Particle-vibration coupling for giant resonances beyond the diagonal approximation

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A fully self-consistent particle-vibration coupling (PVC) model is presented. The main novelty stands in releasing the so-called diagonal approximation that neglects completely the interaction between the doorway states. As applications, isoscalar giant monopole, dipole, and quadrupole resonances in ^{16}\text{O} are investigated based on the use of Skyrme functionals. The diagonal approximation is found to clearly impact on the strength distribution of the giant quadrupole resonance, and the description of the experimental data is improved when we perform the full calculation. The impact of the diagonal approximation is analyzed in detail, especially its effect on the eigenenergies and the induced coupling between neutron and proton particle-hole configurations. The latter is a direct and physically sound effect of the improvement on our formalism. The importance of using self-consistently the full effective interaction in the PVC vertex, and the effect of its renormalization via the subtraction method are also discussed. For completeness, we also analyze the dependence on the Skyrme parameterization in our results.

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I. INTRODUCTION

Probing the response of a nucleus to the scattering of a particle or photon is a powerful tool to study the underlying nuclear structure. In the excitation energy range from 10 MeV to 30 MeV the nuclear systems show prominent and broad resonances, that are called giant resonances. Giant resonances have been experimentally studied for a long time [1], and yet the techniques that are developed are still improving towards unprecedented and advanced levels [2, 3]. These studies provide extremely rich information on the nuclear phenomenology. To name a few highlights, we mention the study of compression modes such as the Isoscalar Giant Monopole and Dipole Resonances that are undertaken in order to understand the incompressibility of uniform nuclear matter [4]; the Isovector Giant Dipole Resonance and the associated dipole polarizability that is studied due to its implication for the symmetry energy [3, 5–7]; the low-lying dipole strength in the Isovector Dipole channel for its possible relation to the neutron skin thickness [8–12]; the Isoscalar Giant Quadrupole Resonance which is tightly connected to the nucleon effective mass close to the Fermi surface [13]; the Gamow-Teller resonance [14] for its key role in astrophysically relevant weak-interaction processes [15] (cf. also the general discussion about giant resonances and the parameters of the nuclear equation of state in Ref. [16], and the report on giant resonances in nuclei far from stability in Ref. [17]).

On the other hand, the rich information on giant resonances also sets a challenge for theoretical descriptions. In the random phase approximation (RPA), the giant resonances are described as coherent superpositions of one particle one hole (1p-1h) excitations. The centroid of giant resonances and the energy weighted sum rule (EWSR) can be well described. However, the experimental resonance width Γ, which directly relates with the lifetime τ ≡ ℏ/Γ, cannot be described by RPA due to the missing of the coupling with more complicated correlations. Two main effects were identified to contribute to the width, the escape of a nucleon from the nucleus (escape width) and the spreading of the excitation energy into more complicated configurations (spreading width) [18]. Different efforts have been made to take into account these effects, for example: continuum RPA [19, 20]; second RPA (SRPA) [21–25]; quasiparticle-phonon model [26–29] quasiparticle-phonon model based on time-blocking approximation (TBA) [30–32]; TBA in the relativistic framework [33–35].

In this work we use the particle-vibration coupling (PVC) model, which takes into account the coupling between a nucleon and the low-lying nuclear collective excitations (phonons) [36]. In early applications, phenomenological inputs were used for the PVC vertex and parameters were adjusted to reproduce the data, making it difficult to have a universal description [18, 37, 38]. A self-consistent treatment for the interaction in the PVC vertex, on top of a mean field associated with Skyrme functionals was worked out in Ref. [39], although only the velocity-independent central term was included in the vertex. The approach was further developed in Refs. [40–43], and now the full Skyrme interaction is used for both the PVC vertex and the mean field. The same consistency has been achieved also in the relativistic PVC [44]. The PVC has been extended to describe open-shell nuclei within the Hartree-Fock (HF) plus BCS framework [45], and later on in the Hartree-Fock-Bogoliubov framework [46]. By including both collective and noncollective exci-
tations, the so-called hybrid configuration mixing model was developed to study the low-lying spectroscopy of odd nuclei, and shell-model-type states like 2p-1h can be well taken into account [47]. To better understand the renormalization of the effective interaction, the subtraction method developed in Ref. [30] has been studied in the PVC [48]. The PVC has been used to investigate, for example, the $\beta$-decay [49, 50] and good descriptions were achieved.

However, in the above studies the so-called diagonal approximation has been used, that is, the 1p-1h state coupled with a phonon, which is also called a doorway state, has no interaction with other doorway states. This is similar to the diagonal approximation in the SRPA where there is no interaction among the 2p-2h states. In the context of SRPA, this approximation has been tested against the fully self-consistent framework, and it has been shown to affect significantly the strength distributions [23]. Therefore, it is of importance to have a closer view into this approximation in the PVC. This will be the main objective of this work, that is, to develop a fully self-consistent PVC without diagonal approximation and study its influence on the giant resonances.

In Sec. II, we give a brief summary of the formalisms of the HF, RPA, and PVC. The numerical details for the calculations are discussed in Sec. III. Results for the isoscalar giant monopole, dipole, and quadrupole resonances of $^{16}\text{O}$ by full PVC are presented in Sec. IV. Finally, the summary and perspectives for future investigations will be given in Sec. V.

II. THEORETICAL FRAMEWORK

A. From Hartree-Fock to Random Phase Approximation

Our starting point is the Skyrme functional which is constructed from the Skyrme effective interaction solved within the Hartree-Fock (HF) approximation. The detail of the Skyrme interaction and the corresponding formulas of the Skyrme Hartree-Fock theory in spherical nuclei have been given in detail [51] and will not be repeated here. In this work we take the doubly magic nucleus $^{16}\text{O}$ as an example, so that effects of pairing and deformation [52] can be ignored. The Hartree-Fock ground state $|\Phi_0^{\text{HF}}\rangle$ is a single Slater determinant. In the second quantized form it can be written as:

$$|\Phi_0^{\text{HF}}\rangle = \prod_i^A a_i^\dagger |\rangle,$$

where $A$ is the number of nucleons of a given nucleus, $a_i^\dagger$ is the creation operator of HF single-particle state $|i\rangle$, and $|\rangle$ is the bare vacuum. The HF equation is solved with a box boundary condition and a set of discrete occupied and unoccupied states $|i\rangle$ are obtained. The Hamiltonian of the system can be expressed as

$$H = H_0 + V_{\text{res}},$$

where $H_0$ is the HF Hamiltonian and $V_{\text{res}}$ the residual interaction:

$$H_0 = \sum_i^A e_i a_i^\dagger a_i - \frac{1}{2} \sum_{ij}^{A} \widetilde{V}_{ijij},$$

$$V_{\text{res}} = \frac{1}{4} \sum_{k'kl} \widetilde{V}_{k'kl} : a_{k'}^\dagger a_{l'}^\dagger a_i a_k :.$$  

In the above equations, $e_i$ is the single-particle energy of state $|i\rangle$, and $\widetilde{V}_{ijij}$ is the antisymmetrized two-body matrix element. The normal ordered product of operators $a_{k'}^\dagger a_{l'}^\dagger a_i a_k$ is labelled as $: a_{k'}^\dagger a_{l'}^\dagger a_i a_k :$ with respect to the HF particle-hole vacuum $|\Phi_0^{\text{HF}}\rangle$.

To study the excited state properties, one can use the RPA, in which all the possible 1p-1h excitations are considered. If we define the HF ground state $|\Phi_0^{\text{HF}}\rangle$ and all the 1p-1h excitations $|ph\rangle$ built upon as the subspace $Q_1$, the RPA solution can be obtained by diagonalizing the Hamiltonian in this subspace $Q_1 H_0 Q_1$. For the derivation of the RPA equations and their solution we refer the reader to Ref. [53]. The RPA equation reads

$$\sum_{ph} \left( A - B^* \right)_{ph'h',ph} \left( X_{ph}^{(n)} Y_{ph}^{(n)} \right) = \omega_n \left( X_{ph'}^{(n)} Y_{ph'}^{(n)} \right),$$

with $\omega_n$ the excitation energy of RPA state $|\Phi_n^{\text{RPA}}\rangle$ (that can be simply labeled as $|n\rangle$ when there is no ambiguity), $X_{ph}^{(n)}$ and $Y_{ph}^{(n)}$ the corresponding RPA wave function coefficients. The matrix elements $A$ and $B$ are

$$A_{ph'h',ph} = \langle 0 | [a_{ph'}^\dagger a_{ph}, [H, a_{ph}^\dagger a_{n}] ] | 0 \rangle,$$

$$B_{ph'h',ph} = \delta_{ph'h',ph} (e_p - e_h) + \tilde{V}_{ph'h',ph},$$

where $|0\rangle$ is the RPA ground state $|\Phi_0^{\text{RPA}}\rangle$, and within the quasiboson approximation it is replaced by the HF ground state $|\Phi_0^{\text{HF}}\rangle$ [53]. Without causing confusion, the simple form $|0\rangle$ of the ground state will be used later on also in the framework of PVC. The RPA excited states, or the phonons, can be expressed as

$$|n\rangle = Q_n^\dagger |0\rangle,$$  

with

$$Q_n^\dagger = \sum_{ph} \left[ X_{ph}^{(n)} a_{ph}^\dagger - Y_{ph}^{(n)} a_{ph}^\dagger a_{ph}^\dagger \right],$$

and the RPA ground state satisfies

$$Q_n |0\rangle \equiv 0.$$
B. Particle-vibration coupling

As we briefly mentioned in the Introduction, RPA can give a good description of the centroid energy of giant resonances as well as of the EWSR exhausted by each mode. However, properties such as the width of the resonances cannot be well described. Part of the width comes from the so-called Landau damping effect and part of it is due to correlations beyond 1p-1h [18]. The Landau damping effect produces a fragmentation of the strength, in contrast with the ideal situation in which there is a single collective peak. Such an effect depends on the intensity of the residual interaction that 1p-1h configurations feel, as well as the density of the unperturbed 1p-1h states around the resonance energy. Coupling with more complicated states than 1p-1h produce the resonance spreading width. Our formalism can also account for the other mechanism giving rise to the resonance width, since the escape of a nucleon can be also described.

To take into account these effects, two subspaces $P$ and $Q_2$ are built. Similar to $Q_1$, subspace $P$ is made up with 1p-1h configurations but now the particle is a continuum state and orthogonal to all the states in $|i\rangle$. For subspace $Q_2$, one can chose the 2p-2h configurations and the resulting framework would be the second RPA [54]. In the particle-vibration coupling model, the $Q_2$ space is composed of the so-called doorway states $|N\rangle$ with 1p-1h excitation coupled to a RPA phonon,

$$|N\rangle = |ph\rangle \otimes |n\rangle.$$  

(10)

The corresponding excitation operator reads

$$Q_N^i = \sum_{ph,n} \left[ \tilde{X}_{ph,n}^N a_p^i a_h^\dagger Q_n - \tilde{Y}_{ph,n}^N Q_n a_h^i a_p^\dagger \right].$$  

(11)

Now, the PVC equation is an eigenequation in the $P + Q_1 + Q_2$ space,

$$H(P + Q_1 + Q_2)\Psi = \omega(P + Q_1 + Q_2)\Psi,$$  

(12)

$\Psi$ being the full-space wave function to be projected out. After truncating higher orders, this equation can be mapped into $Q_1$ with an energy dependent Hamiltonian as [41] (see Appendix A)

$$H(\omega)Q_1 \Psi = \left( \Omega_\nu - i\frac{\Gamma_\nu}{2} \right) Q_1 \Psi.$$  

(13)

Both the effective Hamiltonian $H$ and the eigensolutions are complex. The effective Hamiltonian is composed of three terms,

$$H(\omega) \equiv Q_1 HQ_1 + W^\dagger(\omega) + W(\omega) = Q_1 HQ_1 + Q_1 HP \frac{1}{\omega - PH + i\epsilon} PHQ_1 + Q_1 HQ_2 \frac{1}{\omega - Q_2 HQ_2 + i\epsilon} Q_2 HQ_1,$$  

(14)

i.e., the RPA term, escape term ($W^\dagger$), and spreading term ($W$). For the calculation of the escape term, one is referred to Ref. [41]. For more detail of the spreading term and the diagonal approximation of it, see Section II C.

As one is now working in the $Q_1$ subspace, the RPA solutions can be used as a basis to expand the PVC state as

$$|\nu\rangle = \sum_n F_n^{(\nu)} |n\rangle.$$  

(15)

Then the PVC equation (13) takes the matrix form

$$\sum_n \mathcal{H}_{n'n}(\omega) F_n^{(\nu)} = \left( \Omega_\nu - i\frac{\Gamma_\nu}{2} \right) F_n^{(\nu)},$$  

(16)

with

$$\mathcal{H}_{n'n}(\omega) = \omega_n + W_{n'n}(\omega) + W_{n'n}^\dagger(\omega).$$  

(17)

The matrix of the wave function coefficients is complex orthogonal,

$$F^T F = FF^T = 1.$$  

(18)

The response function associated with the operator $O$ is defined as

$$R(\omega) = \langle 0|O^\dagger \frac{1}{\omega - H(\omega) + i\epsilon} O|0\rangle.$$  

(19)

The corresponding strength function is

$$S(\omega) = -\frac{1}{\pi} \text{Im} R(\omega) = -\frac{1}{\pi} \text{Im} \sum_\nu \langle 0|O|\nu\rangle^2 \frac{1}{\omega - \Omega_\nu + i\frac{\Gamma_\nu}{2}}.$$  

(20)

The sum rules, or the $k$th moments $m_k$ of the strength function, are defined as

$$m_k = \int_0^\infty S(\omega) \omega^k d\omega.$$  

(21)

Among them, the energy-weighted sum rule $m_1$ is of particular interest as it can be expressed in a simple form via a double commutator evaluated in the ground state, namely

$$m_1 = \frac{1}{2} \langle 0|[O^\dagger, [H, O]]|0\rangle.$$  

(22)
C. Spreading term in PVC

The spreading term is the last term in Eq. (14),

\[ W^\dagger(\omega) = Q_1 HQ_2 \frac{1}{\omega - Q_2 HQ_2 + i\epsilon} Q_2 HQ_1. \]  

(23)

It describes the process in which 1p-1h configurations of the Q1 subspace are coupled to the more complicated doorway states of the Q2 subspace. These terms can be derived with the equation-of-motion method [55] as in the SRPA [56]. Similar to the RPA matrix Q1HQ1 in Eq. (5), one has the matrix Q1HQ2 and Q2HQ2 in the particle-hole and phonon representation:

\[ Q_1 HQ_2 = \left( \begin{array}{ccc} A_{ph,p_1 h_1 n} & B_{ph,p_1 h_1 n} \\ -B_{ph,p_1 h_1 n}^* & -A_{ph,p_1 h_1 n}^* \end{array} \right) \]  

(24)

\[ Q_2 HQ_2 = \left( \begin{array}{ccc} A_{p_1 h_1 n_1, p_2 h_2 n_2} & B_{p_1 h_1 n_1, p_2 h_2 n_2} \\ -B_{p_1 h_1 n_1, p_2 h_2 n_2}^* & -A_{p_1 h_1 n_1, p_2 h_2 n_2}^* \end{array} \right) \]  

(25)

with the matrix elements defined similarly to Eq. (6),

\[ A_{ph,p_1 h_1 n} = \langle 0 | [a_{ph}^\dagger a_p, [H, a_p^\dagger a_{h_1} Q_n^1]] | 0 \rangle \]  

(26)

\[ B_{ph,p_1 h_1 n} = \langle 0 | [a_{ph}^\dagger a_p, [H, Q_n a_{h_1}^\dagger a_{p_1}]] | 0 \rangle \]  

(27)

\[ A_{p_1 h_1 n_1, p_2 h_2 n_2} = \langle 0 | [Q_{n_1} a_{h_1}^\dagger a_{p_1}, [H, a_{p_2}^\dagger a_{h_2} Q_n^3]] | 0 \rangle \]  

(28)

\[ B_{p_1 h_1 n_1, p_2 h_2 n_2} = \langle 0 | [Q_{n_1} a_{h_1}^\dagger a_{p_1}, [H, Q_n a_{h_2}^\dagger a_{p_2}]] | 0 \rangle \]  

(29)

They can be evaluated as

\[ A_{ph,p_1 h_1 n} = \delta_{ph} \delta_{p_1 h_1} (p|V|p_1 n) - \delta_{pp_1} \langle h_1 | V | h_n \rangle, \]  

(30)

\[ A_{p_1 h_1 n_1, p_2 h_2 n_2} = \delta_{n_1 n_2} \left[ \delta_{p_1 h_1, p_2 h_2} (\omega_n + e_{p_1 h_1}) + V_{p_1 h_1 p_2 h_2} \right], \]  

(31)

\[ B_{ph,p_1 h_1 n} = B_{p_1 h_1 n_1, p_2 h_2 n_2} = 0, \]  

(32)

with \( \omega_n \) the energy of the phonon \( |n\rangle \), \( e_{ph} = e_p - e_h \), and

\[ (a|V|b, n) = \sum_{ph} \left[ X_{ph}^{(n)} V_{ahp} + Y_{ph}^{(n)} V_{ahp} \right]. \]  

(33)

The matrix element \( A_{ph,p_1 h_1 n} \) in Eq. (30) represents the interaction between the 1p-1h state \( |ph\rangle \) in the Q1 space and the doorway state \( |p_1 h_1 \rangle \otimes |n\rangle \) in the Q2 space. A diagrammatic representation of this interaction is given in the left part of Fig. 1. The matrix element \( A_{p_1 h_1 n_1, p_2 h_2 n_2} \) in Eq. (31) represents the interaction among the doorway states, and its diagrammatic representation is also provided in the right part of Fig. 1.

The full spreading term can then be written as

\[ W^\dagger_{ph'} (\omega) = \sum_{p_1 h_1, p_1 h_1 n} A_{ph', p_1 h_1 n} \times (\omega - A_{ph', p_1 h_1 n} + i\epsilon)^{-1} A_{p_1 h_1 n, ph}. \]  

(34)

\[ \text{FIG. 1: Schematic show of the interaction of } Q_1 HQ_2 \text{ and } Q_2 HQ_2, \text{ corresponding to the matrix elements in Eqs. (30,31).} \]

In the above notation \( (\omega - A_{p, h,n_1 h_1 n_1 + i\epsilon})^{-1} \) is not the inverse of a single matrix element, but the matrix element of the inverted matrix of \( \omega - A_{p, h,n_1 h_1 n_1 + i\epsilon} \).

In previous investigations, the diagonal approximation was used, that is, no interaction among the doorway states was considered [41]. Within this approximation, the matrix element \( A_{p_1 h_1 n_1, p_2 h_2 n_2} \) in Eq. (31) becomes

\[ A_{p_1 h_1 n_1, p_2 h_2 n_2} = \delta_{n_1 n_2} \delta_{p_1 h_1} (\omega_n + e_{p_1 h_1}). \]  

(35)

The matrix \( Q_2 HQ_2 \) then becomes diagonal, and the spreading term can be easily evaluated as

\[ W^\dagger_{ph'} (\omega) = \sum_{p_1 h_1 n} A_{ph', p_1 h_1 n} \frac{1}{\omega - \omega_n - e_{p_1 h_1} + i\epsilon}. \]  

(36)

When the diagonal approximation is not considered, there is an extra step of inverting the matrix \( \omega - Q_2 HQ_2 + i\epsilon \) before evaluating the spreading term. See Appendix B for more details.

Finally, interactions that are fitted at the mean-field level and are used within effective theories that go beyond mean field should in principle be refitted against to experimental data in order to avoid double-counting. That is, a renormalization of the model parameters is compulsory. The parameters will change their value since many-body contributions beyond mean-field are now explicitly included. The purpose of the subtraction method [30, 48] is to provide a recipe for the renormalization of the effective interaction within the adopted model scheme that avoids a refitting of the parameters. For that, the spreading term in Eq. (14) should be replaced by

\[ W^\dagger (\omega) = W^\dagger (\omega) - W^\dagger (\omega = 0). \]  

(37)

III. NUMERICAL DETAILS

The nucleus \(^{16}\text{O}\) is studied as an example since it provides a simple case for various theoretical investigations and tests. As it is a doubly magic nucleus, the effects of pairing and deformation can be ignored. The Skyrme functional SAMi [57] will be used in all calculations except in the last section where a systematic study on the dependence on the parameterization of the Skyrme functional is given. Three isoscalar (IS) non charge-exchange excitation modes will be examined: the giant monopole resonance (GMR, \( J^π = 0^+ \)), giant dipole resonance (GDR, \( J^π = 1^- \)), and giant quadrupole resonance...
we show the strength function of ISGMR, ISGDR, and ISGQR in $^{16}\text{O}$ calculated by RPA (bars) and PVC (lines), in comparison with experimental data [59, 60]. The original data is given in terms of the fraction of EWSR $F(E)$ in Ref. [60], with a total of $(48 \pm 10)\%$, $(32 \pm 7)\%$, and $(53 \pm 10)\%$ of the EWSR in the region $E_r$ from 11 to 40 MeV. This data is transformed to the strength distribution by:

$$S(E) = \frac{F(E)}{F_{\text{cut}}} m_1,$$

with the values of $m_1$ adopted as the double commutator ones in Table I. For the dipole resonance, the level at 7.12 MeV which exhausts 4.2\% of the EWSR is taken from Ref. [59].

In previous studies of PVC such as Refs. [41, 48], the interaction vertex $Q_1HQ_2$ in Eq. (24) includes only the central term of the Skyrme interaction. The effect of other terms on the single-particle properties have been investigated in Ref. [42, 43]. Here we would like to investigate the effect of those terms on the strength function, therefore in Fig. 2 both the results of PVC with central interaction ($V_c$) and with full interaction ($V_{\text{full}}$) are given, within the diagonal approximation (PVC-dia). For PVC without diagonal approximation (PVC-full), only the results with full interaction are given. In all cases, the HF+RPA calculations are performed with full Skyrme interaction.

It can be seen from Fig. 2 that by including the escape and spreading effects within the PVC, the width of the strength distribution appears naturally, unlike in the case of RPA. This makes the comparison with experimental data more realistic. On the other hand, the centroid of the distribution ($m_1/m_0$) is shifted to a lower energy, from few hundreds of keV for the ISGMR and ISGDR to a maximum of about 1.5 MeV for the case of the ISGQR (cf. Table I). It is important to note here that functionals are usually calibrated in order to give a reasonable description of the experimental centroid energy at the RPA level and, therefore, such shift may lead to worse agreement with the data.

By comparing the results with central term only and results with full interaction, it can be seen that by including Coulomb term and spin-orbit term, the strength is generally slightly shifted to a lower energy. In the case of ISGMR and ISGDR, the shape of the strength distribution does not change too much, while in ISGQR such change is more significant.

From the diagonal approximation to the fully self-consistent calculation, the strength function is also much influenced in the ISGQR case. Within the diagonal approximation, there are two major peaks near 17 and 18.5 MeV; while with the full calculation, there are four major peaks near 14.5, 17, 18.5, and 19.5 MeV, with lower strength and wider distribution. The lowest peak near 14.5 MeV is of particular interest as there is no sign of this peak in the diagonal approximation. It will be used as an example in Section IV C to analyze the difference between the diagonal approximation and the full calculation. Regarding the ISGMR, the removal of the diagonal

IV. RESULTS AND DISCUSSION

A. Spectrum and sum rules

In Fig. 2 we show the strength function of ISGMR, ISGDR, and ISGQR in $^{16}\text{O}$ calculated by RPA (bars) ...
approximation also shows some effect, for example: the lowest peak near 16.5 MeV is shifted to a lower energy and the strength increases; The distributions of the peaks near 20, 21.5, 24, and 29.5 MeV are also affected, but, overall, the effect is weaker than the case of ISGQR. Among the three cases, the ISGDR is the one where the diagonal approximation shows less influence.

As mentioned in the introduction, the diagonal approximation has been investigated in the SRPA framework for the giant resonances of $^{16}$O in Ref. [23]. From RPA to SRPA, the strength distributions are shifted downwards, similar to the effect of PVC in Fig. 2. However, quantitatively, the effect of SRPA is larger. For ISGMR, IVGDR, and ISGQR, the main peaks are shifted downwards by about 4, 6, and 8 MeV, respectively [23]; while for PVC the shifts are $\approx 2$–3 MeV. For the ISGMR, the diagonal approximation in SRPA shifts the distribution to a lower energy by about 2 MeV, while in PVC it changes mildly (see Fig. 2 (a) of this work and Fig. 8 (a) of Ref. [23]). For the dipole case, the effect of diagonal approximation is small in both SRPA and PVC (see Fig. 2 (b) of this work and Fig. 15 (b) of Ref. [23]). For the ISGQR, the diagonal approximation in SRPA shifts the distribution downwards by around 2 MeV, similar to ISGMR, while in PVC it is more complicated as the shape has changed much (see Fig. 2 (c) of this work and Fig. 9 (a) of Ref. [23]). In all the cases, the diagonal approximation in SRPA does not change much the shape of the strength distribution, while in PVC this is not the case for the ISGQR.

In Fig. 3 the effects of the subtraction [Eq. (37)] in the full PVC calculation are shown for the ISGMR, ISGDR, and ISGQR strength distributions of $^{16}$O. As a reference, the results of the RPA and experimental data shown in Fig. 2 are also displayed in Fig. 3. It can be seen that by adopting the subtraction procedure, the strength distributions are generally shifted upwards around 1 MeV, except in the ISGDR case where the main peak at 17 MeV vanishes and a new peak at 14 MeV appears. The effects of subtraction presented here are consistent with the findings of previous investigation using PVC with diagonal approximation (see Fig. 4 of Ref. [48]).

In Ref. [61], the quasiparticle-phonon coupling model with time-blocking approximation was used to study the ISGMR, ISGQR, and isovector GDR of $^{16}$O, $^{40}$Ca, and $^{208}$Pb. A systematic downward shift of the centroid energy of the giant resonances was found from RPA to TBA with subtraction. This effect is similar to the one of PVC presented here, though quantitatively it is smaller (see Fig. 3 of this work and Fig. 4 of Ref. [61]). Especially in the case of ISGQR, the full PVC calculation (with or without subtraction) gives very different strength distribution from the one given by RPA, while they are similar for TBA and RPA [61]. This might be related with the diagonal approximation as removing it shows quite some effect here.

The subtraction in SRPA has been investigated for ISGMR and ISGQR and it also pushes the strength distribution to a higher energy [62]. However, comparing with the results of PVC shown in Fig. 3, the effect in SPRA is again larger. With subtraction, the strength are shifted upwards about 2 MeV in SRPA while in PVC it is generally less than 1 MeV, see Figs. 1 and 4 of Ref. [62]. Comparing the results of SRPA including subtraction with RPA given in Ref. [62], the main peaks of ISGMR and ISGQR given by SRPA with subtraction are about 1.5 and 1 MeV lower than those by RPA. These are similar to the differences between PVC with subtraction and RPA shown in Fig. 3.

In comparison with the experimental data, the three peaks of ISGMR around 18, 23, and 26 MeV may correspond to the three peaks given by the PVC, though the energies are slightly lower than the data. This may be understood as the SAMi functional has been developed in such a way that the experimental ISGMR is reproduced at the RPA level, which can be seen from the black vertical lines in Fig. 3. When the PVC is included, though the description of resonance width has been improved, the centroid is pushed to a slightly lower energy and the subtraction remedies to this problem only to some extent. The peaks around 12 and 14 MeV may be due to $\alpha$-clustering effects [63].
In the case of ISGDR the description of PVC with SAMi functional is rather good, especially the low-lying 7.1 MeV level has been nicely reproduced. The peaks around 12 and 18 MeV, and the resonance shape above 20 MeV are also well described. The subtraction worsens the description of the data below 20 MeV.

In the case of the ISGQR, the peak at 15 MeV by PVC might be attributed to the peak at 12 MeV or 14 MeV of the data. The experimental data for the high energy part of ISGQR is concentrated from 18 to 26 MeV, while the theoretical distribution is from 16 to 22 MeV, slightly lower than the data. Again, the subtraction shifts the strength distribution to higher energies but still lower than the experimental data.

The sum rules for the above discussed calculations are shown in Table I, including the results for the RPA, PVC with diagonal approximation and with central term of the interaction (PVC-d, $V_c$), PVC with diagonal approximation and full interaction (PVC-d), full PVC (PVC-f, without diagonal approximation and with full interaction), and full PVC with subtraction (PVC-s). The strength function given by PVC are integrated up to $E = 120$ MeV. The EWSR $m_1$ by the double commutator in Eq. (39) are also shown.

First, the EWSR ($m_1$) values given by the RPA calculation in all three cases, the ISGMR, ISGDR, and ISGQR, are fully exhausted comparing with the ones obtained by the double commutator. For the PVC results, there are small discrepancies. In the case of SRPA without subtraction, the EWSR is proven to be fully exhausted [56], and this has been shown in the calculation [23]. The $Q_2$ subspace in PVC theory is composed of the doorway states (10) and this may violate the Pauli principle. This fact, together with the cut-offs on the phonon model space may possibly induce the violations of the sum rule in the PVC calculations that are shown in Table I.

As it has been discussed in Fig. 2, the strength distributions given by PVC are generally shifted to a lower energy comparing with those by RPA. Therefore, the inverse EWSR ($m_{-1}$) are larger compared with RPA even when the subtraction method is implemented, and the centroid energy ($m_1/m_0$ or $\sqrt{m_1/m_{-1}}$) are smaller. The influence of non-central terms of the interaction (comparing PVC-d, $V_c$ and PVC-d) on the sum rules are negligible in the case of ISGMR, while for ISGDR and ISGQR a small effect shows up. In all cases, the diagonal approximation (comparing PVC-d and PVC-f) has little influence on the sum rules. On the other hand, the subtraction has much influence on the sum rules (comparing PVC-f and PVC-s). The EWSR are significantly larger and agree less with the double commutator sum rule when subtraction is performed, in agreement with the findings in the PVC calculation with diagonal approximation [48] and SRPA [62]. This is a feature of the subtraction method that needs to be better investigated.

We recall here that the subtraction method was devised for exactly keeping the $m_{-1}$ value obtained within the RPA in beyond RPA calculations while no procedure of...
renormalization was imposed on \( m_1 \).

**B. Different components of interaction**

Next, we show how different components of the interaction contribute to the strength function in Fig. 2, using the ISGQR as an example.

![Graph](image)

**FIG. 4:** (Color online) Strength function of ISGQR in \(^{16}\text{O}\) calculated by RPA with full interaction, PVC with central interaction (PVC, \( V_c \)), PVC with central plus Coulomb interactions (PVC, \( V_c + V_{\text{Coul}} \)), PVC with central plus spin-orbit interactions (PVC, \( V_c + V_{\text{s.o.}} \)), and PVC with full interaction (PVC, \( V_{\text{full}} \)). In all cases the SAMi functional is used.

In Fig. 4 the strength distributions calculated by PVC without diagonal approximation and with different terms of interaction are shown, including: with central terms only (\( V_c \)), with central terms and Coulomb term (\( V_c + V_{\text{Coul}} \)), with central terms and spin-orbit term (\( V_c + V_{\text{s.o.}} \)), and with full interaction (\( V_{\text{full}} \)). It can be seen that the Coulomb interaction has a negligible effect on the strength distribution, except for a small influence near 14 and 21 MeV. On the other hand, the spin-orbit term has much influence and clearly changes the distribution. With the central term there is only one minor peak near 14 MeV and one major peak near 18.5 MeV. When including the spin-orbit term, the strength of the major peak decreases much and two other peaks near 17 and 19.5 MeV become larger.

**C. Influence of diagonal approximation: eigen-energies**

In this Subsection, we analyze the difference between PVC with and without diagonal approximation in Fig. 2. The low energy peak at \( \omega = 14.6 \) MeV in the ISGQR will be used as an example, as it is manifestly different in the two calculations. In the following results, all PVC calculations are performed with the full interaction at \( \omega = 14.6 \) MeV. The integration of the strength around this energy \((14.6 \pm 0.4 \text{ MeV})\) within full PVC calculation gives \( \int S_{\text{full}} d\omega = 34.9 \text{ fm}^4 \), whereas within the calculation with diagonal approximation is \( \int S_{\text{dia}} d\omega = 3.7 \text{ fm}^4 \).

Figure 5 shows the strength contributions from different PVC states \( \nu \), as given by Eq. (20). The position of \( \omega = 14.6 \) MeV has been indicated by the vertical dashed line, and the RPA states are given by the gray vertical lines (with unit fm\(^4\)).

**FIG. 5:** (Color online) Contribution to the ISGQR strength function of \(^{16}\text{O}\) at \( \omega = 14.6 \) MeV from different PVC eigenstates \( \nu \) with different excitation energies, see also Eq. (20). Results of (a) fully self-consistent PVC calculation (red lines) and (b) PVC calculation with diagonal approximation (blue lines) are shown. The position of \( \omega = 14.6 \) MeV is given by the vertical dashed line, and the RPA states are given by the gray vertical lines (with unit fm\(^4\)).

Let us express the square of the transition matrix elements explicitly in terms of its real and imaginary parts,

\[
\langle 0|O|\nu\rangle^2 = a_{\nu} + ib_{\nu},
\]

with \( a_{\nu} \) and \( b_{\nu} \) both real numbers. From Eq. (20), the strength function can be written as

\[
S(\omega) = \frac{1}{\pi} \sum_{\nu} \frac{a_{\nu} e^{i \omega \Omega_{\nu}} - b_{\nu}(\omega - \Omega_{\nu})}{(\omega - \Omega_{\nu})^2 + \frac{\Gamma_{\nu}^2}{4}}.
\]

In Fig. 6 the real part of the square of the transition matrix element \( a_{\nu} = \text{Re}(\langle 0|O|\nu\rangle^2) \) is shown. It can be seen that both the transition matrix element of the state at \( \Omega_{\nu} = 15.5 \) MeV in the full calculation, and that of the state at \( \Omega_{\nu} = 18.0 \) MeV in the diagonal approximation, are very large. Although the value of the \( \Omega_{\nu}(\text{full}) = 15.5 \) MeV one is slightly larger than the one
of the $\Omega_\nu(\text{dia.}) = 18.0$ MeV, the difference is not large enough to explain the difference in the final contribution to the strength shown in Fig. 5. Therefore, according to Eq. (42), the much stronger strength in the full calculation from $\Omega_\nu(\text{full}) = 15.5$ MeV state must be due to the position of this state, which is much closer to the energy being evaluated, that is, $\omega = 14.6$ MeV. In this way, the energy denominator in Eq. 42 of this state is much smaller than the $\Omega_\nu(\text{dia.}) = 18.0$ MeV state and as a consequence the strength is larger.

Next, we will study the origin of the large difference in the eigenenergies of these two states. First, one needs to identify the components of these two states, or more specifically, from which RPA states they come from. For this purpose, we will identify them by looking at the corresponding wave functions.

In the upper panel of Fig. 7 we show the real part of the PVC wave function $F_\nu$ (15) of states $\Omega_\nu(\text{full}) = 15.5$ MeV and $\Omega_\nu(\text{dia.}) = 18.0$ MeV in the basis of RPA states $|n\rangle$ by the two PVC calculations: with (dia.) and without (full) diagonal approximation. The transition matrix elements $\langle n|O|0\rangle$ are shown in the lower panel. The transition matrix elements $\langle 0|O|\nu\rangle$ in the PVC representation in Fig. 6 can be calculated as

$$\langle 0|O|\nu\rangle = \sum_n F_n^{(\nu)}|0\rangle|O|n\rangle. \tag{43}$$

It can be seen that these two states have similar RPA components in both PVC calculations. Although not really dominant, the major component of these two states can be identified as the 11th RPA state with the largest transition matrix element $\langle n = 11|O|0\rangle$. This RPA state is the one located at $\omega_n = 21.3$ MeV with the largest strength as shown in Fig. 2 (c) or Fig. 5.

In Fig. 8, the wave function $F_n^{(\nu)}$ of states $\omega_\nu(\text{full}) = 15.5$ MeV and $\omega_\nu(\text{dia.}) = 18.0$ MeV are transformed to the 1p-1h basis for the $X$ amplitude as

$$F_{ph}^{(\nu)} = \sum_n X_{ph}^{(n)} F_n^{(\nu)}. \tag{44}$$
Similar transformation can be done for the $Y$ amplitudes, but as their values are very small they will not be shown here. From this figure it can be seen that the original RPA state $\omega_n = 21.3$ MeV is a very collective state with many 1p-1h components involved in. When considering the escape and spreading effect of the PVC, we noticed that this state becomes even more collective. In both calculations with and without diagonal approximation, the wave functions $F^{(\nu)}_{ph}$ of these states are similar.

After identifying the major RPA components of the PVC states, one can see how the eigenenergies change from RPA to PVC. In Fig. 9 we show the RPA solutions $\omega_n$ for the ISGQR of $^{16}$O, below 23 MeV, obtained by using the SAMi functional, together with the corresponding eigenenergies of the PVC solutions with and without diagonal approximation at $\omega = 14.6$ MeV. The diagonal matrix elements of the PVC Hamiltonian $H_{nn}$ in Eq. (17) are also given.

It can be seen from Fig. 9 that the diagonal PVC matrix elements are attractive. In the calculation with diagonal approximation $W_{nn} = -2.0$ MeV while for full calculation the value is $-2.7$ MeV, that is, the full calculation gives 0.7 MeV more attraction. After diagonalizing the PVC Hamiltonian $H$, the energy level changes from the perturbative approximation $H_{nn}$ (originated from the $\omega_n = 21.3$ MeV RPA state) to the final eigenvalue $\Omega_\nu$ with a further decrease of 1.3 MeV in the diagonal approximation, and of 3.1 MeV in the full calculation. In the end, the eigenenergy of this state in the calculation with diagonal approximation is $\Omega_\nu(\text{dia.}) = 21.3 - 2.0 - 1.3 = 18.0$ MeV, while in the full calculation it is $\Omega_\nu(\text{full}) = 21.3 - 2.7 - 3.1 = 15.5$ MeV.

In Fig. 10, the PVC matrix elements $W$ are shown with the index $n$ referring to the RPA basis. Since the numbering for the RPA state we are interested in is $n = 11$, with excitation energy $\omega_n = 21.3$ MeV, the matrix elements are shown for $W_{n,11}$. In this figure, the big attraction of the diagonal matrix elements $W_{11,11}$ for both calculations can be clearly seen, with 0.7 MeV more in the full calculation. Moreover, the magnitudes of the non-diagonal matrix elements are generally larger in the full calculation, which in the end leads to more mixing of other states and lower eigenvalues after diagonalizing.

As a conclusion, the extra attraction shown by the full PVC model is the main cause of the appearance of the low energy peak in the ISGQR.

D. Influence of diagonal approximation: coupling between neutron and proton particle-hole configurations

In this subsection, we analyze another important difference between PVC with and without diagonal approximation shown in Fig. 2, that is, the coupling of neutron 1p-1h excitations and proton 1p-1h excitations. The low energy peak at $\omega = 16.4$ MeV in the ISGMR will be used as an example. The integration of the strength around this energy (16.4 $\pm$ 0.4 MeV) by full PVC calculation is $\int S_{\text{full}} d\omega = 1.5$ fm$^4$, and by the calculation with diagonal approximation is $\int S_{\text{dia.}} d\omega = 1.3$ fm$^4$.

Figure 11 shows the strength contributions from different PVC states $\nu$, as given by Eq. (20). The position of $\omega = 16.4$ MeV has been indicated by the vertical dashed line, and the contributions from the RPA states are given by the gray vertical lines in the background. For the full
calculation, the largest contribution to the strength at $\omega = 16.4$ MeV comes from the PVC state at $\Omega_{\nu} = 16.7$ MeV while, for the diagonal approximation, the largest contribution comes from the state at $\Omega_{\nu} = 17.2$ MeV. At variance with the situation discussed in Fig. 5, these two PVC states are both close to the energy being evaluated ($\omega = 16.4$ MeV). Therefore, from Eq. (20), one can hint that the difference in the strength should come from the difference in the transition matrix element in these two calculations.

In Fig. 12 the real part of the square of the transition matrix element $\langle 0|O|\nu \rangle$ is shown. As expected, the transition matrix element of the state $\Omega_{\nu}$(full) = 16.7 MeV is larger than the state $\Omega_{\nu}$(dia.) = 17.2 MeV, and this explains the larger strength in the full calculation.

To understand the difference in the transition matrix elements, we show in Fig. 13 the PVC wave function $F^{(\nu)}_n$ (15) of states $\Omega_{\nu}$(full) = 16.7 MeV and $\Omega_{\nu}$(dia.) = 17.2 MeV in the basis of RPA phonons $|n\rangle$, and the transition matrix elements $\langle n|O|0 \rangle$ in the RPA representation. The transition matrix elements $\langle 0|O|\nu \rangle$ in the PVC representation in Fig. 12 can be calculated as in Eq. (43).

Differently, again, from the situation of the lowest peak in the ISGQR, these two states in Fig. 13 have very different RPA components. In the calculation with the diagonal approximation, the major RPA component of the state $\Omega_{\nu}$(dia.) = 17.2 MeV can be identified as the 4th RPA phonon, while the state $\Omega_{\nu}$(full) = 16.7 MeV has the same major component but very much mixed with the 6th RPA phonon. Since the 6th RPA phonon has a larger transition matrix element than the 4th RPA phonon, according to Eq. (43), the transition matrix element for $\Omega_{\nu}$(full) = 16.7 MeV is also larger.

In Fig. 14 we show the 1p-1h components of these two PVC states as well as the related RPA states $\omega_{n=4} = 18.6$ MeV and $\omega_{n=6} = 19.8$ MeV. As mentioned above, the PVC state $\Omega_{\nu}$(dia.) = 17.2 MeV is dominated by the RPA phonon $\omega_{n=4} = 18.6$ MeV and therefore its wave function in the 1p-1h representation is very similar to this.
phonon. For PVC state \( \Omega_{\nu}^{\text{full}} = 16.7 \) MeV, the RPA component \( \omega_n = 18.6 \) MeV, which is mainly a neutron \( p_{1/2} \) excitation, is very much mixed with the component \( \omega_n = 19.8 \) MeV, which is mainly a proton \( p_{1/2} \) excitation. In other words, in the full PVC calculation there is a coupling between a neutron 1p-1h excitation and a proton 1p-1h excitation, which can not show up in the calculation with the diagonal approximation as we discuss in detail in what follows.

The reason for the coupling between neutron and proton 1p-1h states is shown in Fig. 15, in which the matrix elements of the spreading term in both full PVC calculation and calculation with diagonal approximation are plotted. The index \( ph \) is the same as in Fig. 14. As expected, most of the matrix elements are attractive (negative values) and therefore the strength distributions are shifted to a lower energy.

The general pattern of the matrix is similar for both full PVC calculation and PVC with diagonal approximation. However, there is a clear difference that the matrix elements of neutron-proton interaction in full PVC are nonzero while in PVC with diagonal approximation they are zero. This can be understood from the expression of spreading term in Eq. (34) and the diagram in Fig. 1. The matrix element \( A_{p'h'1n,p1h1n} \) in Eq. (34) (or \( Q_2HQ_2 \) in Fig. 1) can not couple the initial 1p-1h excitation \( (p1h) \) with the final 1p-1h excitation \( (p'h') \) that has a different charge, and the same is true for \( A_{p1h1n,p'h} \). Only in the denominator \( A_{p1h1n,p1h1n} \) (or \( Q_2HQ_2 \) in Fig. 1) there is interaction \( \bar{V}_{p1h2n}Q_{2} \) between the initial and final 1p-1h excitations with different charges. When the diagonal approximation is applied in the denominator \( Q_2HQ_2 \), this interaction is removed and as a consequence the spreading term has zero matrix elements in the off-diagonal blocks where the neutron and proton 1p-1h excitations interact.

In the case of ISGQR discussed in Fig. 8, the original RPA phonon is already composed of many neutron and proton 1p-1h excitations. Therefore in that case the coupling between 1p-1h states of different charges nature via the denominator in Eq. (34) is not significant.

E. Dependence of different functionals

To test the dependence of the results on the choice of different functionals, in Fig. 16 we show the strength function of ISGMR, ISGDR, and ISGQR in \(^{16}\text{O}\) calculated by full PVC with and without subtraction using

![FIG. 14: (Color online) RPA wave function (X amplitudes) of the state with excitation energy (a) \( \omega_n = 18.6 \) MeV and (b) \( \omega_n = 19.8 \) MeV in the 1p-1h representation, see Eq. (8). Different regions divided by vertical lines are for different hole states. (c) Real part of the PVC wave functions of states with excitation energies \( \Omega_{\nu}^{\text{full}} = 16.7 \) MeV and \( \Omega_{\nu}^{\text{dia.}} = 17.2 \) MeV, see Eq. (44), by the two PVC calculations: with (dia.) and without (full) diagonal approximation.](image)

![FIG. 15: (Color online) Matrix elements of spreading term in the 1p-1h representation (a) in the full PVC calculation (34) and (b) in PVC calculation with diagonal approximation (36).](image)
For the detail of the experimental data as an example, SKX gives the lowest energy different Skyrme functionals: SAMi [57], SIV [64], SkI3 [65], and SKX [66]. As it can be seen from the figure, the basic features such as the shape of the strength distributions obtained with different functionals are similar to each other, while in detail the results depend very much on the selected functional. Taking the lowest peak in (a-c) of Fig. 16 as an example, SKX gives the lowest energy in all three cases: around 12 MeV in ISGMR, 3.5 MeV in ISGDR, and 12.5 MeV in ISGQR; SIV gives the highest energy, around 18 MeV in ISGMR, 9 MeV in ISGDR, and 15.5 MeV in ISGQR; SAMi and SkI3 sit in between with SkI3 gives slightly lower energy.

For ISGMR, if the states near 12 and 14 MeV are attributed to cluster vibrations [63], the rest of the resonance strength around 18, 24, and 31 MeV is best described by the SIV functional. For ISGDR, SIV gives a very strong lowest excitation near 9 MeV, in agreement with the strong experimental excitation near 7 MeV; however, the strength from 12 MeV to 24 MeV by SIV is not described as well as with the other functionals. The dependence on the functional in the case of the ISGDR when $E > 30$ MeV is very small. In the case of the ISGQR, SIV and SkI3 give a better description, from the excitation near 15 MeV, to 19, 21, and 25 MeV. The strong strength near 12 MeV given by SKX is in agreement with the data, but this model gives a too large strength near 17 MeV where no experimental peak appears.

When subtraction is included in the PVC calculations shown in (d-f) of Fig. 16, the effect for different functionals are similar to the one that has been investigated in Sec. IV A using SAMI. The strength distributions are generally shifted to a higher energy by about $≈ 1 − 2$ MeV. For ISGMR, the first two peaks’ positions given by SIV are now slightly higher than the data, while the major peak near $≈ 22 − 24$ MeV given by SkI3 is in good agreement with the data. For the ISGDR, the strength distribution given by SKX has been improved, and it describes well the experimental structures near 7, 11, and 19 − 22 MeV. In this case the results from other functionals are not as good as they were before subtraction. For the ISGQR, the description by SkI3 is improved with subtraction and the peaks near 19 and 21 MeV are in good agreement with the data.

The correlation between the excitation energy calculated at RPA level and nuclear matter properties has been extensively studied (cf. [16] and references therein). For instance, the compression mode ISGMR and ISGDR are correlated with the incompressibility coefficient $K_\infty$; the ISGQR is correlated with the effective mass $m^*/m$. Such correlations still persist at the PVC level. For example, among the four functionals, SAMI gives the smallest incompressibility coefficient with $K_\infty^{(SAMI)} = 245$ MeV while SIV gives the largest $K_\infty^{(SIV)} = 325$ MeV. Accordingly, the constrained energy $E_c = \sqrt{m_1/m_2}$ given by these two functionals are $E_c^{(SAMI)} = 23.7$ MeV and $E_c^{(SIV)} = 26.7$ MeV for ISGMR, $E_c^{(SAMI)} = 26.2$ MeV and $E_c^{(SIV)} = 28.5$ MeV for ISGDR. SKX gives the largest effective mass with $m_1^{SKX}/m = 0.99$ and SIV the smallest $m_1^{SIV}/m = 0.47$. Accordingly, the centroid energy of ISGQR given by SKX is 15.0 MeV while by SIV is 21.6 MeV. These relations are also reflected in Fig. 16.
V. SUMMARY

In this work we have developed the fully self-consistent particle-vibration model without the diagonal approximation, that is, the interaction among the doorway states has been taken into account. The full PVC has been used to study the isoscalar giant monopole, dipole, and quadrupole resonances of $^{16}$O using Skyrme functionals. The results are compared with the second RPA [23, 62] and time-blocking approximation [61].

The importance of including self-consistently the full interaction in the PVC vertex has been shown, by considering the strength distributions and sum rules. Among the different terms of the Skyrme interaction other than the central term, the spin-orbit term, which has been ignored in most previous PVC studies, plays a significant role in our current study, especially in the case of the ISGQR.

The diagonal approximation has also much influence on the strength distribution of the ISGQR in $^{16}$O. Without diagonal approximation, the strength distribution of the ISGQR is more fragmented and wider, in better agreement with the experimental data. A new peak near $E = 15$ MeV appears in the full PVC calculation (also present at lower energies in the experimental data). Such peak has been used as an example to show the difference induced by the diagonal approximation for the eigenenergies. For the case of ISGMR and ISGDR, the strength distributions in $^{16}$O are less influenced by the diagonal approximation; and in all cases, the sum rules are not influenced much by the diagonal approximation.

Another important drawback of the diagonal approximation is that one implicitly neglects the possibility of coupling between neutron and proton 1p-1h excitations included in the doorway states, that is instead recovered in the full PVC calculation. This difference is more prominent in situations where two phonons are dominated, respectively, by either a neutron or a proton 1p-1h excitation, as the interaction between 1p-1h excitations with different charge in the diagonal approximation is set to zero. When the phonon is already composed with mixed neutron and proton 1p-1h excitations, removing the diagonal approximation may not be significant.

The subtraction method, which has been developed to renormalize the effective interaction beyond RPA, has also been investigated within the framework of full PVC calculations. It solves, to some extent, the problem that the centroid of strength distributions is slightly too low compared with experimental data.

Although we have shown that removing the diagonal approximation is a step to be done, there is still room to improve the PVC models. We plan to perform further investigation on the proper treatment of phonons in the doorway states. A recent investigation within the time blocking approximation [32] might provide some interesting insight in this respect, as the authors propose a way to choose the most relevant phonons and achieve convergence with respect to the model space. At the same time, the full PVC should be tested in more nuclei and, even more importantly, in the case of other types of resonances such as spin-isospin resonances. This may impact on the problem of the Gamow-Teller quenching or on the $\beta$-decay processes of astrophysical interest.

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Appendix A: Effective Hamiltonian in $Q_1$ subspace

The subspaces $P$, $Q_1$ and $Q_2$ have the following properties

$$P^2 = P, \quad Q_1^2 = Q_1, \quad Q_2^2 = Q_2,$$

$$PQ_1 = PQ_2 = Q_1Q_2 = 0,$$

$$P + Q_1 + Q_2 = 1.$$  \hfill (A1)

The eigenequation

$$H\Psi = \omega\Psi$$ \hfill (A2)

becomes

$$H(P + Q_1 + Q_2)\Psi = \omega(P + Q_1 + Q_2)\Psi.$$ \hfill (A3)

Multiply operator $P, Q_1, Q_2$ to both side of Eq. (A3) and using the properties of (A1), one can obtain a set of equations

$$(\omega - H_{PQ_1}) P\Psi = H_{PQ_1}Q_1\Psi + H_{PQ_2}Q_2\Psi,$$ \hfill (A4a)

$$(\omega - H_{Q_1}) Q_1\Psi = H_{Q_1P}P\Psi + H_{Q_1Q_2}Q_2\Psi,$$ \hfill (A4b)

$$(\omega - H_{Q_2}) Q_2\Psi = H_{Q_2P}P\Psi + H_{Q_2Q_1}Q_1\Psi,$$ \hfill (A4c)

with the subscript of the Hamiltonian represents, e.g., $H_{PQ_1} = PHQ_1$. From Eqs. (A4a, A4c), one has

$$P\Psi = \frac{1}{\omega - H_{PP}}H_{PQ_1}Q_1\Psi + \frac{1}{\omega - H_{PP}}H_{PQ_2}Q_2\Psi,$$ \hfill (A5a)

$$Q_2\Psi = \frac{1}{\omega - H_{Q2Q_2}}H_{Q2P}P\Psi + \frac{1}{\omega - H_{Q2Q_2}}H_{Q2Q_1}Q_1\Psi.$$ \hfill (A5b)

A small quantity $i\epsilon$ should be added in the denominator but has not been written out explicitly. Substitute back into Eq. (A4b), one obtains [48]

$$(\omega - H_{Q_1}) Q_1\Psi = [W^\dagger(\omega) + W^\dagger(\omega) + \ldots] Q_1\Psi,$$ \hfill (A6)

with the expression of $W^\dagger(\omega)$ and $W^\dagger(\omega)$ have been given in Eq. (14). Truncating the expansion to the leading order, one has Eqs. (13) and (14).
Appendix B: Matrix elements of spreading term

Following the equation-of-motion method \[55\], the PVC equation is derived in a similar way as the SRPA in Ref. \[56\]. With Eqs. \(24, 25\) and Eqs. \(30-32\), the full spreading term \(23\) reads

\[
W_{p' h', p h}^{\downarrow} = \sum_{p_1 h_1, p_1 h_1 n} \left( \begin{array}{cc} A_{p' h', p' h'}^{\downarrow} & 0 \\ 0 & -A^{\ast}_{p' h', p' h'} \end{array} \right) \left( \begin{array}{cc} 1 & 0 \\ \omega - A^{\ast}_{p' h'} n_{p h} & 1 \end{array} \right) \left( \begin{array}{cc} 1 & 0 \\ \omega + A_{p h} n_{p h} & 1 \end{array} \right) \left( \begin{array}{cc} 0 & -A^{\ast}_{p_1 h_1 n_{p h}} \\ 0 & 1 \end{array} \right)
\]

\(B1\)

This is a two-by-two matrix with dimension corresponding to the RPA matrix in Eq. \(5\). Without causing confusion we can write it as

\[
W_{p' h', p h}^{\downarrow} \rightarrow \left( \begin{array}{cc} W_{p' h', p h}^{\downarrow}(\omega) & 0 \\ 0 & -W^{\ast}_{p' h', p h}(-\omega) \end{array} \right)
\]

\(B2\)

with \(W_{p' h', p h}^{\downarrow}(\omega)\) given in Eq. \(34\). When the PVC equation is solved in the RPA phonon basis, one can transform this matrix to the phonon representation by

\[
W_{n', n}^{\downarrow} = \sum_{p' h', p h} \left[ W_{p' h', p h}^{\downarrow}(\omega) X_{p' h'}^{(n')} \right] X_{p h}^{(n)}, \quad \text{for spherical nuclei, the particle-hole } jj \text{-coupled matrix element can be used, which is defined as}
\]

\[
\langle 12|\hat{V}|34\rangle = \sum_{m_1 m_2 m_3 m_4} (-1)^{j_1-j_3-m_3} C_{j_1 m_1 j_3 m_3}^{j_4 m_2 m_4} (-1)^{j_2-m_2} C_{j_4 m_2 m_4}^{j_3 m_3 m_1} \langle 12|\hat{V}|34\rangle.
\]

\(B4\)

The RPA operator \(8\) in the coupled form is

\[
Q_{n L M}^{\dag} = \sum_{p h} \left[ X_{p h}^{n L} A_{p h}^{\dag}(L M) - \bar{Y}_{p h}^{n L} A_{p h}(L M) \right]
\]

\(B5\)

with

\[
A_{p h}^{\dag}(L M) = \sum_{m_p m_h} (-1)^{j_h-m_h} C_{j_p m_p j_h-m_h}^{L M} a_{m_p}^{\dag} a_{m_h},
\]

\(B6\)

\[
A_{p h}(L M) = \sum_{m_p m_h} (-1)^{L+M+j_h-m_h} C_{j_p m_p j_h-m_h}^{L-M} a_{m_h} a_{m_p}.
\]

\(B7\)

From now on without specification, the quantum number will not include the magnetic one, for example, the summation in Eq. \(B5\) do not include \(m_p\) or \(m_h\). The RPA matrix \(6\) in the \(jj\)-coupled form (with coupled total angular momentum \(J\)) simply becomes

\[
A_{p' h', p h}^{\dag} = \delta_{p' h', p h} (e_p - e_h) + \hat{V}_{p' h', p h}^{\dag}, \quad B_{p' h', p h}^{J} = \hat{V}_{p' h', p h}^{J}.
\]

\(B8\)

The \(jj\)-coupled form of the spreading term \(34\) is more complicated. We first give the \(jj\)-coupled form of Eq. \(31\), with coupled total angular momentum \(\lambda\),

\[
A_{p_1 h_1, p_2 h_2}^{\lambda} = \delta_{p_1 h_1, p_2 h_2} \left[ \delta_{p_1 h_1, p_2 h_2} (\omega_{n_1 L_1} + e_{p_1 h_1}) + \bar{V}_{p_1 h_1, p_2 h_2}^{\lambda} \right],
\]

\(B9\)

Let the inverse of matrix \(\omega - A_{p_1 h_1, p_2 h_2}^{\lambda} + i \epsilon\) be labeled as \(D_{11}(\omega)\), and the inverse of matrix \(-\omega - A_{p_1 h_1, p_2 h_2}^{\lambda} + i \epsilon\) be labeled as \(D_{22}(\omega)\), they satisfy the follow equation (take \(D_{11}\) as an example)

\[
\sum_{p_1 h_1} \left[ \delta_{p_1 h_1} (\omega + i \epsilon - \omega_{n L} - e_{p_1 h_1}) - \bar{V}_{p_1 h_1, p_1 h_1}^{\lambda} \right] \langle p_1 h_1 | D_{11}(\omega) | p_2 h_2 \rangle^{\lambda}_{n L} = \delta_{p_1 h_1, p_2 h_2}.
\]

\(B10\)
Since $D_{22}$ can be obtained in the same equation (B10) by simply replacing $\omega$ to $-\omega$, we will not distinguish these two matrix explicitly and simply write $\langle p_1 h_1 | D(\omega) | p_2 h_2 \rangle_{nL}^\lambda$. In the end, the full spreading term (34) in the $jj$-coupled form can be written as

$$W^{(j)}_{p'h',ph}(\omega) = \sum_{k=1}^4 W^{(j)}_{p'h',ph}(k; \omega),$$

with

$$W^{(j)}_{p'h',ph}(1; \omega) = \sum_{\lambda p_i} \sum_{nL,p_i} F_1 \hat{\lambda}^2 \hat{L}^2 \left\{ j p_i j h' j p \lambda \right\} \left\{ j p_j j h j p \lambda \right\} \langle p'|V|p_1,nL\rangle \langle p_1 h'_1 | D(\omega) | p_1 h \rangle_{nL} \langle nL,p_1 V|p \rangle,$$  \hspace{1cm} (B12a)

$$W^{(j)}_{p'h',ph}(2; \omega) = \sum_{\lambda h_i} \sum_{nL,h_i} F_2 \hat{\lambda}^2 \hat{L}^2 \left\{ j h_i j h' j p \lambda \right\} \left\{ j h_j j h j p \lambda \right\} \langle h'_1 |V|h',nL\rangle \langle p_1 h'_1 | D(\omega) | p_1 h \rangle_{nL} \langle nL,h V|h_1 \rangle,$$  \hspace{1cm} (B12b)

$$W^{(j)}_{p'h',ph}(3; \omega) = \sum_{\lambda p_i} \sum_{nL,p_i} F_3 \hat{\lambda}^2 \hat{L}^2 \left\{ j p_i j h' j p \lambda \right\} \left\{ j p_j j h j p \lambda \right\} \langle p'|V|p_1,nL\rangle \langle p_1 h'_1 | D(\omega) | p_1 h \rangle_{nL} \langle nL,p_1 V|p \rangle,$$  \hspace{1cm} (B12c)

$$W^{(j)}_{p'h',ph}(4; \omega) = \sum_{\lambda h_i} \sum_{nL,h_i} F_4 \hat{\lambda}^2 \hat{L}^2 \left\{ j h_i j h' j p \lambda \right\} \left\{ j h_j j h j p \lambda \right\} \langle h'_1 |V|h',nL\rangle \langle p_1 h'_1 | D(\omega) | p_1 h \rangle_{nL} \langle nL,p_1 V|h_1 \rangle.$$  \hspace{1cm} (B12d)

Schematic diagrams for these terms are shown in Fig. 17 (a-d).

![Diagram](image)

FIG. 17: (a-d) Diagrammatic show of the four terms $W^{(j)}_{p'h',ph}(k; \omega)$ without diagonal approximation in Eq. (B12); (e-h) with diagonal approximation in Eq. (B16).

In the above equation, $\hat{\lambda} = \sqrt{2\lambda + 1}$, $\hat{L} = \sqrt{2L + 1}$. The coupled matrix element $\langle a | V | b, nL \rangle$ is different from the general expression in Eq. (33) by

$$\langle a | V | b, nL \rangle = \sum_{p_1 h_1} \left[ X_{p_1 h_1}^{nL} \bar{V}_{abh}^{L} + (-1)^{L+j_0-j_h} Y_{p_1 h_1}^{nL} \bar{V}_{abh}^{L} \right],$$  \hspace{1cm} (B13a)

$$\langle nL, a | V | b \rangle = \sum_{p_1 h_1} \left[ (-1)^{L+j_0-j_h} X_{p_1 h_1}^{nL} \bar{V}_{abh}^{L} + Y_{p_1 h_1}^{nL} \bar{V}_{abh}^{L} \right].$$  \hspace{1cm} (B13b)

The phases in the above equations are

$$F_1 = (-1)^{j_{h'}+j_{h'}+j_{h}+L+j_{p_1}}, \hspace{1cm} F_2 = (-1)^{j_{h'}+j_{h'}+j_{h}+j_{p}+j_{p_1}},$$

$$F_3 = (-1)^{j_{h'}+j_{h'}+j_{h}+j_{p}+\lambda+j_{p_1}}, \hspace{1cm} F_4 = (-1)^{j_{h'}+j_{h'}+j_{h}+j_{p}+\lambda+j_{p_1}}.$$  \hspace{1cm} (B14)

When the diagonal approximation is adopted, one has

$$\langle p_1 h_1 | D(\omega) | p_1 h_1 \rangle_{nL}^{\lambda} = \frac{1}{\omega - (\omega_{nL} + c_{p_1 h_1}) + i\epsilon}.$$  \hspace{1cm} (B15)
There is no longer $\lambda$ dependence of matrix $D$, and the spreading terms in Eq. (B12) can be reduced to

\begin{align}
W_{p',h',\omega}^{(1)}(1: \omega) &= \delta_{h'h}\delta_{j'p,jp} \sum_{nLp_1} (-1)^{L+jp-jp_1} \frac{\hat{L}^2}{j''_p} \frac{\langle p'|V|p_1,nL\rangle \langle nL,p_1|V|p \rangle}{\omega - (\omega_{nL} + e_{p,h}) + i\epsilon} \\
W_{p',h',\omega}^{(2)}(2: \omega) &= \delta_{p,p'}\delta_{j'p,jp} \sum_{nLh_1} (-1)^{L+jh-jh_1} \frac{\hat{L}^2}{j''_p} \frac{\langle h_1|V|h',nL\rangle \langle nL,h|V|h' \rangle}{\omega - (\omega_{nL} + e_{p,h}) + i\epsilon} \\
W_{p',h',\omega}^{(3)}(3: \omega) &= -(-1)^{J+jp+jh} \sum_{nL} \hat{L}^2 \left\{ \begin{array}{c}
\sum_{j,J} \langle j'p|L \rangle \langle L|j \rangle \langle j'|p|nL\rangle \langle nL|L|j'p \rangle \langle j'h|nL\rangle \langle nL|h'|j'p \rangle \langle j|h'|p|nL\rangle \langle nL|p'|V|p \rangle \\
\omega - (\omega_{nL} + e_{p,h}) + i\epsilon
\end{array} \right\} \\
W_{p',h',\omega}^{(4)}(4: \omega) &= -(-1)^{J+jp+jh} \sum_{nL} \hat{L}^2 \left\{ \begin{array}{c}
\sum_{j,J} \langle j'p|L \rangle \langle L|j \rangle \langle j'|p|nL\rangle \langle nL|L|j'p \rangle \langle j|h'|nL\rangle \langle nL|p'|V|p \rangle \\
\omega - (\omega_{nL} + e_{p,h}) + i\epsilon
\end{array} \right\}
\end{align}

They are in agreement with previous studies [41]. Schematic diagrams for these terms are shown in Fig. 17 (c-h).
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