Optimizing phonon space in the phonon-coupling model

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We present a new scheme to select the most relevant phonons in the phonon-coupling model, named here time-blocking approximation (TBA). The new criterion, based on the phonon-nucleon coupling strengths rather than on $B(EL)$ values, is more selective and thus produces much smaller phonon spaces in TBA. This is beneficial in two respects: first, it curbs down the computational cost, and second, it reduces the danger of double counting in the expansion basis of TBA. We use here TBA in a form where the coupling strength is regularized to keep the given Hartree-Fock ground state stable. The scheme is implemented in an RPA and TBA code based on the Skyrme energy functional. We first explore carefully the cutoff dependence with the new criterion and can work out a natural (optimal) cutoff parameter. Then we use the freshly developed and tested scheme to a survey of giant resonances and low-lying collective states in six doubly magic nuclei looking also on the dependence of the results when varying the Skyrme parametrization.

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I. INTRODUCTION

The most often applied approach to collective phenomena in nuclear physics is the random phase approximation (RPA) [1]. It provides a reliable description of the spectral distribution of multipole excitations from low energy collective states to the giant resonance region. If one includes the single-particle (sp) continuum we end up with the continuum RPA [2] which allows to calculate the escape width of giant resonances. In medium and heavy mass nuclei the experimental width however is dominated by the spreading width which involves higher order effects. These may be explicitly two-particle two-hole correlations [3] or the coupling to phonons which also give rise to a broadening [4] of the strength. The most complete formulation of the quasiparticle-phonon coupling has been developed in Ref. [9] which is the basis of the present investigation. This approach is called quasiparticle time blocking approximation (TBA). As input one needs sp energies, sp wavefunctions and a particle-hole (ph) force. Here we have to distinguished two different approaches. In the first case the sp quantities are taken from a shell model which parameters are adjusted to the experimental sp energies. The ph force is, e.g., modeled as zero-range, density dependent interaction and the corresponding parameters are adjusted to appropriate nuclear structure properties (Refs. [10, 11]). In the second case, one starts from an effective Lagrangian or Hamiltonian which allows a fully self-consistent description of nuclear ground state and subsequent dynamics, see Ref. [12] and references therein. Both approaches can equally well be complemented by TBA to account for complex configuration.

As compared to other treatments of complex configurations (e.g. second RPA [13]), the phonon-coupling method (i.e. TBA) is particularly efficient by confining the complex configurations to a well manageable amount of phonons. Thus the key task of TBA is to select properly the most relevant phonons (i.e. RPA modes). It is obvious that we should chose those phonons which incorporate a large amount of the interaction. These are the collective phonons which consist of a coherent superposition of many ph states. Besides delivering the strongest contributions, using collective phonons is not so much plagued by double counting as predominantly sp excitations do. In the present paper we present a new method of selecting the phonon space for TBA which is applicable to light and heavy nuclei. This method is presented in section II and compared with previously used selection criteria.

As a preview, figure 1 illustrates the effect of TBA and the impact of phonon space for the example of isovector dipole strength in $^{208}$Pb (details of the method will be explained later). The RPA result resides correctly in the region of the giant dipole resonance (GDR), but has a marked double-peak structure which is at variance with data. The spreading width described with TBA dissolves the upper peak through substantial broadening and so recovers nicely the experimental one-peak structure. TBA results are shown for three different choices of phonon space. Formerly, we used the $B(EL)$ strength as measure of collectivity taking into account only phonons above a certain cutoff value. The curve

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FIG. 1. (Color online) The giant dipole resonance in $^{208}$Pb calculated using RPA (red solid line) and the TBA with different selection criteria for phonons: $B$-criterion with $b_{\text{cut}} = 0.2$ (green solid line) and $V/E$-criterion with $v_{\text{min}} = 0.1$ (black dashed line) and $v_{\text{min}} = 0.01$ (black dotted line). The Skyrme parametrization SV-bas was used. Details of the methods and numerical parameters are described in Sec. I. Experimental data from [13].

marked $b_{\text{cut}} = 0.2$ stems from this old recipe. In this paper, we will present a new and more selective criterion relying on the phonon-nucleon coupling. We denote this method the $V/E$-criterion and the corresponding cutoff parameter $v_{\text{min}}$. The curve $v_{\text{min}} = 0.1$ yields practically the same results as previously, however, employing much less phonons. The dependence on cutoff is indicated with the curve $v_{\text{min}} = 0.01$ which makes a slight difference as compared to $v_{\text{min}} = 0.1$. In the following, we will discuss in detail the optimal choice of the cutoff parameter.

Section II starts in subsection II A with a brief summary of RPA, in subsection II B of TBA, and explains in subsection II C the criteria for selecting the space of most relevant phonons. The latter subsection is decisive as it provides the formal basis for the new selection criterion from which we show later on that it is more efficient than previous choices. Section III present details of the practical treatment, the continuum-response formalism in subsection III A numerical aspects in subsection III B and the actual nuclear mean field related to the Skyrme energy-density functional in subsection III C Section IV addresses the central question, namely the dependence of the TBA results on the selection of phonons. In subsection A the previously used $B$-criterion which relies on the magnitude of the $B(E1)$ values is compared with the new $V/E$-criterion and in subsection B we discuss the dependence on the new cutoff parameter $v_{\text{min}}$. Here we demonstrate in several figures that this new selection criterion gives rise to a plateau in nearly all cases. Surprisingly also the energies of the low-lying collective $3^-$ resonances, which are the most sensitive quantities in this respect, depend only smoothly on the new parameter. This is connected with the stability conditions [15] introduced into the TBA approach. In Section V we present our results for the giant multipole resonances, giant monopole resonance (GMR), GDR and giant quadrupole resonance (GQR) for light, medium and heavy mass nuclei. Three Skyrme parameter sets were used with different effective masses. In Section VI, the excitation energies and transition probabilities for the low-lying collective $3^-$ and $2^+$ states are compared with the experimental values. In both cases, the influence of the phonons is discussed. Finally in Section VII we summarize the paper and give an outlook on further improvements.

II. NEW CRITERION FOR THE SELECTION OF THE PHONONS

A. Summary of RPA

The RPA modes $n$ are characterized by the energies $\omega_n$ and transition amplitudes $z_n^{12}$ which describe the composition of $n$ from the $ph$ and $hp$ states. These are determined by the eigenvalue equation

$$\sum_{34} \Omega_{12,34}^{RPA} z_n^{34} = \omega_n z_n^{12},$$

where

$$\Omega_{12,34}^{RPA} = \Omega_{12,34}^{(0)} + \sum_{56} M_{12,56}^{RPA} V_{56,34},$$

$$\Omega_{12,34}^{(0)} = h_{13} \delta_{42} - h_{13} \delta_{42},$$

$$M_{12,34}^{RPA} = \delta_{13} \rho_{42} - \delta_{13} \delta_{42},$$

$\rho$ is the single-particle density matrix, $h$ is the single-particle Hamiltonian, and $V$ is the amplitude of the residual interaction. In symbolic notation, Eqs. 1 and 2 read

$$\Omega^{RPA} | z^n > = \omega_n | z^n > ,$$

$$\Omega^{RPA} = \Omega^{(0)} + M^{RPA} V .$$

The transition amplitudes $| z^n >$ are normalized to

$$\langle z^n | M^{RPA} | z^{n'} > = \text{sgn}(\omega_n) \delta_{n,n'} .$$

We will suppose that the RPA is self-consistent (though this is not essential for the subsequent formulas), i.e. that the following relations are fulfilled:

$$h_{12} = \frac{\delta E[\rho]}{\delta \rho_{21}},$$

$$V_{12,34} = \frac{\delta^2 E[\rho]}{\delta \rho_{21} \delta \rho_{34}},$$

where $E[\rho]$ is an energy density functional. In the basis diagonalizing the operators $h$ and $\rho$ we have:

$$h_{12} = \varepsilon_1 \delta_{12},$$

$$\rho_{12} = n_1 \delta_{12} .$$
where \( n_1 = 0, 1 \) is the occupation number. In what follows the indices \( p \) and \( h \) will be used to label the single-particle states of the particles \( (n_p = 0) \) and holes \( (n_h = 1) \) in this basis.

### B. Summary of TBA

In TBA, Eq. \[1\] takes the form

\[
\sum_{34} \Omega_{12,34}^{\mathrm{TBA}}(\omega_p) z_{34}^p = \omega_p z_{12}^1,
\]

where

\[
\Omega_{12,34}^{\mathrm{TBA}}(\omega) = \Omega_{12,34}^{\mathrm{RPA}} + \sum_{56} M_{12,56}^{\mathrm{RPA}} W_{56,34}(\omega),
\]

\[
W_{12,34}(\omega) = W_{12,34}(\omega) - W_{12,34}(0).
\]

The matrix \( W(\omega) \) in \[11\] and \[12\] represents the induced interaction and is defined in the \( ph \) subspace as

\[
W_{12,34}(\omega) = \sum_{c, \sigma} \sigma F_{12}^{c(\sigma)} F_{34}^{c(\sigma)*} \left( \omega - \sigma \Omega_c \right),
\]

where \( \sigma = \pm 1 \), \( c = \{ p', h', n \} \) is an index of the subspace of \( ph \otimes \text{phonon} \) configurations, \( n \) is the phonon’s index,

\[
\Omega_c = \varepsilon_{p'} - \varepsilon_{h'} + \omega_n, \quad \omega_n > 0,
\]

\[
F_{12}^{c(-)} = F_{21}^{c(+)*}, \quad F_{ph}^{c(-)} = F_{hp}^{c(+)} = 0,
\]

\[
g_{12}^{n} = \delta_{p'p} g_{n}^{n} - \delta_{h'h} g_{n}^{n},
\]

\[
g_{12}^{n} = \sum_{34} V_{12,34} z_{34}^{n}.
\]

It is important to note the subtraction of the zero-frequency interaction in the induced interaction \( W(\omega) \). This serves to confine the induced interaction only to dynamical excitations while the ground state remains unaffected \[16\]. Moreover, this solves part of the double counting problem and recovers the stability condition (see \[15\]).

### C. Selection of most relevant phonons

In the self-consistent TBA, in which the relations \[8\] are fulfilled, we formally have no free parameters in addition to the parameters of the energy density functional. Nevertheless, there is the question of what number and what kind of phonons should be included in the \( ph \otimes \text{phonon} \) space of the model. This question concerns the problem of convergence with respect to enlarging the \( ph \otimes \text{phonon} \) subspace. So, it is important to select a small amount of phonons producing the strongest coupling between the \( ph \) and \( ph \otimes \text{phonon} \) configurations. Moreover, including only sufficiently collective phonons minimizes violation of the Pauli principle and reduces the problem of double counting connected to the second-order contributions. However, the quest of a well-justified and clear criterion of collectivity is still matter of debate.

For example, the values of the contributions of the separate \( ph \) components (first of all, the main component) of the RPA transition amplitude \( z_n^m \), for a positive frequency state, \( \omega_n > 0 \), into the norm \[7\] can be chosen as this criterion (see, e.g., Refs. \[17\] \[18\]). This is quantified by the quantity \( \xi_n^2 \)

\[
\xi_n^2 = \max_{\ell \in \{ph\}} \sum_{m_p, m_h} \left( |z_n^{p,\ell}|^2 - |z_n^{h,\ell}|^2 \right),
\]

where \( m_p \) and \( m_h \) are the projections of the total angular momentum of the particles and holes, \( (ph) \) denotes the set of the remaining single-particle quantum numbers. For the non-collective phonons the value of \( \xi_n^2 \) should be close to 1. The maximum value of \( \xi_n^2 \) for the collective phonons \( (\xi_{n,\max}^2) \) lies typically in the interval 0.5-0.6 \[17\]. This method estimates the spread of the RPA state over the \( 1p1h \) configurations, but it does not introduce any energy cutoff of the phonon’s basis that would be desirable to limit the phonon subspace. In addition, this criterion does not give information about the magnitude of the particle-phonon coupling for the selected phonons.

Frequently, also in our earlier work, the probability criterion is used in which the phonons are selected according to the values of the reduced probability of the electric transition \( B(EL) \) calculated with the transition amplitude \( |z_n^m| \) of the phonon (see, e.g., \[10\] \[12\] \[19\]). This means that only phonons with \( B(EL)/B(EL)_{\max} > \beta_{\text{cut}} \) are included in the phonon basis, where \( B(EL)_{\max} \) is the maximal \( B(EL) \) for the given multipolarity \( L \). \( \beta_{\text{cut}} \) is the cutoff parameter typically ranging from 1/10 to 1/5. In Ref. \[19\] this criterion is formulated in terms of the phonon’s contribution to the energy weighted sum rule (EWSR). This integral method of the selection of the phonons (we will refer to it as the \( B \)-criterion) is based on the assumption that the excitation modes having the largest transition probabilities are the most collective ones and should have the strongest coupling to the single-particle states (see discussion at the end of this section). However, the connection of the \( B \)-criterion to collectivity is, in fact, not so obvious.

Here we suggest another method in which the connection to collectivity and interaction strength becomes more explicit. Let us introduce the average interaction strength in mode \( n \) and average \( ph \) energy as

\[
\langle V \rangle_n = \langle z_n^m | V | z_n^m \rangle,
\]

\[
|\omega_n^{(0)}| = \langle z_n^m | M_{\mathrm{RPA}} \Omega^{(0)} | z_n^m \rangle.
\]
In terms of the basis \( \{ |n\rangle \) we have:

\[
|\omega_n^{(0)}\rangle = \sum_{ph} (\varepsilon_p - \varepsilon_h)(|z_{pn}^n|^2 + |z_{hp}^n|^2).
\] (21)

From Eqs. (3) and (7) we obtain

\[
\langle z^n | M^{\text{RPA}} \Omega^{\text{RPA}} | z^n \rangle = |\omega_n|.
\] (22)

From Eqs. (6), (19), (20), (22) and from the property \((M^{\text{RPA}})^2 = 1 \) in the \(ph\) space it follows that

\[
\langle V \rangle_n = |\omega_n| - |\omega_n^{(0)}|.
\] (23)

As follows from Eq. (19), the quantity \( \langle V \rangle_n \) represents the average value of the residual interaction in the RPA state \( |z^n\rangle \). The values of \( \langle V \rangle_n \) can be easily calculated using Eqs. (21) and (23) if the solutions of the RPA equation are known.

The new criterion for selection of phonons (positive frequency: \( \omega_n > 0 \)) is

\[
|v_n| > v_{\text{min}} \quad v_n = \langle V \rangle_n / \omega_n.
\] (24)

This means that only those phonons will be included in the TBA basis whose dimensionless interaction strength \( v_n \) exceeds the cutoff value \( v_{\text{min}} \). Note that the negative (positive) sign of \( v_n \) indicates that the residual interaction in the state \( |z^n\rangle \) has on average attractive (repulsive) character. We call this selection the \( V/E \)-criterion in the following.

There are several arguments to justify the \( V/E \)-criterion. First, from Eqs. (17) and (19) we obtain

\[
\langle V \rangle_n = \langle z^n | g^n \rangle.
\] (25)

In the macroscopic approach (see, e.g., Refs. 26, 27) both the transition amplitudes \( z_{12}^n \) and the amplitudes \( g_{12}^n \) are proportional to the dimensionless deformation amplitudes \( \beta_n \) of the respective vibrational modes. So, in this approach \( |v_n| \propto \beta_n^2 \). Therefore, the selection of the phonons with the largest values of \( |v_n| \) corresponds to the selection of the low-energy vibrational modes with the largest deformation amplitudes having thus the strongest coupling to the single-particle states.

Second, we take the point of view that \( |v_n| \) is a measure of collectivity. Large values make a large (collective) shift of energy as shown by Eq. (23). Small values correspond to uncorrelated (non-collective) RPA modes which are dominated by what is called a one-loop diagram. But just such uncorrelated RPA modes taken as the phonons produce the second-order contributions in the response function of the TBA which should be eliminated to avoid double counting.

Third, the \( V/E \)-criterion seems to be preferable as compared with the \( B \)-criterion because it requires no additional assumptions. Note that the \( B \)-criterion relies on \( B(EL) \) values which refer to an external multipole operator and it requires additional cutoff value \( L_\text{max} \) and multipolarity whereas the \( V/E \)-criterion is the same for all the multipoarities and automatically eliminates all states with too large values of \( L \).

Nevertheless, it is interesting to establish a connection between the \( V/E \)- and \( B \)-criterion. Consider a residual interaction \( V \) in a separable form as a multipole decomposition (see, e.g., [3])

\[
V = \sum_{\alpha,L,M} \kappa_{\alpha L M}^2 |Q_{\alpha L M}^n\rangle \langle Q_{\alpha L M}^n|,
\] (26)

where \( Q_{\alpha L M}^n \) are the multipole operators, index \( \alpha \) labels different kinds of these operators (electric, magnetic, isoscalar, isovector, etc.), \( \kappa_{\alpha L M}^2 \) are the force parameters. If the same \( Q_{\alpha L M}^n \) is taken as the multipole operator for the \( B(EL) \) value, the respective reduced probability in the RPA reads

\[
B_n(\alpha L_n) = \sum_{M_n} |\langle z^n | Q_{\alpha L_n M_n}^n\rangle|^2.
\] (27)

From Eqs. (19), (26) and (27) we obtain

\[
\langle V \rangle_n = \sum_{\alpha} \frac{\kappa_{\alpha}^2}{2L_n + 1} B_n(\alpha L_n).
\] (28)

Thus the \( B(EL) \) values are indeed strongly related to the average interaction strength \( \langle V \rangle_n \). There are, however, different weight factors which impact the criteria. The \( V/E \)-criterion employs a weight \( \kappa_{\alpha}^2 \) while the \( B \)-criterion is weighted with \( B(EL)_{\text{max}} \). Different weights create different selectivity and we have yet to see how the two criteria compare in practice. Realistic residual interactions are not strictly separable, but are found often rather close to a sum of separable terms. Thus the above relation maintains some general relevance.

## III. DETAILS OF CALCULATIONS

### A. Basic Equations

Our approach is based on the version of the response function formalism developed within the Green function method (see [24, 25]). Details are described in [12, 26]. The basic calculated quantity is the response \( R(\omega) \) which is a solution of the Bethe-Salpeter equation. In RPA and TBA, it reads

\[
R^{\text{RPA}}(\omega) = R^{(0)}(\omega) - R^{(0)}(\omega) V R^{\text{RPA}}(\omega),
\] (29)

\[
R^{\text{TBA}}(\omega) = R^{(0)}(\omega) - R^{(0)}(\omega)(V + \tilde{W}(\omega)) R^{\text{TBA}}(\omega),
\] (30)

where

\[
R^{(0)}(\omega) = - (\omega - \Omega^{(0)})^{-1} M^{\text{RPA}}
\] (31)
is the uncorrelated \( ph \) propagator. The \( ph \)-interaction \( V \) is defined in Eq. \( [8] \) and the induced interaction \( W(\omega) \) in Eqs. \( [12,13] \).

Knowledge of the response function allows us to calculate the distribution of the nuclear transition strength \( S(E) \) caused by an external field which is represented by a single-particle operator \( Q \). It reads

\[
S(E) = -\frac{1}{\pi} \text{Im} \Pi(E + i\Delta), \tag{32}
\]

\[
\Pi(\omega) = -\langle Q | R(\omega) | Q \rangle, \tag{33}
\]

where \( E \) is an excitation energy, \( \Delta \) is a smearing parameter, and \( \Pi(\omega) \) is the (dynamic) polarizability.

### B. Details of the numerical treatment

The two approaches studied here, RPA and TBA, are realized with the same numerical representation. The \( sp \) energies, \( sp \) wavefunctions, and the residual \( ph \) interaction are obtained from stationary Skyrme-Hartree-Fock (SHF) calculations based on the Skyrme energy functional. All terms of the residual interaction are treated in the RPA and TBA fully self-consistently, according to the formulas given in Ref. \[27\], but with one exception: the spin-spin terms are omitted. This does not break self-consistency because the terms are not active in the ground state of the double-magic nuclei. The new treatment of the single-particle continuum \[12\] is used both in the RPA and TBA calculations. There, the RPA and the TBA equations are solved in a discrete basis that simplifies calculations of matrix elements of the residual interaction. However, the uncorrelated \( ph \) propagator \( R^{(0)}(\omega) \) is constructed with Green functions properly taking into account the nucleon continuum. Therefore the uncorrelated as well as the correlated propagators do not contain discrete poles at positive energies but a smooth cut.

The box sizes were 15 fm for \(^{16}\text{O}, 40,48\text{Ca} \) and 18 fm for \(^{56}\text{Ni}, 132\text{Sn}, 208\text{Pb} \). The maximal angular momentum of the \( sp \) basis was limited to \( l_{\text{max}}^{\text{sp}} = 17 \) which was found by several tests to be a sufficiently large value. We checked the dependence of the results on the maximum s.p. energy \( \varepsilon_{\text{sp}}^{\text{max}} \). For light \(^{16}\text{O} \) and medium mass nuclei \((\text{Ca and Ni}) \) we found saturation at \( \varepsilon_{\text{sp}}^{\text{max}} = 500 \text{ MeV} \), and for heavy nuclei \(^{132}\text{Sn} \) and \(^{208}\text{Pb} \) at \( \varepsilon_{\text{sp}}^{\text{max}} = 100 \text{ MeV} \). The maximal \( sp \) energies were thus set as: \( \varepsilon_{\text{sp}}^{\text{max}} = 500 \text{ MeV} \) for \(^{16}\text{O}, 40,48\text{Ca}, 56\text{Ni} \) and \( \varepsilon_{\text{sp}}^{\text{max}} = 100 \text{ MeV} \) for \(^{132}\text{Sn} \) and \(^{208}\text{Pb} \). The phonon basis is restricted by the cutoff \( \varepsilon_{\text{min}} \), or \( B(EL) \) respectively, and the dependence on the cutoff will be studied in section \[IV \]. The maximal phonon energy is \( E_{\text{max}}^{\text{ph}} = 40 \text{ MeV} \). The maximal phonon angular momentum \( L_{\text{max}}^{\text{ph}} \) is determined by these conditions. The maximal angular momentum of the quasiparticle-phonon configurations is \( L_{\text{max}}^{\text{ph}} = 27 \). In the following, we keep these parameters of representation \((sp \text{ space, maximum phonon energy, and maximum angular momentum}) \) fixed at rather large values because we want to concentrate on the trends with the phonon cutoff \( \varepsilon_{\text{min}} \), or \( B(EL) \) respectively. The question of convergence with these parameters of representation and possible saving at this site will spared for a forthcoming publication.

Each resonance positions were characterized by the energy centroid defined as the ratio \( E_0 = m_1/m_0 \) of the first and zeroth energy moments of the corresponding strength \( S(E) \). For the GDR (here we considered the photo absorption cross section) as well as for the GMR and GQR in \(^{132}\text{Sn}, 208\text{Pb} \) (here we considered the fraction of the EWSR), the centroids were calculated in the energy windows \( E_0 \pm 2\delta \) where \( \delta \) was the spectral dispersion. To avoid too small energy windows, we used the constraint \( \delta > \delta_{\text{min}} \) where \( \delta_{\text{min}} = 2.5 \text{ MeV} \) for the GDR in \(^{16}\text{O} \), 2 MeV for the GDR in \(^{40,48}\text{Ca}, 132\text{Sn}, 208\text{Pb} \) and for all resonances in \(^{56}\text{Ni} \), 0.5 MeV for the GMR and GQR in \(^{132}\text{Sn}, 208\text{Pb} \). The width \( \Gamma \) and dispersion for these resonances were defined as

\[
\Gamma = 2\delta \sqrt{2\ln 2}, \quad \delta = \frac{\int (E - E_0)^2 S(E) dE}{m_0} \tag{34}
\]

These \( E_0 \) and \( \Gamma \) are approximate values of the Lorentzian parameters.

The isoscalar strengths in light nuclei are distributed in large energy ranges and have a complex structure therefore for these strengths we used the large windows: \( 11 < E < 40 \text{ MeV} \) for GMR and GQR in \(^{16}\text{O} \), \( 10 < E < 30 \text{ MeV} \) for GMR in \(^{40,48}\text{Ca} \), and \( 10 < E < 25 \text{ MeV} \) for GQR in \(^{40,48}\text{Ca} \). The peak position of the low-lying dipole strength in \(^{132}\text{Sn} \) was determined as the energy with the maximum cross section. The resonance widths \( \Gamma \) depend slightly on the smearing parameter \( \Delta \). In all the RPA and TBA calculations, we used in Eq. \[32\] \( \Delta = 400 \text{ keV} \). It is questionable to represent the broad and strongly fragmented spectral distribution in \(^{16}\text{O} \) by only two numbers (peak energy, width). But it suffices for the purpose of comparison because we handle the experimental data the same way.

### C. Choice of Skyrme Parametrization

From the variety of self-consistent nuclear mean-field models \[28\], we consider here the Skyrme-Hartree-Fock (SHF) functional, for a detailed description see \[28,30\]. It's essential features are: The functional depends on a couple of local densities and currents (density \( \rho \), gradient of density \( \nabla \rho \), kinetic-energy density \( \tau \), spin-orbit density \( J \), current \( j \), spin density \( \sigma \), kinetic spin-density \( T \)). All densities and currents exist twofold, for isospin zero and isospin one. It consists of quadratic combinations of these local quantities, corresponding to pairwise contact interactions. In principle, all parameters in front of these contact terms could be density dependent. In practice, density dependence is considered only for the term \( \propto \rho^2 \) (both isospins). Pairing is incorporated by
TABLE I. Nuclear matter properties (NMP) for the three Skyrme forces used here: incompressibility \( K \), isoscalar effective mass \( m*/m \), symmetry energy \( a_{\text{sym}} \), Thomas-Reiche- Kuhn sum rule enhancement \( \kappa_{\text{TRK}} \). Parametrizations SV-bas, and SV-mas07 [32], SV-m64k6 from [33].

| NMP   | \( K \) [MeV] | \( m*/m \) | \( a_{\text{sym}} \) [MeV] | \( \kappa_{\text{TRK}} \) |
|-------|---------------|-----------|------------------|------------|
| SV-bas| 234           | 0.90      | 30               | 0.4        |
| SV-mas07 | 234         | 0.70      | 30               | 0.4        |
| SV-m64k6 | 241         | 0.64      | 27               | 0.6        |

Adding a separate pairing functional. The typically 13–14 model parameters are considered as being universal parameters applying throughout the whole nuclear landscape and bulk matter. They are determined by a fit to a large body of experimental data of the nuclear ground state (binding energies, radii, spin–orbit splittings, pairing gaps). For recent examples see [31,33].

Nuclei span a large range in mass number, but a small one in neutron-proton difference. Their ground states are stationary states. This means that the ground state fits determine predominantly isoscalar static properties and leave some leeway in other respects. Thus there exist many Skyrme parametrizations which perform comparably well in ground state properties but differ in the less well determined aspects amongst them many response properties, equivalent to nuclear matter properties (NMP). As a consequence, a study using Skyrme forces should employ a couple of different parametrizations to explore the possible variety of predictions. To quantify the variation, we consider the key response properties of the forces in terms of NMP, i.e. equilibrium properties of symmetric nuclear matter, namely 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). These four NMP have a one-to-one relation to nuclear giant resonances in \(^{208}\text{Pb} \) [22]: \( K \) to GMR, \( m*/m \) to GQR, \( \kappa_{\text{TRK}} \) to GDR, and \( a_{\text{sym}} \) to dipole polarizability [34]. In order to allow well defined explorations, the survey [32] provides a series of Skyrme parametrizations with systematically varied NMP. The present survey aims at exploring the effect of phonon coupling on excitation properties. Here, the response properties are crucial and we take a minimal subset of these systematically varied parametrizations to discriminate robust features from changing ones. Table I lists the chosen parametrizations and their NMP. SV-bas is the base point of the variation of forces. 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 RPA calculations. SV-mas07 varies the effective mass while keeping the other NMP fixed. SV-m64k6 was developed in [35] 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 in \(^{208}\text{Pb} \) which was achieved by low \( a_{\text{sym}} \) in combination with high \( \kappa_{\text{TRK}} \). To avoid unphysical spectral bunching for the GDR, a low \( m*/m \) was used.

IV. DEPENDENCIES

In this section, we investigate the dependence of mean energy and width of giant resonances on the cutoff parameter for the phonon space as was introduced in Section II. Recall, that the crucial ingredient in the phonon-coupling model is the number of active phonons. As already discussed in Section II, we propose as selector the parameter \( v_{\text{min}} \) which is connected with the collectivity of the phonons. Large \( v_{\text{min}} \) exclude automatically phonons which are dominated by one or two \( ph \) components only.

A. Comparing \( B \)-criterion with \( V/E \)-criterion

Fig. 2 compares mean energies of GR (lower panel) and number of active phonons (upper panel) as function of the cutoff parameters \( v_{\text{min}} \) and \( b_{\text{cut}}/5 \). As one can see, the two criteria give very similar results for the GR energies (lower panel) when scaling \( b_{\text{cut}} \) by factor 1/5. However, the number of phonons (upper panel) is much different. The \( V/E \)-criterion achieves the same GR peak energies with substantially less phonons. This indicates that the \( V/E \)-criterion is more efficient in selecting the relevant phonons.

B. Dependence on the cutoff \( v_{\text{min}} \)

The distribution of relative strength of the phonon’s states \( |v_n| \) defined by Eq. (24) in \(^{208}\text{Pb} \) is shown in Fig. 3. The calculations were performed in the discrete self-consistent RPA for the Skyrme parametrization SV-m64k6 [34] with \( \varepsilon_{\text{max}} = 500 \text{ MeV} \). For the most collective low-lying vibrational states in \(^{208}\text{Pb} \) (first \( 2^+ \), \( 3^- \), \( 4^+ \), \( 5^- \), and \( 6^+ \) levels), \( v_n \) takes the values in the interval from \(-4.0 \) for the \( 3^- \) state up to \(-0.3 \) for the \( 6^+ \) state. The distribution in Fig. 3 representing \( V/E \)-criterion shows a clear distinction between collective phonons, which stick out well above background indicated by the dashed horizontal line, and the non-collective ones below this line. This suggests that a cutoff at \( v_{\text{min}} = 0.05 \) is an optimal choice.

The increase of collective states above \( \omega_{\text{phon}} = 50 \text{ MeV} \) is an artifact of the Skyrme force. This does not appear if we perform calculations with a Migdal \( ph \)-interaction which possesses no momentum dependence. We have produced similar scatter plots for other nuclei in this survey and find the same pattern suggesting the practically the same optimal cutoff. To corroborate this choice, we will investigate in the following the dependence of results on resonance energies and width on the choice of cutoff.

Figs. 4–6 show the dependence of GR properties and low-lying collective states in \(^{16}\text{O} \), \(^{48}\text{Ca} \), and \(^{208}\text{Pb} \) on the cutoff parameter \( v_{\text{min}} \). The most sensitive dependence on
\[ v_{\text{min}} \text{ is seen in the light nucleus } ^{16}\text{O}. \text{ But even in this case the variation of these key quantities between the } v_{\text{min}} = 0.2 \text{ and 0.05 (the value which we finally use) are not very large: The energies of GR are stable and the variation of the width of the GDR as well as the excitation energy of the } 3^- \text{ state is still moderate. Much less dependence on } v_{\text{min}} \text{ is seen with increasing mass number } A. \text{ In all cases, we see steep changes starting sooner or later below } v_{\text{min}} = 0.05. \text{ Thus we encounter a plateau of robust results within which we can chose pertinent } v_{\text{min}}. \text{ We finally take the lower end of the plateau which complies nicely with the optimum value suggested in the scatter plot in Fig. 3.} \]

\section*{V. GIANT MULTIPOLAR RESONANCES}

RPA and TBA were designed to describe nuclear excitation spectra in the realm of giant multipole resonances \cite{13} and so GR are to be the first test case for new developments. We will compare in this section RPA with TBA results for the three most prominent modes, GDR, GMR, and GQR. In order to demonstrate the influence of the underlying energy functional, we will use three different Skyrme parametrizations as explained in section \ref{sec:III-C}. Before going on, let us briefly recall basic properties of GR. The heavier the nucleus the more concentrated the
resonance spectra such that isoscalar GMR and GQR and isovector GDR display one prominent and rather narrow resonance peak. Spectral fragmentation takes over for GMR and GQR towards light nuclei whereas the GDR still remains a compact, though fragmented, resonance. Finally in $^{16}$O we observe for GMR and GQR a multi-peak structure, which is distributed over a large energy band. As mentioned before to define here a mean energy is somewhat questionable. Nevertheless we can evaluate experimental mean energies the same way which can then be compared with our results.

Fig. 7 shows the RPA and TBA results on GR together with experimental data for the selected nuclei and parametrizations. Although our main emphasis lies on the changes induced by phonon coupling in the step from RPA to TBA, let us briefly comment on the trends with parametrization. The heavy nucleus $^{208}$Pb being closest to bulk displays a nearly one-to-one correspondence between NMP and GR peak energies [32], namely between GMR and incompressibility, GQR and effective mass, GDR and TRK sum-rule enhancement, and dipole polarizability and asymmetry energy. We see this in the upper right panel of Fig. 7: our set of three parametrizations varies $m^*/m$ and accordingly most changing is the GQR, the set SV-m64k6 varies additionally $\kappa_{TRK}$ and the GDR peak comes visibly higher. Smaller nuclei gather increasingly surface effects which, in turn, mixes the dependencies. For example, changing $m^*/m$ affects all other modes too. Unfortunately, we have to realize that the trend with system size $A$ is not reproduced by only one of the parametrizations. Take the example SV-bas. It is tuned to reproduce GR in $^{208}$Pb but all three GR show large deviations for the lightest nuclei in the sample. SV-m64k6 was tuned to cover the GDR in $^{16}$O as well as in $^{208}$Pb [35] and it does so, but it fails still for GMR and GQR. The problem remains yet unsolved that the present form of the Skyrme functional cannot yet cover GR in all nuclei [44]. We will not solve it in this paper. The aim is to check the impact of phonon coupling on the trends which is also an important ingredient in further improving the functional.

Now let us look at effect of phonon coupling in Fig. [7] The step from RPA to TBA shifts the peak energies to lower energies. The prominent result of this summary view is that this down-shift is rather small and constant for all forces and nuclei. It varies only in a small band of 0.5–1.5 MeV. The major effect of phonon coupling remains the smoothing of the spectral distributions towards realistic profiles as seen in Fig. 1 and Figs. 8. The effect on peak energies is much smaller than the variations with parametrizations. Thus the solution for the yet unresolved trends with $A$ has to come from improved...
FIG. 7. Mean energies of resonances for three Skyrme parametrizations and six doubly magic nuclei. The experimental data for GMR and GQR in $^{16}$O were taken from Ref. [36] and for GDR in $^{40}$O from [37], in $^{40}$Ca and $^{48}$Ca for GDR from [38] and GMR/GQR from [39], in $^{56}$Ni for GDR from [41] and for GQR from [42], in $^{132}$Sn for GDR from [42], in $^{208}$Pb for GDR from [14] and for GMR/GQR from [43].

The structure of the cross sections of the GR resonances are qualitatively changed by the TBA compared to the RPA. This can not be seen by comparing the widths of the resonances but one has to look at the detailed cross sections, or strength distributions respectively.

Fig. 8 show detailed strength distributions for the three GR in $^{56}$Ni and $^{208}$Pb. It demonstrates the impact of phonon coupling in detail. The down-shift of peak energy is, though small, well visible. We see also that the total width is not so much affected. It is dominated by spectral fragmentation due to the different energies of the various $ph$ components. This effect, the Landau damping, is already present in RPA and in general larger than the escape widths due to the coupling to the continuum. TBA adds what is called spreading width or collisional width [21] which has moderate impact on the total width, but functionals. However, the fine-tuning of parametrization should stay aware of the small down-shift.

FIG. 8. Strength distributions of giant resonances in $^{56}$Ni and $^{208}$Pb. Compared are RPA and TBA results computed using the Skyrme parametrization SV-m64k6. The blue dashed and full red lines represent RPA and TBA results, respectively. Experimental data (dashed-dotted lines in the upper block) are for $^{56}$Ni Gaussians obtained from experimental values of $E_0$ and $\Gamma$ [41] and (lines with error bars in the lower block) for $^{208}$Pb from [43] for GMR and GQR and from [14] for GDR.
shapes significantly the profile of the spectral distribution by reducing, in most cases considerably, the height of the main peak. This feature that phonon coupling works predominantly on the detailed profile is new as compared to earlier publications. It is due to the subtraction scheme in Eq. (12) which eliminates double counting of static corrections.

VI. LOW-LYING COLLECTIVE STATES

A. General considerations

In all nuclei reported here exists a low lying collective $3^{-}$ state. As the parity changes from shell to shell one obtains only low-lying ($ph$) pairs with negative parity. From $^{48}$Ca on the spin-orbit splitting is so large that the lower partner of the first unoccupied shell is shifted beneath the Fermi edge in the next lower shell. The coupling of this hole state with the states of the same shell just above the Fermi edge gives rise to low-lying $ph$ pairs with positive parity. For this reasons, in heavy nuclei, the gap between the $ph$ states and the spin-orbit splitting are crucial for the energies of the low-lying states having negative or positive parity. The energy gaps between the particle and hole spectra in $^{208}$Pb shown in Table II are the differences $1h_{9/2} - 3s_{1/2}$ for protons and $2g_{9/2} - 3p_{1/2}$ for neutrons.

As we can see from Table II in the case of $^{208}$Pb the experimental gaps and the spin-orbit splittings are nicely reproduced by the SV-bas parametrization whereas the results from the SV-m64k6 especially for the neutron data deviate strongly from the experimental values. Therefore we expect that in this case the results for the low-lying $3^{-}$ and $2^{+}$ states derived with the SV-bas parameters agree much better with the data than the ones obtained with SV-m64k6. In Table III we show spin-orbit splitting and the energy gaps for $^{40}$Ca, $^{48}$Ca, $^{56}$Ni and $^{132}$Sn. Here we compared only the theoretical results for SV-bas with the data. For the spin-orbit splitting the agreement between theory and experimental data is good, with the exception of the proton $1f$ pair in $^{48}$Ca. Also the energy gaps between the particle and hole species are well reproduced. Here we have to bear in mind that the SV-bas parameter set was not adjusted to any of these quantities but to the usual nuclear matter properties and the monopole, quadrupole and dipole giant resonances [45].

B. Effective mass, spin-orbit splitting and phonons

Fig. 9 shows energies and $B(EL)\uparrow$ values of the low-lying collective $3^{-}$ and $2^{+}$ states in all doubly magic nuclei. The three Skyrme parametrization have different $m^*/m$: 0.9 (SV-bas), 0.7 (SV-n07) and 0.64 (SV-m64k6). As mentioned above, the low-lying collective $3^{-}$ state depends on $m^*/m$ in a sensitive and systematic way, the lower $m^*/m$ the higher $E(3^{-})$ because these energies are dominated by the energy gap between the shells with opposite parity which increases with decreasing $m^*/m$. The parameter set SV-bas gives for all doubly magic nuclei $^{40}$Ca, $^{48}$Ca, $^{56}$Ni and $^{132}$Sn. All values are given in MeV.

| | $\Lambda_p$ | $\Lambda_N$ | $\Delta_p$ | $\Delta_N$ |
|---|---|---|---|---|
| $^{208}$Pb | | | | |
| SV-bas | 5.22 | 6.83 | 4.09 | 3.86 |
| SV-m64k6 | 5.80 | 7.87 | 4.35 | 5.11 |
| Exp. | 5.57 | 5.84 | 4.21 | 3.43 |

| | $\Lambda_p$ | $\Lambda_N$ | $\Delta_p$ | $\Delta_N$ |
|---|---|---|---|---|
| $^{40}$Ca | | | | |
| SV-bas | 7.06 | 7.45 | 4.99 | 5.10 |
| Exp. | 5.69 | 5.71 | 7.24 | 7.28 |
| $^{48}$Ca | | | | |
| SV-bas | 7.48 | 7.36 | 5.42 | 2.93 |
| Exp. | 5.08 | 8.75 | 6.18 | 4.80 |
| $^{56}$Ni | | | | |
| SV-bas | 7.14 | 7.33 | 4.11 | 4.15 |
| Exp. | 7.45 | 7.17 | 6.42 | 6.40 |
| $^{132}$Sn | | | | |
| SV-bas | 5.59 | 7.42 | 5.59 | 4.68 |
| Exp. | 6.13 | 6.75 | 6.13 | 4.94 |

*a For $^{132}$Sn, $\Lambda_p$ and $\Lambda_N$ are given for the shells $1g$ and $1h$, respectively. For all other nuclei, $\Lambda_p$ and $\Lambda_N$ are given for $1f$.**
The theoretical $E(2^+)$ in the medium mass nuclei are slightly too low although the spin-orbit orbit splitting is rather appropriate as seen from Table III. For heavier nuclei, the theoretical value increases relative to data. In all cases, the deviations are, in fact, small. In spite of the differences which we probably pointed out too much, it is astonishing that the Skyrme functionals place the two low-lying states so well although their energies are not fitted and emerge from subtle interplay of several ingredients.

The effect of phonon coupling (difference between open and filled symbols) is generally small (usually 0.2 MeV, occasionally 1 MeV), smaller than for GR but relative to the lower excitation energies comparable. The down-shift is usually beneficial for coming closer to data in case of $E(3^-)$. The situation is mixed for $E(2^+)$ because the relation of theory to data varies with parametrization and nucleus. The general conclusions remains the same as for GR: the general trends are not changed by phonon coupling, but the small down-shift should be considered when going for fine tuning a model.

C. Transition probabilities $B(EL)$ of the low-lying collective states

The transition probabilities, $B(EL)$ values shown in the upper block of Fig. 9 are an even more sensitive test for the quality of a theoretical approach compared with the energies as they test the structure of the wave functions. Fig. 9 shows both, energies and $B(EL)$ values, for the low lying $2^+$ and $3^-$ collective states together in comparison with data. The agreement is satisfactory. Not only the energies but also $B(EL)$ values in most cases stay within 10% to 20% from data. Only the $B(E3)$ values in $^{16}O$ deviate by a factor of three. This might be connected with the single-particle energies. It has been shown in Ref. 92 that if one starts with the experimental $ph$-energies and includes the excitation energy of the $3^-$ state in the fitting procedure of the $ph$-force than the $B(E3)$ value is in good agreement with the data. In the present approach the energy gap between the particle and hole states is 4 MeV smaller compared with the experimental values. As the energy of the $3^-$ is well reproduced it is obvious that the (self-consistent) $ph$-force is too weak to create collectivity. To much lesser extend, this can be said of the other cases too. With the exception of the $B(E2)$ value of $^{56}Ni$ all $B(E2)$-values are already in RPA too small. As mentioned before, the fragmentation of the single-particle strength gives an additional reduction in TBA.

In this connection one has to bear in mind that in the present approach (like in most other approaches of this kind) correlations beyond RPA are included only in the excited states but not in the ground state. One of the few exceptions is Ref. 93. Here magnetic dipole states were investigated and in this case, as expected, ground-state correlations beyond RPA give rise to a reduction of the strength. In an other investigation 63 the authors treated 2p2h correlations consistently in the excited states as well as in the ground state. Here giant resonances were investigated and in the case of the isoscalar the GQR in $^{40}Ca$ the peak shows, as expected, an enhancement. Unfortunately no results for low-lying collective states were here reported.

Comparing TBA with RPA we see that phonon cou-
Spectral always reduces the $B(EL)$ strength, not much but very systematically. This is explained by the fact that, on the one hand, the TBA excitation energies are shifted down with respect to the RPA ones. On the other hand, the RPA-IWWSR (inverse energy-weighted sum rule) is conserved in the TBA with subtraction (see [15]) and therefore the $B(EL)$ values should change in the same direction. The same coincidence of lowering energy together with lowering $B(EL)$ could be observed already in Fig. [7].

VII. SUMMARY

In this publication we present a new selection criterion for phonons in phonon coupling models. The criterion relies on the inverse-energy weighted average interaction strength $v_{\text{min}}$, in given RPA modes and so is independent of additional assumptions about external field operators. It is found to sort out (and discard) unambiguously all non-collective states. In this way, it restricts in a natural way the energies and angular momenta of the phonons included in the model space. As a formal motivation, we could show that our new criterion may be compared with the macroscopic method where the low-lying vibrations with the largest deformation parameter give rise to the strongest coupling to the single-particle states. We investigated within the framework of the time-blocking approximation (TBA) the dependence of the results on the magnitude of the new cutoff parameter $v_{\text{min}}$. It is demonstrated that there exists a plateau where the numerical results depend only weakly on the parameter $v_{\text{min}}$. From this investigations we extract the quantity $v_{\text{min}} = 0.05$.

We applied the newly tuned scheme to a systematic survey of giant resonances as well as of the low-lying collective $2^+$ and $3^-$ resonances in light, medium and heavy double magic nuclei where we used three different Skyrme parametrizations to explore the variances of predictions. Thereby we looked at two aspects, first, we studied the effect of phonon coupling in a wide range of nuclei and modes, and second, we looked at the performance in comparison to data. The phonon coupling in TBA has three effects: a shift of the resonances peak energies, an enhancement of their width, and a smoothing of the spectral distributions. The shift is always downward to lower resonance energies and remains rather small (0.5–1.5 MeV for giant resonance, 0.2–1 MeV for low lying states). Most importantly, the down-shift is for a given mode much the same for all nuclei and forces such that trends (with mass number, with force) are not changed as compared to RPA. The effect on the width is hardly recognizable as this is dominated by RPA’s fragmentation width. The largest effect appears in the detailed spectral distributions which are efficiently smoothed such that the TBA profiles comes very much closer to the experimental strength distributions.

What agreement of the results with data is concerned, we have mentioned already the beneficial effect of TBA for spectral distributions. The only small shift of the peak energies leaves the burden of matching resonance positions mainly to RPA while delivering some fine tuning from phonon coupling. And here we find again as has been worked out in several earlier RPA studies namely that the Skyrme energy density functional allows a pertinent description of giant resonances in heavy nuclei but has still unsolved problems with covering the full A dependence of the collective resonances. The present survey gives a direction for further search. The problem of A dependence has first to be resolved roughly within RPA and then TBA comes into play when fine tuning.

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