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Microscopic multiphonon method for odd nuclei and its application to ^{17}O

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An equations of motion phonon method is extended to odd nuclei. It generates an orthonormal basis out of an odd particle coupled to n-phonon core states ($n = 0,1,2,\dots$), built of Tamm-Dancoff phonons, and formulates the eigenvalue problem in such a multiphonon particle-core space. ^{17}O is chosen as testing ground. An intrinsic chiral Hamiltonian is adopted in a large configuration space to perform a calculation using a Hartree-Fock (HF) basis in a space encompassing up to two and, under simplifying assumptions, three phonons. The impact of the different phonon components on spectrum, moments, transitions, and dipole cross section is discussed.

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The excitations of the core are known to modify the single-particle states. The basic mechanism is illustrated within the particle-vibration coupling (PVC) model [1,2] in which a particle is coupled to the collective excitations of the core, commonly described in the random-phase approximation (RPA).

More refined PVC calculations were performed in recent years, mostly within the framework of energy density functionals deduced from Skyrme forces [3–9] or relativistic meson-nucleon Lagrangians [10–13] or from the theory of finite Fermi systems [14]. It was claimed, however, that the contribution of the core vibrations is largely incorporated into the functional [15].

Other approaches used the Gogny interaction [9] or emphasized the role of the Pauli principle within the quasiparticle-phonon context [16] or the importance of the RPA ground-state correlations [17].

Calculations focused mainly on the impact of three-body forces on bulk properties and energy levels were carried out within the no-core shell model [18,19], self-consistent Green's function theory [20], and coupled-cluster theory [21–25].

We proposed for even-even nuclei an equations of motion phonon method (EMPM), in the particle-hole (p-h) [26–28] and quasiparticle [29] schemes, which derives a set of equations generating an orthonormal basis of multiphonon states, built of phonons obtained in the Tamm-Dancoff approximation (TDA), and formulates the eigenvalue problem in such a basis. The method was adopted to study the spectroscopic properties of neutron-rich nuclei with special attention to the dipole response [29–32].

Here, we derive analogous equations for odd nuclei which yield an orthonormal basis out of states composed of an odd particle coupled to n phonons ($n = 1,2,\dots n\dots$), describing the excitations of a doubly magic core and, then, adopt such a basis to solve the full eigenvalue problem. The formalism has the same accuracy of the shell model. On the other hand, it lends naturally to an approximate treatment in virtue of the particle-phonon structure of the basis. It is possible, for instance, to truncate the phonon space while keeping the effects of p-h configurations of very high energy, since these are incorporated into the phonons included in the truncated space. An analogous formalism holds also for hole-phonon and quasiparticle-phonon schemes.

For way of illustration, we apply the method to ^{17}O and perform a calculation in a HF basis using an optimized chiral nucleon-nucleon potential at next-to-next leading order ($\mathrm{NNLO_{opt}}$), which minimizes the contribution of the three-body term [33]. This potential gives too much attraction in heavy nuclei and forced us to add a phenomenological repulsive density-dependent term to reproduce the peak of the giant dipole resonance in ^{208}Pb [32]. Here, this phenomenological term is unnecessary since $\mathrm{NNLO_{opt}}$ reproduces well the experimental binding energies of light nuclei and oxygen isotopes. We will therefore use only the $\mathrm{NNLO_{opt}}$ potential.

The complex shell structure of the low-lying states in ^{17}O was pointed out in the pioneering work of Brown and Green [34] and investigated further within a weak-coupling model [35,36].

More recently, the low-lying spectra of $A = 17$ nuclei were studied within the coupled cluster theory using a chiral potential at next-to-next-to-next leading order ($\mathrm{N^3LO}$) [22]. The electric dipole strength distribution was determined by a shell-model calculation using the empirical WB10 interaction [37] in a restricted space.

The method. We adopt the formalism of second quantization and denote by $a_r^\dagger = a^\dagger_{x_r j_r m_r}$ and $b_r = (-)^{j_r+m_r} a_{x_r j_r -m_r}$ the creation and annihilation operators, respectively.

In even nuclei, we determined an orthonormal basis of n-phonon states of the form

$$|\beta_n\rangle = \sum_{\lambda\alpha_{n-1}} C^{\beta_n}_{\lambda\alpha_{n-1}} |(\lambda \times \alpha_{n-1})^{\beta_n}\rangle$$
$$= \sum_{\lambda\alpha_{n-1}} C^{\beta_n}_{\lambda\alpha_{n-1}} \{O^\dagger_\lambda \times |\alpha_{n-1}\rangle\}^{\beta_n}, \quad (1)$$

where $|\alpha_{n-1}\rangle$ are assumed to be known and

$$O^\dagger_\lambda = \sum_{\mathrm{ph}} c^\lambda_{\mathrm{ph}} (a^\dagger_{\mathrm{p}} \times b_{\mathrm{h}})^\lambda \quad (2)$$

is a TDA operator of energy E_λ.

The key for achieving this goal was provided by the equations of motion

$$\langle\beta\|[H,O^\dagger_\lambda]\|\alpha\rangle = (E_\beta - E_\alpha)X^\beta_{\lambda\alpha}, \tag{3}$$

having omitted the subscript n for simplicity. Here H is a two-body Hamiltonian and

$$X^{(\beta)}_{\lambda\alpha} = \langle\beta\|O^\dagger_\lambda\|\alpha\rangle = \sum_{\lambda'\alpha'}\mathcal{D}^\beta(\lambda\alpha\lambda'\alpha')C^\beta_{\lambda'\alpha'}, \tag{4}$$

where use has been made of Eq. (1). $\mathcal{D}$ is the overlap or metric matrix

$$\mathcal{D}^\beta(\alpha\lambda\alpha'\lambda') = \langle(\lambda\times\alpha)^\beta|(\lambda'\times\alpha')^\beta\rangle, \tag{5}$$

which reintroduces the exchange terms among different phonons and therefore restores the Pauli principle.

After expanding the commutator and expressing the amplitudes X in terms of the C coefficients, we obtained

$$\sum_{\lambda'\alpha'}(\mathcal{AD})^\beta(\lambda\alpha\lambda'\alpha')C^\beta_{\lambda'\alpha'} = E_\beta\sum_{\lambda'\alpha'}\mathcal{D}^\beta(\lambda\alpha\lambda'\alpha')C^\beta_{\lambda'\alpha'}, \tag{6}$$

where

$$\mathcal{A}^{(\beta)}_{\lambda\alpha\lambda'\alpha'} = (E_\lambda + E_\alpha)\delta_{\lambda\lambda'}\delta_{\alpha\alpha'} + \mathcal{V}^{(\beta)}_{\lambda\alpha\lambda'\alpha'}. \tag{7}$$

$\mathcal{V}^{(\beta)}_{\lambda\alpha\lambda'\alpha'}$ is a phonon-phonon potential, whose expression can be found, for instance, in Ref. [32]. This is a generalized eigenvalue equation in the overcomplete basis $|(\lambda\times\alpha)^\beta\rangle$. Following a procedure [26,27] based on the Cholesky decomposition method, we selected a basis of linearly independent states $|(\lambda\times\alpha)^\beta\rangle$ spanning the physical subspace of the correct dimensions $N_n < N_r$ and construct a $N_n\times N_n$ nonsingular matrix $\mathcal{D}_n$. By left multiplication in the N_n-dimensional subspace, we got

$$\big[\mathcal{D}_n^{-1}\mathcal{H}\big]C = \big[\mathcal{D}_n^{-1}(\mathcal{AD})\big]C = EC. \tag{8}$$

This equation determines only the coefficients $C^\beta_{\lambda\alpha}$ of the N_n-dimensional physical subspace, thereby yielding a basis of orthonormal correlated n-phonon states of the form (1).

For the odd systems we intend to construct an orthonormal basis of states $|\nu_n\rangle$ of spin v having the structure

$$|\nu_n\rangle = \sum_{\mathrm{p}\alpha_n}C^{\nu_n}_{\mathrm{p}\alpha_n}|(\mathrm{p}\times\alpha_n)^v\rangle = \sum_{\mathrm{p}\alpha_n}C^{\nu_n}_{\mathrm{p}\alpha_n}(a^\dagger_\mathrm{p}\times|\alpha_n\rangle)^v, \tag{9}$$

where $a^\dagger_\mathrm{p}$ creates a particle of energy ϵ_p, and $|\alpha_n\rangle$, of energy E_{α_n}, are orthonormal n-phonon ($n = 1,2,\dots$) core states of the form (1).

In close analogy with the even nuclei, we start with

$$\langle\alpha_n\|[b_\mathrm{p},H]^\mathrm{p}\|\nu_n\rangle = \big(E_\nu - E_{\alpha_n}\big)X^{(\nu_n)}_{\mathrm{p}\alpha_n}, \tag{10}$$

where

$$X^{(\nu_n)}_{\mathrm{p}\alpha_n} = \langle\alpha_n\|b_\mathrm{p}\|\nu_n\rangle. \tag{11}$$

After expanding the commutator, we obtain

$$\sum_{\mathrm{p}'\alpha'}\big\{\big(\epsilon_\mathrm{p} + E^{(n)}_\alpha - E_{\nu_n}\big)\delta_{\mathrm{p}\,\mathrm{p}'}\delta^{(n)}_{\alpha\alpha'} + \mathcal{V}^{(\nu_n)}_{\mathrm{p}\alpha\mathrm{p}'\alpha'}\big\}X^{(\nu_n)}_{\mathrm{p}'\alpha'} = 0. \tag{12}$$

The particle-phonon interaction is

$$\mathcal{V}^{(\nu_n)}_{\mathrm{p}\alpha\mathrm{p}'\alpha'} = \sum_\sigma[\sigma]^{1/2}W(\alpha\sigma\upsilon\mathrm{p}';\alpha'\mathrm{p})\mathcal{F}^\sigma_{\mathrm{p}\alpha\mathrm{p}'\alpha'}(n), \tag{13}$$

where $[\sigma] = 2J_\sigma + 1$, W is the Racah coefficient, and

$$\mathcal{F}^\sigma_{\mathrm{p}\alpha\mathrm{p}'\alpha'}(n) = \sum_{tq}F^\sigma_{\mathrm{p}\,\mathrm{p}'tq}\rho^{(n)}_{\alpha'\alpha}([t\times q]^\sigma). \tag{14}$$

The sum runs over particles ($tq = \mathrm{p}_1\mathrm{p}_2$) and holes ($tq = \mathrm{h}_1\mathrm{h}_2$), $\rho^{(n)}_{\alpha\alpha'}([t\times q]^\sigma) = \langle n,\alpha\|(a^\dagger_t\times b_q)^\sigma\|n,\alpha'\rangle$ is the density matrix, and

$$F^\sigma_{rsqt} = \sum_\Omega[\Omega](-)^{r+t-\sigma-\Omega}W(rsqt;\sigma\Omega)V^\Omega_{rqst} \tag{15}$$

is the Pandya transformed of the two-body potential V.

Equation (12) is not an eigenvalue equation yet. We have to insert in X the expression (9) of $|\nu_n\rangle$, obtaining

$$\sum_{\mathrm{p}_1\gamma\mathrm{p}'\alpha'}\big\{\big(\epsilon_\mathrm{p} + E^{(n)}_\alpha - E_{\nu_n}\big)\delta_{\mathrm{p}\,\mathrm{p}_1}\delta^{(n)}_{\alpha\gamma} + \mathcal{V}^{(\nu_n)}_{\mathrm{p}\alpha\mathrm{p}_1\gamma}\big\}\mathcal{D}^{(\nu_n)}_{\mathrm{p}_1\gamma\mathrm{p}'\alpha'}C^{\nu_n}_{\mathrm{p}'\alpha'} = 0, \tag{16}$$

where

$$\begin{aligned}\mathcal{D}^{(\nu_n)}_{\mathrm{p}_1\gamma\mathrm{p}'\alpha'} &= \langle(\mathrm{p}_1\times\gamma)^v|(\mathrm{p}'\times\alpha')^v\rangle\\ &= \delta_{\mathrm{p}_1\mathrm{p}'}\delta_{\gamma\alpha'} - (-)^{\mathrm{p}'-v+\alpha'}\sum_\sigma[\sigma]^{1/2}\\ &\quad\times W(\mathrm{p}_1\mathrm{p}'\gamma\alpha';\sigma\upsilon)\rho^{(n)}_{\gamma\alpha'}([\mathrm{p}_1\times\mathrm{p}']^\sigma)\end{aligned} \tag{17}$$

is the overlap matrix which reintroduces, through the density matrix ρ, the exchange terms among the odd particle and the n-phonon states, thereby restoring the Pauli principle.

Equation (16) represents an eigenvalue equation in the overcomplete basis $|(\mathrm{p}\times\alpha_n)^v\rangle$ within the n-phonon particle-core subspace. Following the same procedure adopted for the even nuclei, we extract a basis of linearly independent states $|(\mathrm{p}\times\alpha_n)^v\rangle$ and obtain a nonsingular eigenvalue equation. Its iterative solution, starting from $n = 1$, yields the particle-core states $|\nu_n\rangle$ (9) of energies E_{ν_n} for $n = 1,2,\dots$, which, together with the single-particle states $|\nu_0\rangle$, form an orthonormal basis.

We are now ready to formulate the eigenvalue problem in the full space spanned by $\{|\nu_0\rangle,|\nu_1\rangle,\dots,|\nu_n\rangle\dots\}$

$$\sum_{\nu_{n'}}\big\{\big(E_{\nu_n} - \mathcal{E}_\nu\big)\delta_{\nu_n\nu_{n'}} + \mathcal{V}^{(v)}_{\nu_n\nu_{n'}}\big\}\mathcal{C}^{(v)}_{\nu_{n'}} = 0. \tag{18}$$

Here

$$\mathcal{V}^{(v)}_{\nu_n\nu_{n'}} = [v]^{-1/2}\sum_{\mathrm{p}\alpha_n\mathrm{p}'\alpha_{n'}}C^{(\nu_n)}_{\mathrm{p}\alpha_n}\mathcal{V}^{(v)}_{\mathrm{p}\alpha_n\mathrm{p}'\alpha_{n'}}X^{(\nu_{n'})}_{\mathrm{p}'\alpha_{n'}} \tag{19}$$

are nonvanishing for $n' = n+1$ and $n' = n+2$ and

$$\begin{aligned}\mathcal{V}^{(v)}_{\mathrm{p}\alpha_n\mathrm{p}'\alpha_{n'}} &= \delta_{\mathrm{p}\,\mathrm{p}'}\langle\alpha_n|H|\alpha_{n'}\rangle + \delta_{n'(n+1)}\sum_\lambda[\lambda]^{1/2}W\\ &\quad\times(\alpha_{n'}\lambda\upsilon\mathrm{p};\alpha_n\mathrm{p}')\mathcal{F}^\lambda_{\mathrm{p}\,\mathrm{p}'}\langle\alpha_{n'}\|O^\dagger_\lambda\|\alpha_n\rangle,\end{aligned} \tag{20}$$

where

$$\mathcal{F}^\lambda_{\mathrm{p}\,\mathrm{p}'} = \sum_{\mathrm{p}_1\mathrm{h}_1}F^\lambda_{\mathrm{p}\,\mathrm{p}'\mathrm{p}_1\mathrm{h}_1}c^\lambda_{\mathrm{p}_1\mathrm{h}_1}. \tag{21}$$

Equation (18) yields all the eigenvalues allowed by the space dimensions. The eigenfunctions have the structure

$$|\Psi_\nu\rangle = \sum_{\nu_n} \mathcal{C}^{\nu}_{\nu_n} |\nu_n\rangle = \sum_{\mathrm{p}\alpha_n} \mathcal{C}^{\nu}_{\mathrm{p}\alpha_n} |(\mathrm{p}\times\alpha_n)^{\nu}\rangle, \tag{22}$$

where $\mathcal{C}^{\nu}_{\mathrm{p}\alpha_n} = \sum_{\nu_n} \mathcal{C}^{\nu}_{\nu_n} C^{\nu_n}_{\mathrm{p}\alpha_n}$, having made use of Eq. (9).

A numerical application. A Hamiltonian composed of an intrinsic kinetic term T_{int} and the NNLO$_{\mathrm{opt}}$ potential [33] was employed to generate the HF basis in a space encompassing all harmonic oscillator (HO) shells up to $N_{\max} = 15$. A subset of these states, spanning a space of dimensions corresponding to twelve major shells up to $N = 11$, was used to determine the TDA phonon basis. The center of mass spurious admixtures were eliminated by a Gramm-Schmidt orthogonalization of the 1^- p-h configurations to the spurious state $\propto \vec{R}_{CM}|0\rangle$ [39].

The multiphonon basis included all $|(\mathrm{p}\times\alpha_1)^{\nu}\rangle$, the $|(\mathrm{p}\times\alpha_2)^{\nu}\rangle$ of two-phonon energies $E_{\alpha_2} \leqslant 35$ MeV, and the $|(\mathrm{p}\times\alpha_3)^{\nu}\rangle$ of energies $\epsilon_{\mathrm{p}} + E_{\alpha_3} \leqslant 55$ MeV.

The inclusion of three phonons has required several shortcuts. We ignored the interaction $\mathcal{V}^{(\nu)}_{\mathrm{p}\alpha_3\mathrm{p}'\alpha'_3}$ [Eq. (13)] and put $\mathcal{D}^{(\nu)}_{\mathrm{p}\alpha_3\mathrm{p}'\alpha'_3} \simeq \delta_{\mathrm{p}\,\mathrm{p}'}\delta_{\alpha_3\alpha'_3}$ in Eq. (16), thereby neglecting the exchange terms. Under these approximations, the three-phonon eigenstates are simply $|\nu_3\rangle \sim |(\mathrm{p}\times\alpha_3)^{\nu}\rangle$ and the couplings (19) become

$$\mathcal{V}^{(\nu)}_{\nu_n\nu_3} = \sum_{p\alpha_n} C^{(\nu_n)}_{\mathrm{p}\alpha_n} \mathcal{V}^{(\nu)}_{\mathrm{p}\alpha_n\mathrm{p}'\alpha_3}. \tag{23}$$

We further determined the core states $|\alpha_3\rangle$ in the diagonal approximation by putting $\mathcal{V}^{(\alpha_3)}_{\lambda\alpha_2\lambda'\alpha'_2} = 0$ in Eq. (7). The lack of antisymmetrization between the particle and $|\alpha_3\rangle$ may yield some redundant particle-core three-phonon states and overestimate their couplings to the other n-phonon components. The other approximations affect the redistribution of the three-phonon levels lying at very high energy.

The one-phonon coupling brings several low-lying HF levels, especially those of positive parity, fairly close to the single-particle experimental levels (Fig. 1). The calculation, however, is far from reproducing the rich low-lying spectrum. In fact, the particle-core one-phonon states fall at energies that are too high ($\gtrsim$11 MeV).

The low-energy levels are unaffected by the two phonons. These components, in fact, couple weakly to the low-lying one-phonon states just as in ^{16}O [27,28]. Their inclusion contributes to enhancing further the level density in the high-energy sector of the spectrum. The two phonons can admix only with the one-phonon components of comparable energies. This is possible only in the high-energy sector of the spectrum.

The three phonons have a much stronger impact and push few states of negative parity into the low-energy sector. Their number is modest, though. Moreover, the positive-parity one-phonon states remain at high energies. The net result is that the level density increases greatly with the number of phonons at high energy but remains too low at low energy.

The importance of three phonons was established already in ^{16}O [27,28] and can be understood by observing that the one-phonon to three-phonon coupling is intimately correlated with the zero-phonon to two-phonon coupling through the

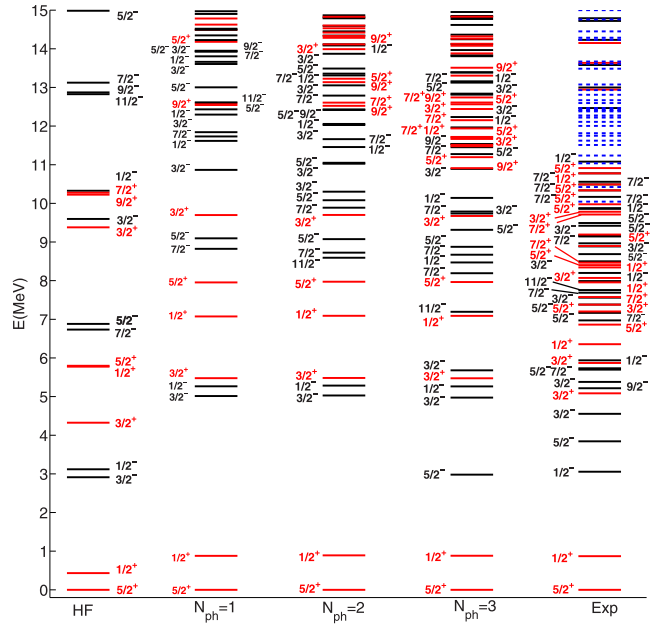

FIG. 1. Theoretical vs experimental [38] spectra of ^{17}O. N_{ph} indicates the maximum phonon number. The dashed levels have unknown spin or parity or both.

formula

$$\langle\alpha_3|V|\alpha_1\rangle = \sum_{\alpha_2} \langle\alpha_3|(\alpha_1\times\alpha_2)^{\alpha_1}\rangle\langle\alpha_2|V|0\rangle. \tag{24}$$

One should therefore expect that such a coupling is strong since the one connecting the HF vacuum to two phonons is very strong. An analogous formula shows that the two phonons couple strongly to four phonons.

The different behavior of states of different parities may be traced back to the HO constituents of the HF states. The HF p-h configurations are built of p-h HO states, whose energies are $(2n+1)\hbar\omega$ and $(2n+2)\hbar\omega$ ($n = 0,1,2,\ldots$) for negative and positive parities, respectively. Correspondingly, the negative-parity phonons have in general lower energies than the corresponding ones of positive parity. Moreover, several three-phonon states are composed entirely of negative phonons and, therefore, have lower energies as well. Two negative-parity phonons are the constituents of the lowest positive-parity two-phonon states. These states, however, would be pushed down in energy by four phonons, which are not included here. They, therefore, do not intrude into the low-energy sector of our level scheme.

For the transition amplitudes of a multipole operator $\mathcal{M}(\lambda)$ we used the truncated formula

$$\langle\psi_{\nu'}\|\mathcal{M}(\lambda)\|\psi_\nu\rangle = \mathcal{M}^{\nu\nu'}_{00}(\lambda) + \mathcal{M}^{\nu\nu'}_{01}(\lambda) + \mathcal{M}^{\nu\nu'}_{10}(\lambda), \tag{25}$$

valid if initial and/or final states have dominant single-particle character. The first term gives the particle-particle transitions

$$\mathcal{M}^{\nu\nu'}_{00} = \sum_{\mathrm{p}\,\mathrm{p}'} \mathcal{C}^{\nu}_{\mathrm{p}} \mathcal{C}^{\nu'}_{\mathrm{p}'} \langle\mathrm{p}'\|\mathcal{M}(\lambda)\|\mathrm{p}\rangle. \tag{26}$$

TABLE I. Ground-state electric quadrupole (Q) and magnetic moments (μ), and $B(E2; 5/2_1^+ \to 1/2_1^+)$. The experimental data are taken from Ref. [38].

	$Q(e\ \mathrm{fm}^2)$	$B(E2\uparrow)(e^2\,\mathrm{fm}^4)$	$\mu(\mu_N)$
HF	0	0	−1.91
EMPM	−0.841	0.17	−1.83
Exp.	−2.578	2.18(16)	−1.89

The second gives the particle-phonon transition

$$\mathcal{M}_{01}^{\nu\nu'}(\lambda) = \sum_{px} \mathcal{C}_p^{\nu} \langle (x\lambda) \| \mathcal{M}(\lambda) \| 0 \rangle P_{\mathrm{p}(x\lambda)}^{(\nu')}, \tag{27}$$

where

$$P_{\mathrm{p}(x\lambda)}^{(\nu')} = \sum_{\nu_1'} \mathcal{C}_{\nu_1'}^{\nu'} X_{\mathrm{p}(x\lambda)}^{\nu_1'} \tag{28}$$

is the weight incorporating the joint contributions of the one-phonon components $|\nu_1'\rangle$ of the final states $|\Psi_{\nu'}\rangle$ and of the particle-phonon configurations of multipolarity λ $|[\mathrm{p} \times (x\lambda)]^{\nu_1'}\rangle$ present in $|\nu_1'\rangle$. The third term gives the phonon-particle amplitude related to the second term by $\mathcal{M}_{10}^{\nu\nu'}(\lambda) = (-)^{\nu-\nu'}\mathcal{M}_{01}^{\nu'\nu}(\lambda)$.

The calculation underestimates the absolute value of the ground-state quadrupole moment by a factor three and the strength of the transition to $1/2_1^+$ by an order of magnitude (Table I).

Let us try to understand why the theoretical quantities assume so small values. Since the odd particle is a neutron ($e_n = 0$), the contribution to the moment and transition strength comes entirely from the terms $\mathcal{M}_{01}(E2)$ [Eq. (27)] and $\mathcal{M}_{10}(E2)$ coupling the single-particle components of $5/2_1^+$ and $1/2_1^+$ to the $\lambda = 2^+$ particle-phonon pieces of $1/2_1^+$ and $5/2_1^+$, respectively. Now $5/2_1^+$ and $1/2_1^+$ have a prominent single-particle character. The one-phonon components account for ∼5% of $|\Psi_{5/2_1^+}\rangle$ and ∼6% of $|\Psi_{1/2_1^+}\rangle$, respectively.

Much smaller are the weights W of the multipole components $|(\mathrm{p} \times \lambda)^{\nu}\rangle$ entering the total wave functions $|\Psi_{\nu}\rangle$. They are calculated using the formula

$$W_{\lambda}^{\nu} = \frac{1}{[\nu]^{1/2}} \sum_{xp\nu_1} |\mathcal{C}_{\nu_1}^{\nu}|^2 C_{\mathrm{p}(x\lambda)}^{\nu_1} X_{\mathrm{p}(x\lambda)}^{\nu_1}, \tag{29}$$

which follows from expanding $\langle\Psi_{\nu}|$ in the normalization condition

$$\langle\Psi_{\nu}|\Psi_{\nu}\rangle = \sum_{\alpha_n} W_{\alpha_n}^{\nu} = 1. \tag{30}$$

The weights of the quadrupole components $|[5/2_i^+ \times (x2^+)]^{\nu}\rangle$ amount only to ∼0.2% for $|\Psi_{5/2_1}\rangle$ and to ∼0.7% for $|\Psi_{1/2_1}\rangle$, while $|[1/2_i^+ \times (x2^+)]^{5/2}\rangle$ account for ∼0.3% of $|\Psi_{5/2_1}\rangle$.

These small amplitudes indicate that single-particle and one-phonon components are not sufficiently admixed by the phonon coupling. We will propose later a possible recipe for strengthening such a coupling.

The quenching of the magnetic moment originates from the spin-flip partners present in the HF p-h configurations of the

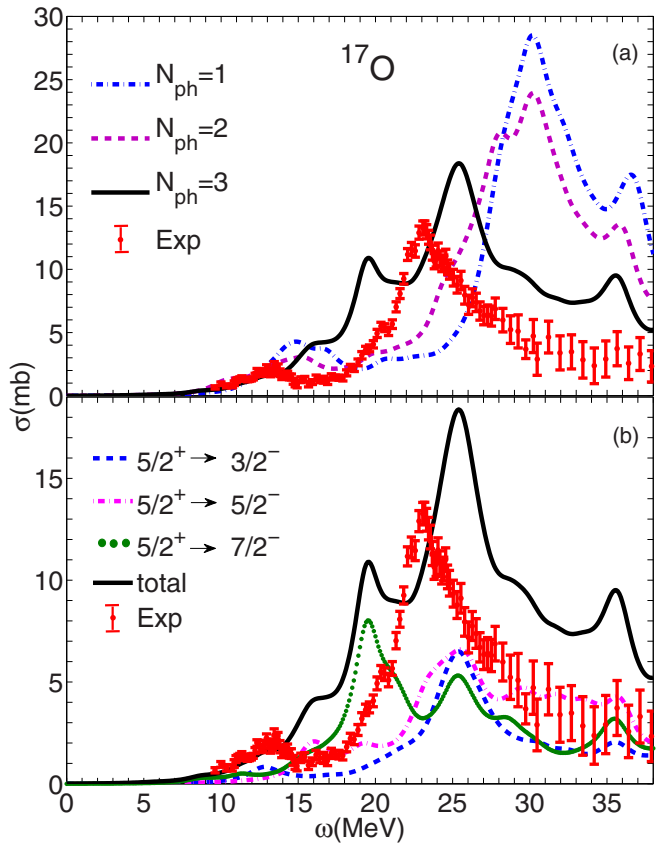

FIG. 2. Theoretical vs experimental [40] $E1$ cross sections (a) and the contributions from the different transitions (b). A Lorentzian of width $\Delta = 2$ MeV was used.

phonons. Though small, it tends to deteriorate the agreement with the experimental value.

The dipole cross section gets damped by the two-phonon coupling and shifted slightly downward in energy. The three phonons cause more substantial damping and push the strength down toward the experimental region. The strong impact of the three phonons can be explained by observing that the contribution to the $B(E1)$ strengths, yielding the cross section, comes mainly from the amplitudes $\mathcal{M}_{01}(E1)$ [Eq. (27)] of the transitions to the one-phonon components of the states $\Psi_{\nu'}$ ($\nu' = 3/2_i^-, 5/2_i^-, 7/2_i^-$). As already pointed out, these components couple strongly to three phonons and are weakly affected by two phonons.

The energy of the resonance peak, however, is still ∼2 MeV above and its height is too high. Figure 2(b) shows that peak and shape of the total cross section depend critically on the way energies and strengths of the groups of transitions to $3/2^-$, $5/2^-$, and $7/2^-$ relate to each others. The contribution of the transitions to $3/2^-$ and $5/2^-$ is concentrated just above the experimental peak, while the one coming from $7/2^-$ is more spread and especially dominant in the low-energy sector.

A massive contribution to the main peak comes from the strengths of a huge number of weak and very weak transitions lying mostly at high energies ($\gtrsim$21 MeV). The states involved have a multiphonon character with two-phonon components comparable in amplitude or larger than the

one-phonon pieces. The contribution at lower energies comes from appreciably strong transitions involving states of dominant one-phonon character. The one-phonon components, in fact, account for 80% to 90% of the total wave functions $\Psi_{\nu'}$ ($\nu' = 3/2_i^-, 5/2_i^-, 7/2_i^-$). They incorporate dipole configurations $|[5/2_i^+ \times (x1^-)]^{\nu_i}\rangle$, the only ones excited by the dipole operator, whose weights [Eq. (29)] range from $W \sim 5\%$ to $W \sim 15\%$.

The integrated cross section up to ∼40 MeV accounts for ∼91% of the Thomas-Reiche-Kuhn sum rule, about twice the fraction (∼50%) exhausted by the data. An appreciable share goes to the pygmy resonance, ∼5.6% versus the measured ∼3.5% for $E \lesssim 16.5$ MeV. Its shape is not reproduced, though.

This large cross section is to be ascribed to the concentration of too much strength at high energy, responsible for the position and height of the main peak, and to the strong transitions at lower energies with consequent overestimation of the cross section below the main peak. Apparently, it would be necessary to reduce the amplitudes of the one-phonon components or, at least, their dipole configurations not only in the states at low energies, of one-phonon character, but also in those at high energies of multiphonon nature.

The analysis of theoretical spectra, transitions, and dipole cross section versus the corresponding experimental quantities indicates that the admixtures among different phonon components are too weak. The phonon composition of the states shows indeed that the one-phonon components have weights that are too small in the states of dominant single-particle character, lying generally at low energies, and amplitudes that are too large in the multiphonon particle-core states.

This insufficient admixing might be traced back to HF. As Fig. 1 shows, its levels or groups of levels above the Fermi surface are too far apart, especially as the energy increases, a common feature of HF spectra derived from nucleon-nucleon interactions [39,41,42]. The phonon coupling fills only partially these gaps.

It is therefore desirable to investigate if it is possible to obtain a smoother HF level scheme by a refinement of the $\mathrm{NNLO_{opt}}$ potential or by adopting other versions of chiral potential like the $\mathrm{NNLO_{sat}}$ [43], which includes the three-body contribution and improves the description of binding energies and nuclear radii as well [44]. A more compact single-particle spectrum would yield more closely packed TDA phonons and would couple them more effectively to HF and the other n-phonon states.

Acting on HF only is not sufficient. Most low-lying positive parity states in ^{16}O have dominant 2p-2h and/or 4p-4h configurations [34,45] and, correspondingly, many states in ^{17}O are mainly 3p-2h) and/or 5p-4h [34]. Thus, for a realistic description of positive-parity spectra it is mandatory to include at least four phonons. As pointed out already, these would push the two phonons down in energy, thereby favoring their mixing with low-lying one-phonon components. Including four phonons is a difficult task which can be accomplished only by resorting to approximations analogous to the ones made for three phonons.

In conclusion, the present formalism makes feasible large-scale, parameter-free calculations, especially under some approximations, starting from bare nucleon-nucleon forces. Due to their particle-phonon structure, the eigenfunctions incorporate configurations of increasing complexity up to arbitrarily high energy and allow a selective analysis of the impact of the different n-phonon states of each multipolarity on all observables. They offer thereby a unified and transparent description of the spectroscopic properties at low and high energy and reliable recipes for curing the deviations from experiments.

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