strategy. In a first step, we build the discrete single-particle basis consisting of the eigenfunctions of the Skyrme–Hartree–Fock (SHF) single-particle Hamiltonian satisfying box boundary conditions. This basis forms the  $ph$  space in which all quantities entering Eq. (2) are defined. In a second step, the matrix elements of the amplitudes  $V$  and  $W$  are calculated in this discrete  $ph$  space. In a third step, we calculate the uncorrelated  $ph$  propagator  $R^{(0)}(\omega)$  in coordinate representation following the method [37] which imposes outgoing-wave (continuum) boundary conditions for the mean-field Green functions. In a fourth step we calculate the matrix elements of the thus determined  $R^{(0)}(\omega)$  in the discrete  $ph$  space. By construction, these matrix elements include the continuum. Finally, Eq. (2) is solved in the discrete  $ph$  space. All the calculations presented below were performed with the use of

this scheme, effectively realizing continuum RPA (CRPA) and continuum TBA (CTBA).

In our calculations, the SHF equations were solved by making use of the Numerov method with the radial mesh size  $h = 0.05$  fm (and with decreasing  $h$  at  $r < 1$  fm, see [38]). The box radius was taken to be 15 fm for  $^{16}\text{O}$  and  $^{40}\text{Ca}$  and 18 fm for  $^{208}\text{Pb}$ . The discrete  $ph$  space was restricted by the cutoff energy  $E_{\text{cut}}$  of the single-particle states equal to 100 MeV. In this space, the isovector  $E1$  EWSR in  $^{208}\text{Pb}$  is fulfilled within 0.02% and the spurious dipole mode (SDM) has an energy about 1 MeV and negligible probability  $B(E1) \lesssim 10^{-5} B(E1)_{\text{max}}$ . For the Skyrme parametrization SV-bas (see below) we have checked that the increase of  $E_{\text{cut}}$  up to 1000 MeV brings the SDM energy in  $^{208}\text{Pb}$  down to the value 5.4 keV, but does not change significantly the RPA strength functions in the regime of giant resonances.

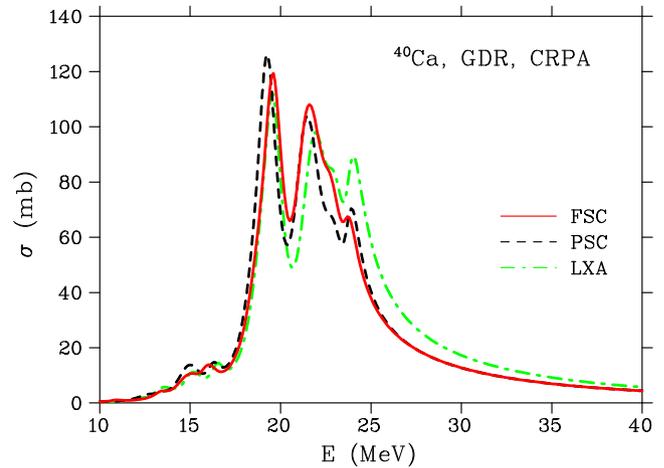
The phonon's basis in the TBA calculations included the solutions of the discrete RPA eigenvalue equation in the neutral channel having natural parity and multipolarities  $L$  in the interval  $0 \leq L \leq 10$ . The maximal energy of the phonons  $E_{\text{max}}^{\text{phon}}$  was taken to be 40 MeV. A crucial criterion for the selection of the phonons was their reduced transition probability  $B(EL)$ : only phonons with  $B(EL)$  greater than 1/5 of the maximal  $B(EL)$  for the given  $L$  were included in the basis. This selects states with some collectivity and reduces the risk of double counting in the present scheme where the Pauli principle is not explicitly enforced in  $2p2h$  space. In particular, for the Skyrme parametrization SV-bas, the so-determined phonon's basis includes 70 phonons for  $^{16}\text{O}$ , 74 phonons for  $^{40}\text{Ca}$ , and 95 phonons for  $^{208}\text{Pb}$ .

It is known that TBA can be plagued by ultraviolet divergences as any beyond-mean-field theories based on the Skyrme energy functionals (see, e.g., [39]). In fact, this problem is avoided in our TBA calculations by virtue of the subtraction method mentioned above. The convergence of TBA with respect to enlarging the phonon basis has been demonstrated in Ref. [32] in the case of the first  $2^+$  and  $3^-$  levels in the nucleus  $^{208}\text{Pb}$ . In the calculations presented here we have checked that the strength functions of the giant resonances have no noticeable differences for  $E_{\text{max}}^{\text{phon}} = 40$  MeV and  $E_{\text{max}}^{\text{phon}} = 20$  MeV in the TBA with subtraction.

In LXA for the exchange terms, one replaces the momentum dependence of the interaction by the magnitude of the momentum near the Fermi level. This could have an especially large effect for Skyrme parametrizations with small effective masses like the ones we used in [20]. To establish a connection with our previous publication, we take the GDR in  $^{40}\text{Ca}$  as test case and compare in Fig. 1 the fully self-consistent CRPA (indicated as FSC) with the partially self-consistent CRPA where spin-orbit and Coulomb terms are neglected (indicated as PSC) and with CRPA at the level of LXA. The Skyrme force which was used has a very low effective mass of  $m^*/m = 0.56$ . Even in this extreme case, the LXA gives reasonable results. Nonetheless, we are going to use here the exact continuum scheme throughout.

The present investigations aim at exploring the effect of phonon coupling under varying conditions. Thus we have picked seven different Skyrme parametrizations which were developed by systematic variation of key properties, five sets from [7] and two from [20]. The parametrizations are characterized by nuclear matter properties (NMP), i.e. equilibrium properties of homogeneous, symmetric nuclear matter, for which we have some intuition from the liquid-drop model [40]. Of particular interest for resonance excitations are the NMP which are related to response to perturbations: incompressibility  $K$  (isoscalar static), effective mass  $m^*/m$  (isoscalar dynamic), symmetry energy  $a_{\text{sym}}$  (isovector static), TRK sum rule enhancement  $\kappa_{\text{TRK}}$  (isovector dynamic).

In Table 1, we list the selection of parametrizations and their NMP. The set SV-bas is the base point of the variation of forces.



**Fig. 1.** (Color online.) Photo absorption cross section for  $^{40}\text{Ca}$ . The fully self-consistent CRPA (solid red line indicated as FSC) is compared with the CRPA where spin-orbit and Coulomb terms are omitted (dashed black line indicated as PSC) and with the CRPA where the exchange terms are calculated in LXA (dash-dotted green line). The results are obtained with the SV-m56k6 [20] parametrization. Smearing parameter  $\Delta = 400$  keV.

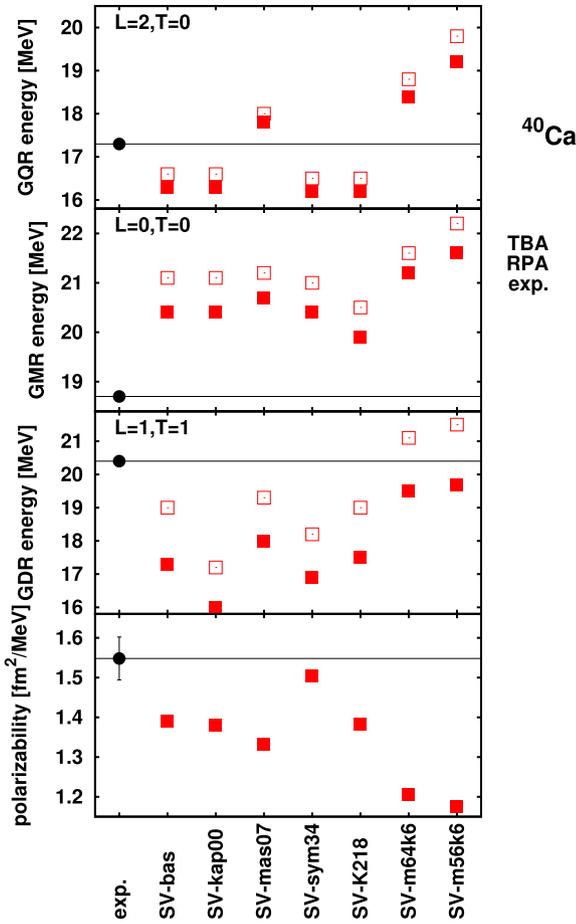
**Table 1**

Nuclear matter properties for the Skyrme parametrizations used in this study: incompressibility  $K$ , isoscalar effective mass  $m^*/m$ , symmetry energy  $a_{\text{sym}}$ , Thomas-Reiche-Kuhn sum rule enhancement  $\kappa_{\text{TRK}}$ . The first five parametrizations stem from [7], the last two from [20].

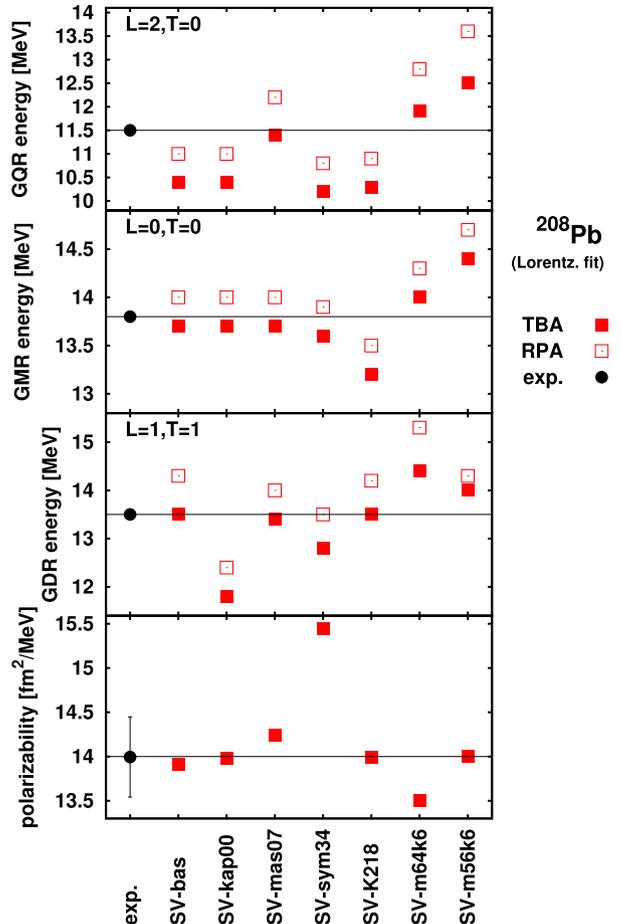
	$K$ [MeV]	$m^*/m$	$a_{\text{sym}}$ [MeV]	$\kappa_{\text{TRK}}$
SV-bas	234	0.90	30	0.4
SV-kap00	234	0.90	30	0.0
SV-mas07	234	0.70	30	0.4
SV-sym34	234	0.90	34	0.4
SV-K218	218	0.90	30	0.4
SV-m64k6	241	0.64	27	0.6
SV-m56k6	255	0.56	27	0.6

Its NMP are chosen such that dipole polarizability and the three most important giant resonances (GMR, GDR, and GQR) in  $^{208}\text{Pb}$  are well reproduced by Skyrme-RPA calculations. Each one of the next four parametrizations vary exactly one NMP while keeping the other three at the SV-bas value. These 1 + 4 parametrizations allow to explore the effect of each NMP separately. The last two parametrizations in Table 1 were developed in [20] with the goal to describe, within TBA, simultaneously the GDR in  $^{16}\text{O}$  and  $^{208}\text{Pb}$ . This required to push up the RPA peak energy which was achieved by low  $a_{\text{sym}}$  in combination with high  $\kappa_{\text{TRK}}$ . To avoid unphysical spectral distributions for the GDR, a very low  $m^*/m$  was used, see [20].

Giant resonances are usually well concentrated modes and can be characterized by their energy centroid. This allows a compact comparison of different parametrizations and nuclei. Figs. 2 and 3 summarize the centroids for the three major giant resonances (giant dipole GDR, isoscalar giant monopole GMR, isoscalar giant quadrupole GQR) in  $^{208}\text{Pb}$  and  $^{40}\text{Ca}$  (upper and middle panels) and the dipole polarizability  $\alpha_D$  (lower panel). Let us briefly recall the trends for RPA (see Ref. [7] for more details). Changing  $\kappa_{\text{TRK}}$  affects almost exclusively the GDR such that lower  $\kappa_{\text{TRK}}$  yields a lower peak position. Changing  $m^*/m$  affects the GQR where lower  $m^*/m$  means higher peak position. Changing  $a_{\text{sym}}$  affects the dipole polarizability  $\alpha_D$  [41] with larger  $a_{\text{sym}}$  enhancing  $\alpha_D$  although we see also a small side effect on  $\alpha_D$  from changing  $m^*/m$ . Changing  $K$  has an impact predominantly on the GMR where lower  $K$



**Fig. 2.** (Color online.) Energies (all in MeV) for GDR, GMR, and GQR, and dipole polarizability for  $^{40}\text{Ca}$  computed with a couple of Skyrme parametrizations as indicated and compared with experimental data. Compared are results from continuum RPA and continuum TBA. The values are energy centroids for GMR and GQR, and peak energies from Lorentzian fit for GDR.



**Fig. 3.** The same as Fig. 2 for  $^{208}\text{Pb}$ .

lowers the peak energy. The combined changes of NMP in the two parametrizations SV-m64k6 and SV-m56k6 affect every mode.

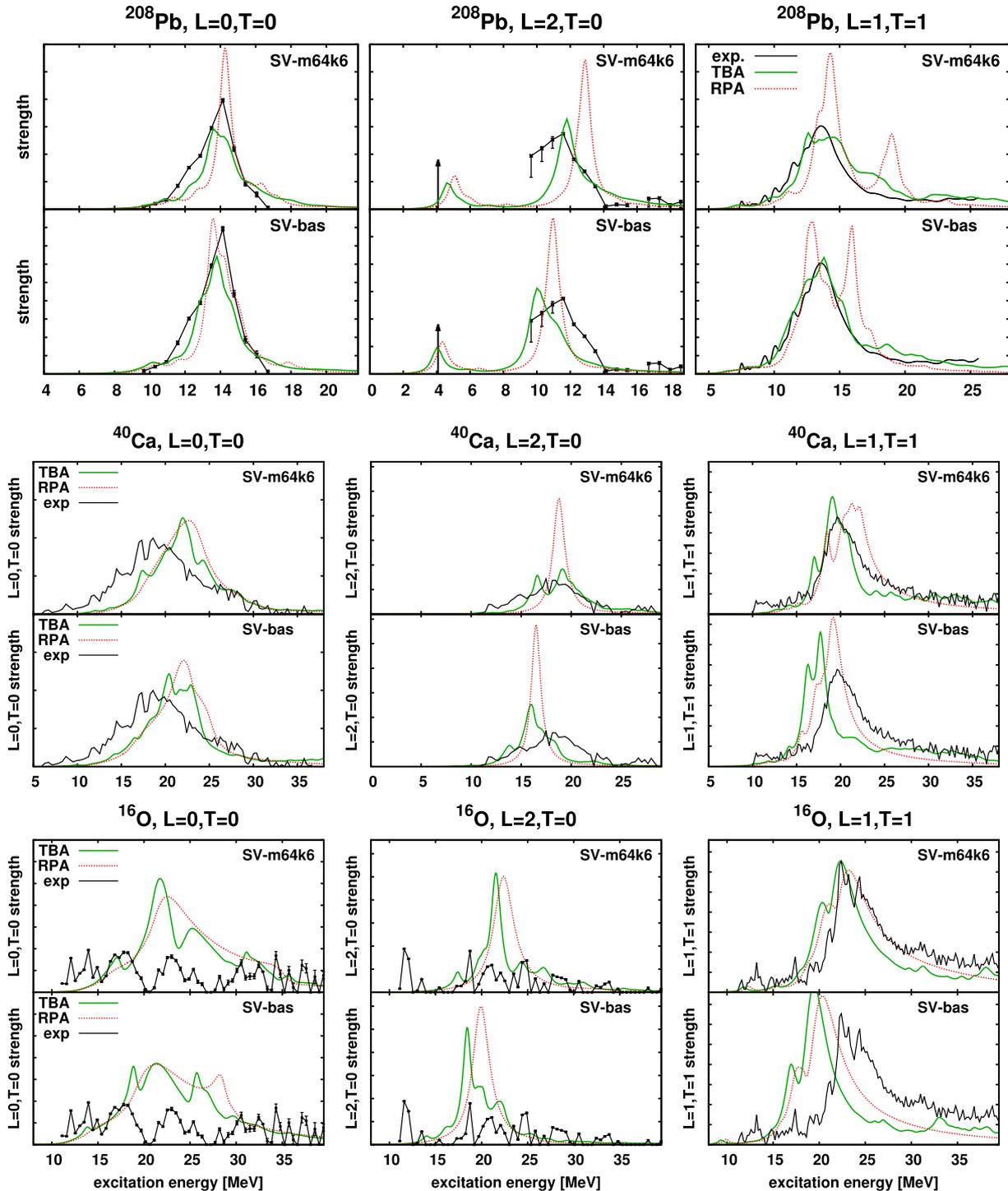
The effect of the phonons (move from open to closed symbols) does not change these trends in general. Detailed effects depend very much on the actual parametrization. Generally, one may say that the quasiparticle-phonon interaction leads to a downshift of the centroid energies. Concerning the GDR, the results for SV-m56k6 basically reproduce those shown in [20] for CRPA. The quantitative effect obtained in CTBA here is somewhat different due to the difference in the improvements of the calculation scheme (see above discussion), though the qualitative effect (decrease of the CTBA mean energies with respect to the CRPA) is the same.

In the upper panel of Fig. 4, we present detailed strength distributions  $S_Q(E)$  for the GDR, GMR and GQR in  $^{208}\text{Pb}$  for SV-bas and SV-m64k6. CTBA works best in heavy nuclei and produces nearly a quantitative agreement with data concerning the magnitude of the cross sections, its widths and (smooth) profiles. In particular for the GDR, TBA manages to smooth the too fragmented structure seen in CRPA. But also for GMR and GQR we recognize the strong reduction of peak height and corresponding broadening of the cross sections due to the phonon coupling. The reason for that efficient smoothing is the high density of levels and of phonons in  $^{208}\text{Pb}$ . It is noteworthy that all three modes, GDR, GMR and GQR, are well reproduced in TBA by the force SV-m64k6. The same is true for GDR and GMR in the case of SV-bas. For the GQR, CTBA

shifts the peak to a slightly too low value. Note that SV-bas was designed to fit the GQR peak within RPA. The phonon coupling in CTBA shifts the GQR centroid downward thus spoiling the former agreement. The GQR is known to be strongly related to the effective mass [42,7]. SV-bas with  $m^*/m = 0.9$  delivered the correct peak while CTBA down-shifts it. SV-m64k6 with CTBA is still a bit too high. Fig. 3 indicates that a better compromise for CTBA may be found at an intermediate mass  $m^*/m \approx 0.7$ . It is a task for future development to further optimize the compromise for CTBA [21].

The situation for isoscalar resonances is different in light nuclei as one can see for  $^{16}\text{O}$  in the lower panel of Fig. 4. The dominant decay channel of the GQR is the  $\alpha$ -decay into the ground state and first excited state of  $^{12}\text{C}$  [43]. In the range between 18–23 MeV the  $\alpha$ -decay width is 90% of the total decay width and between 23–27 MeV 70%. This reaction mechanism is not included in RPA nor in TBA. This is probably the reason why theory overestimates the magnitude of the cross section and does not reproduce the very broad experimental distribution. A theoretical investigation of the  $\alpha$ -decay can be found in Ref. [44]. The visible phonon effect in our continuum approach is weaker than in the discrete calculation in Ref. [11] as the escape width is dominating in the GQR region in the case of  $^{16}\text{O}$ . The theoretical monopole distribution is very broad as no narrow single-particle resonances can contribute. It resembles more the experimental pattern but is probably for the same reason a factor of two too large in the resonance region.

Our theory works better for the GMR and GQR in  $^{40}\text{Ca}$  as shown in the middle panel of Fig. 4. In the case of the GQR, the phonon coupling has a large effect and gives rise to broad resonances in



**Fig. 4.** (Color online.) Detailed spectral strength distributions for  $^{208}\text{Pb}$  (upper),  $^{40}\text{Ca}$  (middle), and  $^{16}\text{O}$  (lower panels) and for the three modes under consideration: isoscalar monopole (left panels), isoscalar quadrupole (middle panels), and isovector dipole (right panels). Photo-absorption cross section is shown in case of the dipole mode. Fractions  $E0$  and  $E2$  EWSR/MeV are shown in the case of the monopole and quadrupole modes. Results are obtained with the SV-bas [45] and SV-m64k6 [20] parametrizations. Compared are strengths from CRPA and CTBA with experimental data. The latter are taken from [46–48] for the GDR and from [49–53] for the GMR and GQR.

agreement with the data. For the same reason as in  $^{208}\text{Pb}$ , the GQR for the force SV-m64k6 is in nice agreement with the strength distribution, whereas for SV-bas the theoretical distribution is placed at slightly too low energies. For the GMR, the phonon effect is small as the dominant particle configurations are still in the continuum. This fact gives rise to a broad distribution which, however, is the same in RPA and TBA. Moreover, the mean energies for both forces deviate from the experimental peak by about two MeV.

The situation is completely different for the GDR. The reason is that the GDR is dominated by the  $1\hbar\omega$  transitions which practically exhaust the TRK-sum rule in heavy and light nuclei, i.e. the continuum states are less important. For the force SV-m64k6 the GDR in all three nuclei is well reproduced. But this force was designed for this situation [20]. The force SV-bas shows the well known effect: if the GDR in  $^{208}\text{Pb}$  is reproduced, it is in  $^{16}\text{O}$  by few MeV too low.

To summarize: We present results for isoscalar and isovector giant resonances in light and heavy mass nuclei obtained within the fully self-consistent RPA and the RPA extended by including the quasiparticle-phonon coupling. A new method for treating the single-particle continuum was developed and applied in these calculations. For one of the Skyrme parametrizations which were specifically adjusted to reproduce the GDR in  $^{208}\text{Pb}$  and  $^{16}\text{O}$  [20], we obtain also good results for the isoscalar resonances in  $^{208}\text{Pb}$  and  $^{40}\text{Ca}$ . The results for  $^{16}\text{O}$  are not satisfying and we discuss the origin of this mismatch.

### Acknowledgements

The authors thank S.P. Kameronzhiev for fruitful discussions. This work was supported by the Deutsche Forschungsgemeinschaft (grant RE322-13/1). N.L. and V.T. acknowledge Saint Petersburg State University for a research grant 11.38.648.2013. We thank Dave Youngblood for providing us with the experimental data of the isoscalar giant resonances.

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