Proper treatment of the Pauli principle in mirror nuclei within the microscopic particle(hole)-phonon scheme

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(Received 3 October 2019; accepted 6 February 2020; published 19 February 2020)

It is shown that the Cholesky decomposition method, implemented in mirror nuclei to extract an orthonormal basis from a redundant set of states composed of a valence particle (hole) coupled to Tamm-Dancoff approximation (TDA) phonons, yields a few levels which violate the mirror symmetry, at variance with the shell model. A more appropriate implementation of the method is suggested which eliminates this inconsistency.

DOI: 10.1103/PhysRevC.101.024308

I. INTRODUCTION

The particle-vibration coupling (PVC) model is an efficient method for studying the polarizing action of the core excitations on the valence nucleon in odd nuclei [1]. The core vibrations were described in the random-phase-approximation (RPA), based on nonrelativistic [2–4] and relativistic [5] energy density functionals (EDF), and in the quasiparticle phonon model (QPM) [6].

In all these approaches, only a restricted number of phonons is taken into account. They are chosen arbitrarily according to the specific problem to be solved. Moreover, the antisymmetrization between the odd particle (or quasiparticle) and the phonons is neglected.

We have developed for even nuclei a multiphonon approach, dubbed the equation of motion phonon method (EMPM), where, by resorting to the Cholesky method, an orthonormal basis of *n*-phonon states $|\alpha_n\rangle$ (n = 0, 1, 2, ...) is extracted from a redundant set of tensor products of particlehole (p-h) [7–9] or quasiparticle [10] Tamm-Dancoff approximation (TDA) phonons $|\alpha_1 = \lambda\rangle$ and then adopted for solving the eigenvalue problem in such a multiphonon space.

More recently, the method was extended to odd nuclei [11–15]. For these systems, an orthonormal basis was extracted from the overcomplete set of states $|(p \times \alpha_n)^v\rangle$ [$|(h^{-1} \times \alpha_n)^v\rangle$], of spin *v*, composed of a valence particle [hole] coupled to the states $|\alpha_n\rangle$ describing the excitations of the core.

We should expect that this multiphonon formulation should be equivalent to shell model within the same configuration space, as is the case for even nuclei. Let us consider, for illustrative purposes, the specific case of a hole-phonon basis (n = 1), which spans the space usually adopted in the PVC.

An approach using an orthonormal basis extracted from the set of states $|(h^{-1} \times \lambda)^v\rangle$ should be equivalent to one adopting the basis states $|((h_1^{-1} \times h_2^{-1})^\Omega \times p)^v\rangle$ composed of two holes coupled to a particle as in the shell model.

Calculations using the optimized chiral potential NNLO_{opt} [16] confirm such a consistency for nuclei of the oxygen region with neutron excess [14,15]. However, in ¹⁵O and ¹⁵N [15] and, to a less extent, in ¹⁷O and ¹⁷F [11,12], a few levels were found to violate the mirror symmetry, which is instead preserved in phenomenological shell model calculations, consistent with experiments [17–19].

Such a symmetry breaking is only partly induced by the violation of the charge symmetry of the NNLO_{opt} potential. As anticipated in Ref. [15] and discussed here, it is caused in large part by the selection of the linearly independent states operated by the Cholesky method.

In order to obviate this inconsistency one may try alternative methods for selecting the linearly independent basis. An obvious possible candidate is the direct diagonalization of the overlap matrix proposed by Rowe [20]. Unfortunately this method would spoil the structure of the equations of motion. These would become too involved and of problematic, practically impossible, numerical implementation if extended to spaces spanned by two or more phonon basis states.

We need therefore to preserve the Cholesky method and find a prescription which brings minimal changes on the equations. This is the case of the recipe proposed here.

We consider the space spanned by states composed of a particle (hole) coupled to TDA phonons and argue that the treatment in this restricted space guarantees the conservation of the mirror symmetry in any multiphonon space. We use the NNLO_{sat} [21] chiral potential, which incorporates the contribution coming from the three-body force and violates the charge symmetry more weakly than the NNLO_{opt} adopted in Refs. [11,12].

II. THE METHOD

We intend to generate an orthonormal basis of hole-core states $|v_1\rangle$ of spin v and energy E_{v_1} having the form

$$|\nu_{1}\rangle = \sum_{h\lambda} C_{h\lambda}^{\nu_{1}} |(h^{-1} \times \lambda)^{\nu}\rangle = \sum_{h\lambda} C_{h\lambda}^{\nu_{1}} (b_{h} \times O_{\lambda}^{\dagger})^{\nu} |0\rangle, \quad (1)$$

TABLE I. Energies and dominant p-h compositions of a few TDA phonons in ¹⁶O with (I) and without (II) $V_{\pi\nu}$.

	1	Ξ			$ C_{ph}^{\lambda} ^2$
J^{π}	Ι	II	$(p \times h)_{\tau}$	Ι	II
1^{-}_{1}	7.2793	7.8604	$ \begin{array}{c} (1/2^+_1 \times 1/2^1)_{\pi} \\ (1/2^+_1 \times 1/2^1)_{\nu} \end{array} $	60.22 24.30	79.58 13.57
1_{2}^{-}	8.7068	8.6276	$(1/2^+_1 \times 1/2^1)_{\pi}$ $(1/2^+_1 \times 1/2^1)_{\nu}$	31.67 66.06	13.36 75.43
2_{1}^{-}	8.4730	8.7871	$(5/2^+_1 \times 1/2^1)_{\pi} (5/2^+_1 \times 1/2^1)_{\nu}$	71.53 21.60	97.26 0.00
2_{2}^{-}	9.2414	9.2136	$\begin{array}{c} (5/2^+_1 \times 1/2^1)_\pi \\ (5/2^+_1 \times 1/2^1)_\nu \end{array}$	72.50 24.15	0.00 96.97
3_{1}^{-}	6.4808	8.1211	$(5/2^+_1 \times 1/2^1)_{\pi} (5/2^+_1 \times 1/2^1)_{\nu}$	51.05 40.16	99.25 0.00
3_{2}^{-}	9.1313	8.4912	$\begin{array}{c} (5/2^+_1 \times 1/2^1)_\pi \\ (5/2^+_1 \times 1/2^1)_\nu \end{array}$	44.12 53.63	0.00 99.18
4_{1}^{-}	15.8451	16.1035	$(5/2^+_1 \times 3/2^1)_{\pi} (5/2^+_1 \times 3/2^1)_{\nu}$	80.53 19.02	99.70 0.00
42	16.8085	16.7096	$\begin{array}{c} (5/2^+_1 \times 3/2^1)_\pi \\ (5/2^+_1 \times 3/2^1)_\nu \end{array}$	18.76 80.10	0.00 99.66

where $O_{\lambda}^{\dagger} = \sum_{ph} c_{ph}^{\lambda} (a_p^{\dagger} \times b_h)^{\lambda}$ is the p-h TDA phonon operator of energy E_{λ} acting on the Hartree-Fock (HF) vacuum $|0\rangle$. The operators $a_p^{\dagger} = a_{x_p j_p m_p}^{\dagger}$ and $b_h = (-)^{j_h + m_h} a_{x_h j_h - m_h}$ create a particle and a hole of energies ϵ_p and ϵ_h , respectively.

The phonons and their energies are determined by solving the equation

$$\langle (p \times h^{-1})^{\lambda} | (H_{\nu\nu} + H_{\pi\pi} + V_{\pi\nu}) | \lambda \rangle = E_{\lambda} c_{ph}^{\lambda}, \qquad (2)$$

where π and ν denote protons and neutrons.

Our formalism starts with the equations of motion

$$\langle \lambda \parallel [a_h^{\dagger}, H] \parallel \nu \rangle = (E_{\nu} - E_{\lambda}) \langle \lambda \parallel a_h^{\dagger} \parallel \nu \rangle.$$
(3)

Expanding the commutator, we obtain after several manipulations [11] the generalized eigenvalue equation

$$(\mathcal{A} - E)\mathcal{D}C = 0. \tag{4}$$

The matrix \mathcal{A} is given by

$$\mathcal{A}^{\nu_1}_{h\lambda h'\lambda'} = (\epsilon_h + E_\lambda)\delta_{hh'}\delta_{\lambda\lambda'} + \mathcal{V}^{\nu}_{h\lambda h'\lambda'}, \qquad (5)$$

where $\mathcal{V}_{h\lambda h'\lambda'}^{\upsilon}$ describes the interaction between hole-phonon states. Its expression is given by

$$\mathcal{V}_{h\alpha h'\alpha'}^{v} = \sum_{\sigma} [\sigma]^{1/2} (-)^{h+h'-\sigma} W(\alpha \sigma v h'; \alpha' h) \mathcal{F}_{h\alpha h'\alpha'}^{\sigma}, \quad (6)$$

where $W(\sigma h \lambda' v; h' \lambda)$ are Racah coefficients and

$$\mathcal{F}^{\sigma}_{h\alpha h'\alpha'} = \sum_{tq} F^{\sigma}_{hh'tq} \langle \alpha \parallel (a^{\dagger}_t \times b_q)^{\sigma} \parallel \alpha' \rangle.$$
(7)

Here the sum runs over particles $tq = p_1p_2$ and holes $tq = h_1h_2$ and F^{σ} is related to the nucleon-nucleon potential V^{Ω} by the Pandya transformation

$$F_{rsqt}^{\sigma} = \sum_{\Omega} [\Omega](-)^{r+t-\sigma-\Omega} W(rsqt;\sigma\Omega) V_{rqst}^{\Omega}.$$
 (8)

TABLE II.	Energy	and s	structure	of	some	selected	states	deter-
mined using TI	DA phor	ions v	vith (I) a	nd	withou	it (II) $V_{\pi\nu}$		

		E	Σv		И	$W^{ u}_{v\lambda}$	
	ν	¹⁵ O	¹⁵ N	$(v \times \lambda)^{\nu}$	¹⁵ O	¹⁵ N	
	$3/2_1^+$	8.205	10.013	$(1/2^1 \times 1^1)$	81.47		
				$(1/2^1 \times 1^2)$		68.76	
	1			$(3/2^1 \times 3^1)$		12.83	
Ι	$7/2_1^+$	9.002	11.758	$(1/2^{-}_{1} \times 3^{-}_{1})$	91.77		
	0.42+	12 015	15.000	$(1/2_1^- \times 3_2^-)$	05.24	82.83	
	$9/2_1$	13.915	15.880	$(3/2_1 \times 3_1)$ $(3/2^- \times 2^-)$	95.24	26.44	
				$(3/2_1 \times 3_2)$ $(1/2^- \times 4^-)$	3 4 5	61 37	
	2.42+	0.702	0 (01	$(1/2_1 \land -1_1)$	71.77	01.57	
	$3/2_1$	9.782	9.681	$(1/2_1 \times 1_1)$ $(1/2^- \times 1^-)$	/1.6/	77 80	
п	$7/2^{+}$	10 891	11 204	$(1/2_1 \times 1_2)$ $(1/2^- \times 3^-)$	85.06	77.80	
п	//21	10.071	11.204	$(1/2_1 \times 3_1)$ $(1/2_1 \times 3_2)$	05.00	85.17	
	$9/2^+_1$	15.510	15.661	$(1/2_1 \times 3_2)$ $(3/2_1 \times 3_1)$	66.77	00.17	
	- / -1			$(3/2_1^- \times 3_2^-)$		69.60	
				$(1/2_1^- \times 4_1^-)$	26.38	19.11	
		¹⁷ O	¹⁷ F		¹⁷ O	¹⁷ F	
Ι	$11/2^{-}_{1}$	7.714	10.081	$(5/2^+_1 \times 3^1)$	99.92		
	/ 1			$(5/2^+_1 \times 3^2)$		96.75	
Π	$11/2^{-}_{1}$	9.351	9.564	$(5/2^+_{1} \times 3^{1})$	95.80		
	/-1			$(5/2^+_1 \times 3^2)$		96.01	
		³⁹ Ca	³⁹ K	1 2	³⁹ Ca	³⁹ K	
T	$13/2^{-}$	9 1 5 1	11 100	$(3/2^+ \times 5^-)$	98 56		
•	10/-1	,	111100	$(3/2^+_1 \times 5^1)$	20100	97.28	
п	$13/2^{-}$	10 306	10 412	$(3/2^+ \times 5^-)$	97.03		
11	15/21	10.500	10.412	$(3/2^+_1 \times 5^1)$	27.05	96.97	
				(2) = 1 (2) (2)		, 5.77	

 \mathcal{D} is the overlap matrix given by

$$\mathcal{D}_{h\lambda h'\lambda'}^{v} = \langle (h^{-1} \times \alpha)^{v} | (h'^{-1} \times \alpha')^{v} \rangle$$

= $\delta_{hh'} \delta_{\lambda\lambda'}$
+ $\sum_{\sigma} [\sigma]^{1/2} W(\sigma h\lambda' v; h'\lambda) \langle \lambda' \parallel (a_{h'}^{\dagger} \times b_{h})^{\sigma} \parallel \lambda \rangle.$
(9)

The second piece reintroduces the exchange terms among the odd hole and the TDA states.

The eigenvalue equation (4) is ill defined. Since the set of states $|(h^{-1} \times \lambda)^v\rangle$ is overcomplete, the overlap matrix \mathcal{D} is singular. The redundancy is eliminated by resorting to the Cholesky decomposition method which extracts from the set $|(h^{-1} \times \lambda)^v\rangle$ a basis of linearly independent states spanning the subspace of the correct dimensions. We can then construct in such a subspace the overlap matrix \mathcal{D}_n and, by left multiplication, obtain from Eq. (4)

$$\mathcal{D}_n^{-1}(\mathcal{A}\mathcal{D})_n C^n = EC^n.$$
(10)

The solution of the above equation determines only the coefficients C^n of the selected states. Those of the redundant states are undetermined and, therefore, can be safely put equal to zero. The orthonormal basis $\{|v_1\rangle\}$ [Eq. (1)] we searched for is determined thereby.



FIG. 1. Spectra of ¹⁵O and ¹⁵N using TDA phonons generated (I) with the proton-neutron potential $V_{\pi\nu}$ included, (II) without $V_{\pi\nu}$. The positive and negative parity levels are in red and black, respectively.

We can now solve the full eigenvalue problem in the space spanned by the single hole plus the hole-phonon basis states $\{|v_0\rangle, |v_1\rangle\}$, obtaining the eigenfunctions

$$|\psi_{\nu}\rangle = \sum_{\nu_{n}} \mathcal{C}_{\nu_{n}}^{\nu} |\nu_{n}\rangle, \qquad (11)$$

where $|v_0\rangle = |v^{-1}\rangle$ and $|v_1\rangle$ is given by Eq. (1).

III. MIRROR SYMMETRY BREAKING

We focus our analysis mainly on ¹⁵O and ¹⁵N. The adopted Hamiltonian is composed of an intrinsic kinetic operator T_{int} and the chiral potential NNLO_{sat}. The HF basis states were generated in a space encompassing all harmonic oscillator shells up to $N_{max} = 12$. A subset of them, up to N = 7, was used to generate the TDA phonons. We checked

that the inclusion of higher energy shells does not affect the results. The $J^{\pi} = 1^{-}$ TDA phonons are free of spurious admixtures induced by the center-of-mass (CM) motion. They have been removed by resorting to a method based on the Gramm-Schmidt orthogonalization of the p-h basis to the CM state [22].

One may notice in Table I the large energy splitting between the nearby 1^- and, especially, the 3^- states and the corresponding strong mixing between proton and neutron p-h components.

As shown in Table II and Fig. 1, the mirror symmetry is strongly violated by the $3/2_1^+$, $7/2_1^+$, and $9/2_1^+$ levels. In ¹⁵N, these levels differ from the corresponding ones in ¹⁵O by ≈ 1.8 , ≈ 2.8 , and ≈ 2.0 MeV, respectively. The other corresponding levels of ¹⁵N and ¹⁵O are fairly close, in general. Their energy differences range from ≈ 0.1 to ≈ 0.6 MeV.



FIG. 2. The same as in Fig. 1 for 17 O and 17 F.

The symmetry breaking is also apparent from the asymmetric neutron-proton composition of the wave functions (Table II). This asymmetry, however, gets manifest only in a few states.

As anticipated in Ref. [15], the reason of such a breaking can be understood by analyzing the structure of the $7/2_1^+$. In shell model, we get for ¹⁵O

$$|7/2_1^+\rangle_{SM} \sim \left| \left[\left(0p_{1/2}^{-1}(\nu) \times 0p_{1/2}^{-1}(\pi) \right)^1 \times 0d_{5/2}(\pi) \right]^{7/2} \right\rangle.$$
(12)

The component $[(0p_{1/2}^{-1}(\nu) \times 0p_{1/2}^{-1}(\nu))^1 \times 0d_{5/2}(\nu)]^{7/2}$, involving identical particles, is excluded by the Pauli principle. The $7/2_1^+$ state of ¹⁵N is deduced from (12) by interchanging neutrons with protons. Thus, in the shell model, the $7/2_1^+$ levels in ¹⁵O and ¹⁵N are almost degenerate, consistently with experiments.

In our scheme, the $7/2_1^+$ arises from coupling the neutron or proton hole $0p_{1/2}^{-1}$ mainly to 3⁻ phonons. The two lowest $3_1^$ and 3_2^- are ≈ 2.5 MeV far apart and have the proton-neutron mixed structure

$$|3_i^-\rangle \sim c_i^{\pi} \left| (0d_{5/2} \times (0p_{1/2})^{-1})_{\pi}^3 \right| + c_i^{\nu} \left| (0d_{5/2} \times (0p_{1/2})^{-1})_{\nu}^3 \right|,$$
(13)

where $|c_1^{\pi}|^2 \approx 0.51$ and $|c_1^{\nu}|^2 \approx 0.40$ for 3_1^- and $|c_2^{\pi}|^2 \approx 0.44$ and $|c_2^{\nu}|^2 \approx 0.54$ for 3_2^- . Such a large energy splitting and proton-neutron mixing are induced by the strong protonneutron interaction.

The Cholesky method selects hole-phonon components rather than single shell model configurations. Thus, it picks the $[0p_{1/2}^{-1}(\nu) \times 3_1^{-}]^{7/2}$ component for ¹⁵O (Table II) since the 3_1^{-} has a proton dominance (Table I) and discards as redundant the $[0p_{1/2}^{-1}(\nu) \times 3_2^{-}]^{7/2}$ which contains the neutron dominant 3_2^{-} phonon. In contrast, it selects the $[0p_{1/2}^{-1}(\pi) \times 3_2^{-}]^{7/2}$ state for ¹⁵N and discards the $[0p_{1/2}^{-1}(\pi) \times 3_1^{-}]^{7/2}$.

The above selection, though formally correct, has the effect of breaking the mirror symmetry. In fact, the $7/2_1^+$



FIG. 3. The same as in Fig. 1 for 39 Ca and 39 K.

level in ¹⁵O differs from the corresponding one in ¹⁵N by ≈ 2.8 MeV because of the energy splitting between the 3_1^- and 3_2^- .

The strong proton-neutron mixing in the two 3⁻ states seems to cause an additional inconsistency with shell model. The $7/2_1^+$ contains the Pauli principle forbidden configurations $|(0p_{1/2})_{\nu}^{-1} \times (0d_{5/2} \times (0p_{1/2})^{-1})_{\nu}^3\rangle$ in ¹⁵O through 3_1^- and $|(0p_{1/2})_{\pi}^{-1} \times (0d_{5/2} \times (0p_{1/2})^{-1})_{\pi}^3\rangle$ in ¹⁵N through 3_2^- . This, however, is an artifact of the hole-phonon scheme. It is possible to show that, once we perform an angular momentum recoupling, the coefficient of the forbidden shell model configuration $[(0p_{1/2}^{-1}(\nu) \times 0p_{1/2}^{-1}(\nu))^1 \times 0d_{5/2}(\nu)]^{7/2}$ vanishes.

Analogous conclusions can be drawn for the $9/2_1^+$ and $3/2_1^+$ corresponding levels. In the first case, the 3_1^- and 3_2^- phonons couple to the neutron and proton $0p_{3/2}$ holes, while the $3/2_1^+$ states result from coupling the 1_1^- and 1_2^- phonons to the neutron and proton $0p_{1/2}$.

The mirror symmetry is also strongly violated by the $11/2^-$ state in 17 O and 17 F (Fig. 2 and Table II). This state arises from coupling the $0d_{5/2}$ neutron to the 3_1^- phonon with proton dominance in 17 O and the $0d_{5/2}$ proton to the 3_2^- with neutron dominance in 17 F. Thus the corresponding levels get ≈ 2.5 MeV far apart.

In ³⁹Ca and ³⁹K as well as in ⁴¹Ca and ⁴¹Sc, the states which violate strongly the mirror symmetry have high spins and energies. In ³⁹Ca and ³⁹K, for instance, the corresponding levels of spin $13/2_1^-$ differ by ≈ 2 MeV (Fig. 3 and Table II) due to the energy difference between 5_1^- and $5_2^$ which couple to neutron and proton $0d_{3/2}$ holes, respectively.

IV. RESTORATION OF THE MIRROR SYMMETRY

It is clear from the above analysis that it is necessary to investigate if and how the mirror symmetry can be restored. The recipe we propose is simple. Since the redundancy is caused



FIG. 4. Theoretical versus experimental spectra of ¹⁵O. The levels of unknown parity and (or) spin are in blue.

only by the unsymmetrized configurations involving identical nucleons, like $[0p_{1/2}^{-1}(v) \times (0d_{5/2} \times 0p_{1/2}^{-1})_v^3]^{7/2}$ present in the $[0p_{1/2}^{-1}(v) \times 3^{-}]^{7/2}$ component of ¹⁵O, it is more appropriate to implement Cholesky in separate neutron and proton hole-phonon subspaces. This can be achieved by the following simple prescriptions:

- Neglect the neutron-proton interaction V_{πν} in the TDA eigenvalue equation (2). Its solution yields doublets of quasidegenerate TDA phonons: one of proton (|λ⟩ = |λ_π⟩) and the other of neutron (|λ⟩ = |λ_ν⟩) nature.
- (2) Apply the Cholesky method to the overlap matrix \mathcal{D} computed using the states $|(h^{-1} \times \lambda)^{\nu}\rangle$ with the new phonons.
- (3) Recover the proton-neutron potential neglected in the TDA equation (2) by inserting $V_{\pi\nu}$ between TDA phonons directly in the hole-phonon eigenvalue equation (4). This can be done by the simple replacement

in the matrix \mathcal{A} ,

$$E_{\lambda}\delta_{\lambda\lambda'} \to E_{\lambda}\delta_{\lambda\lambda'} + \langle \lambda | V_{\pi\nu} | \lambda' \rangle. \tag{14}$$

The corresponding states selected by Cholesky from the \mathcal{D} matrix are $|(h_{\nu}^{-1} \times \lambda_{\pi})^{\nu}\rangle$ for ¹⁵O and $|(h_{\pi}^{-1} \times \lambda_{\nu})^{\nu}\rangle$ for ¹⁵N. They are quasidegenerate and proton-neutron symmetric since the corresponding proton and neutron phonons are quasidegenerate. Moreover, the terms violating the Pauli principle present in the old hole-phonon basis do not appear at all in the new one.

The restoration of the mirror symmetry is confirmed by the numerical calculations. As shown in Fig. 1, the energy differences between corresponding levels are of the same order of the differences between proton and neutron HF p-h energies. The proton-neutron symmetry is also amply recovered in the wave functions (Table II).

Analogous results are obtained for A = 17 (Fig. 2) and in nuclei around ⁴⁰Ca (Fig. 3). The appreciable deviations one may notice for some levels are due to the differences between proton and neutron HF p-h energies.



FIG. 5. Theoretical versus experimental spectra of ¹⁵N.

The effect of the new basis on the transitions is significant quantitatively but not qualitatively. Those resulting strong or weak in the old basis remain strong or weak in the new basis (Table III). Such a result was expected since the mirror symmetry breaking affects only and partially the structure of a few states.

The correct implementation of the Cholesky method within the restricted space spanned by a particle (hole) coupled to TDA phonons guarantees the conservation of the mirror symmetry also in the multiphonon spaces. In fact, since our method generates doublets of quasidegenerate TDA phonons of proton and neutron nature, to each multiphonon state of proton character must correspond a specular quasidegenerate one with the same neutron dominance. Cholesky selects the first state for the nucleus with a valence proton and the second for the system with a valence neutron.

The conservation of the symmetry beyond the particle(hole)-phonon scheme is of the uttermost importance since the multiphonon states are badly necessary for a fairly realistic description of the spectra of the N = Z doubly magic

nuclei, whose complexity is well known [26–28]. In fact, the one-phonon space considered here is far from providing a faithful description of these spectra. Let us focus for instance on the A = 15 nuclei.

As shown in Figs. 4 and 5, the low-lying theoretical positive parity levels in A = 15 are ≈ 4 MeV above the corresponding experimental levels. Such a discrepancy is surprising at first sight since, as shown in Fig. 6, the low-lying negative parity TDA levels overlap with those measured in ¹⁶O. On the other hand, as we go to the A = 15 nuclei, the ground state, of single-hole character, gets shifted downward in energy due to its strong coupling to the hole-phonon states while the energies of the latter states remain unchanged.

It is worthwhile to point out that the NNLO_{opt} produces a stronger discrepancy with experiments. The energies of TDA negative parity phonons are \approx 5 MeV above the experimental levels and those obtained by using the NNLO_{sat} (Fig. 5). Consequently, the hole-phonon energies of the *A* = 15 nuclei are \approx 3 MeV above those obtained using NNLO_{sat} and \approx 7 MeV above the experimental levels (Fig. 4). The discrepancy with



FIG. 6. TDA versus experimental spectra of ¹⁶O.

respect to NNLO_{sat} is attenuated by the fact that, due to the higher energy of the phonons, the coupling to the hole-phonon state is weaker and induces a smaller energy shift of the ground state.

The multiphonon configurations are expected to improve considerably the description of the spectra.

A substantial downward energy shift of the theoretical levels should be induced from the *n*-phonon to (n + 2)-phonon coupling given by

$$\langle (h^{-1} \times \alpha_n)^{\nu} | H | (h'^{-1} \times \alpha_{n+2})^{\nu} \rangle$$

= $\sum_{\alpha_2} \langle 0 | H | \alpha_2 \rangle \langle (h^{-1} \times [\alpha_2 \times \alpha_n])^{\nu} | (h'^{-1} \times \alpha_{n+2})^{\nu} \rangle.$ (15)

This equation shows that the 1-to-3 and the 2-to-4 phonon couplings are governed simply by the matrix elements between the HF vacuum and the two-phonon states. Such couplings are known to be strong.

We have exploited already the above equation to compute the 1-to-3 phonon coupling in calculations using NNLO_{opt} [12] and obtained a \approx 3–4 MeV shift of the low-lying positive parity levels. Since an analogous effect should be induced by NNLO_{sat}, we expect to obtain a substantial overlap between theoretical and experimental positive parity spectra.

The case of the low-lying negative parity states is more critical. Most of them have a dominant two-phonon structure and, therefore, can be pushed down in energy toward the experimental levels only by the coupling to four phonons. Treating exactly these configurations is very challenging. We rely on the simple structure of the above formula to extract, under some simplifying assumptions on the overlap, the main contribution to the energy shift of the hole (two-phonon) states coming from their coupling to four phonons.

The multiphonon states are necessary also for getting a better description of moments and transitions.

Most of the ground state moments and β -decay *ft* values (Table III) as well as a few transition strengths (Table IV) are fairly close to the experimental data due to the dominantly single particle (hole) nature of the states involved.

TABLE III. Moments and β -decay *ft* values computed with (I) and without (II) $V_{\pi\nu}$ in TDA. Experimental data were taken from Refs. [23–25]. The sign of the experimental quadrupole moments of ¹⁷F and ³⁹Ca is unknown.

		Ι	II	Expt.
¹⁵ O	$\mu (\mu_N) \\ \log ft$	+0.6010 3.650	+0.5967 3.649	+0.7189 (8) 3.637
¹⁵ N	$\mu \left(\mu_N ight)$	-0.24885	-0.24848	-0.28319
¹⁷ O	$Q~(e { m fm}^2) \ \mu(\mu_N)$	-1.442 -1.81	-1.341 -1.81	-2.578 -1.89370(9)
¹⁷ F	$\begin{array}{c} Q \ (e \mathrm{fm}^2) \\ \mu \ (\mu_N) \\ \mathrm{log} ft \end{array}$	-8.3 +4.55 3.337	-8.2 +4.54 3.336	5.8(4) +4.72 3.358(2)
³⁹ Ca	$Q(em^2)$ $\mu(\mu_N)$ $\log ft$	+0.9 +1.05540 3.5521	+0.7 +1.06749 3.5512	3.6 (7) +1.02168 (12) 3.6326 (10)
³⁹ K	$Q (e fm^2) \ \mu (\mu_N)$	+5.74 +0.12422	+5.88 +0.11665	+5.85 (6) +0.39146616 (33)

Most E1 and E3 transition strengths are of the same order as the corresponding experimental strengths (Table IV) indicating that the excited states involved have a dominant particle(hole)-phonon component.

TABLE IV. Transition strengths computed with (I) and without (II) $V_{\pi\nu}$ in TDA. The *M*1 and $E\lambda$ strengths are given in μ_N^2 and $e^2 \text{fm}^{2\lambda}$, respectively. The experimental data are from Refs. [23–25].

¹⁵ O		Ι	II	Expt.
$1/2^1 \rightarrow 3/2^2$	<i>M</i> 1	0.04	0.09	0.75
$1/2^{-}_{1} \rightarrow 3/2^{+}_{1}$	E1	0.03	0.07	$> 1.5 \times 10^{-4}$
$1/2^{-}_{1} \rightarrow 5/2^{-}_{1}$	E2	8.2	8.8	98
$1/2_1^- \to 5/2_1^+$	E3	334	307	160 ± 28
¹⁵ N				
$1/2^1 \to 3/2^2$	M1	0.03	0.04	$(1.04 \pm 0.14) \times 10^{-1}$
$1/2_1^- \to 3/2_1^+$	E1	0.02	0.05	$(5.2 \pm 0.2) \times 10^{-2}$
$1/2^1 \to 5/2^1$	E2	0.05	0.02	8.6 ± 0.6
$1/2^1 \to 5/2^+_1$	E3	382	356	280 ± 27
¹⁷ O				
$1/2^+_1 \rightarrow 5/2^1$	E1	0.0005	0.0004	0.0005
$5/2^+_1 \to 1/2^+_1$	E2	0.54	0.47	2.18 ± 0.16
$5/2^+_1 \to 3/2^1$	E3	45	27	20 ± 12
¹⁷ F				
$5/2^+_1 \to 5/2^1$	E1	0.42	0.19	0.0018
$5/2^+_1 \rightarrow 1/2^+_1$	E2	19.86	19.78	21.64
$5/2^+_1 \to 5/2^1$	E3	119	106	
³⁹ Ca				
$3/2^+_1 \to 1/2^+_1$	E2	0.15	0.05	18.8 ± 2.3
$3/2^+_1 \to 7/2^1$	E3	1248	551	487^{+1066}_{-415}
³⁹ K				
$3/2^+_1 \to 5/2^1$	E1	0.0043	0.0032	$0.0014\substack{+0.0006\\-0.0003}$
$3/2^+_1 \to 1/2^+_1$	E2	14.4	9.1	$20.4^{+5.9}_{-4.7}$
$3/2^+_1 \to 7/2^4$	E3	617	973	903^{+379}_{-289}

The discrepancies with experiments are more pronounced for the negative (positive) parity states in A = 15 (A = 17). The calculations underestimate the M1 and E2 strengths by orders of magnitudes (Table IV). These states have a twophonon character, at least, and therefore can be described properly only within a multiphonon space.

V. SUMMARY AND PERSPECTIVES

We have proposed a variant of the particle(hole)- phonon scheme which preserves the mirror symmetry in the odd neighbors of the N = Z nuclei. Though applied to one-phonon states, the new method guarantees the restoration of the symmetry in any multiphonon space.

The restoration of such a symmetry represents the precondition for an accurate description of the complex spectra of the odd neighbors of doubly closed shell nuclei like ¹⁶O. This accuracy can be reached by trying to improve the nuclear potential and, in parallel, by enlarging the configuration space.

We have seen that the discrepancies with experiments discussed in the text are reduced significantly by replacing the NNLO_{opt} potential, used in previous calculations [11,12], with the more realistic NNLO_{sat}. For a further significant improvement it is necessary to go to spaces spanned by basis states with a sufficiently large number of phonons. We have argued that the inclusion of three and four phonons has a strong impact on the one-phonon and two-phonon states, respectively.

We are able to include up to three phonons which, through their coupling, should shift considerably downward in energy the low lying one-phonons states, as was the case for the NNLO_{opt} potential [11,12]. In virtue of such a shift, for instance, a substantial overlap between theoretical and experimental positive parity spectra is expected for the A = 15mirror nuclei.

In order to improve the description of the negative parity spectra it is necessary to enlarge further the space so as to include four phonons.

Treating exactly these states is numerically very challenging. Nonetheless, we intend to exploit the simple structure of formula (15) governing the coupling between two and four phonons in order to get, under some simplifying assumptions, an approximate estimate of the downward energy shift of the low lying two-phonon states and, therefore, get an insight on the impact of four phonons on the low-lying negative parity states.

ACKNOWLEDGMENTS

We thank Petr Navrátil for having provided the matrix elements of the NNLO_{sat} potential. This work was partly supported by the Czech Science Foundation (Czech Republic), P203-19-14048S and by the Charles University Research Center UNCE/SCI/013. F.K. and P.V. thank the INFN for financial support. Computational resources were provided by the CESNET LM2015042 and the CERIT Scientific Cloud LM2015085, under the program "Projects of Large Research, Development, and Innovations Infrastructures."

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