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The Equation of Motion Phonon Method and its application to neutron rich odd nuclei

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Abstract. We report on the extension to odd nuclei of a microscopic multiphonon approach known as equation of motion phonon method and its application to the odd neighbors of the neutron rich ^{22}O. A calculation using the chiral potential NNLO$_{opt}$ and encompassing up to two phonon basis states provides a description of the spectroscopic properties which is good quantitatively for ^{23}O and qualitatively for ^{21}O and ^{21}N. Serious discrepancies between theory and experiments occur in ^{23}F. A possible recipe for curing them is under investigation.

1. Introduction

Extensive experimental studies have been devoted to the region of neutron rich oxygen isotopes and have produced a rich amount of spectroscopic data for even and odd nuclei in proximity of the new neutron magic numbers N = 14 and N = 16 [1, 2, 3, 4, 5, 6, 7, 8, 9]. They have also stimulated several theoretical investigations adopting different approaches like shell model [10], self-consistent Green's function [11, 12], many-body perturbation theory [13], and coupled cluster [14, 15, 16].

A thorough study of the spectroscopic properties of the neutron rich nuclei in the oxygen region has been carried out within the equation of motion phonon method (EMPM) [17, 18]. It derives and solves iteratively a set of equations of motion to generate an orthonormal basis of multiphonon states built of phonons obtained in particle-hole (p-h) or quasi-particle (qp) Tamm-Dancoff aproximation (TDA). Such a basis simplifies the structure of the Hamiltonian matrix and makes feasible its diagonalization in large configuration spaces. The diagonalization produces at once the totality of eigenstates allowed by the dimensions of the multiphonon space. The formalism does not rely on any approximation, takes into account the Pauli principle, and holds for any Hamiltonian.

This method was applied to doubly closed shell [19, 20, 21, 22] and open shell nuclei [23]. It was also extended to odd nuclei with one valence particle or hole external to a doubly magic core [24, 25, 26, 27]. Here, we focus our attention on the neutron rich neighbors of ^{22}O.

2. The Equation of Motion Phonon Method for odd nuclei

The primary goal of the method is to derive a basis of orthonormal states of the form

$$\mid \nu_n\rangle = \sum_{p\alpha_n} C^{\nu}_{p\alpha_n} \mid (p \times \alpha_n)^v\rangle = \sum_{p\alpha_n} C^{\nu}_{p\alpha_n} (a^\dagger_p \times \mid \alpha_n\rangle)^v, \tag{1}$$

where $\mid \alpha_n\rangle$ are the n-phonon core states also derived within the EMPM. They have the stucture

$$\mid \alpha_n\rangle = \sum_{\lambda\alpha_{n-1}} C^{\alpha_n}_{\lambda\alpha_{n-1}} \mid (\lambda \times \alpha_{n-1})^{\alpha_n}\rangle = \sum_{\lambda\alpha_{n-1}} C^{\alpha_n}_{\lambda\alpha_{n-1}} \left\{ O^\dagger_\lambda \times \mid \alpha_{n-1}\rangle \right\}^{\alpha_n}, \tag{2}$$

where

$$O^\dagger_\lambda = \sum_{ph} c^\lambda_{ph} \left(a^\dagger_p \times b_h \right)^\lambda \tag{3}$$

are the TDA phonon operators acting on the $(n-1)$-phonon states. In the above equations we have also introduced the creation and annihilation operators $a^\dagger_p = a^\dagger_{x_p j_p m_p}$ and $b_h = (-)^{j_h+m_h} a_{x_h j_h m_h}$.

In close analogy with the even-even case outlined in Ref. [18] we start with the equations of motion

$$\langle \nu_n \parallel [H, a^\dagger_p]^p \parallel \alpha_n\rangle = (E_{\nu_n} - E_{\alpha_n})\langle \nu_n \parallel a^\dagger_p \parallel \alpha_n\rangle, \tag{4}$$

where

$$\langle \nu_n \parallel a^\dagger_p \parallel \alpha_n\rangle = \sum_{p'\alpha'_n} \mathcal{D}^{(v)}_{p\alpha_n p'\alpha'_n} C^{\nu_n}_{p'\alpha'_n} = \sum_{p'\alpha'_n} \langle (p \times \alpha_n)^v \mid (p' \times \alpha'_n)^v\rangle C^{\nu_n}_{p'\alpha'_n}. \tag{5}$$

Here H is a two body Hamiltonian of general form and $\mathcal{D}$ is the overlap matrix which reintroduces the exchange terms among the odd particle and the n-phonon states and, therefore, re-establishes the Pauli principle.

After expanding the commutator in Eq. (4) we obtain

$$\sum_{p'\alpha'_n p''\alpha''_n} \left\{ (\epsilon_p + E_{\alpha_n} - E_{\nu_n})\delta_{pp'}\delta_{\alpha_n\alpha'_n} + \mathcal{V}^{(v)}_{p\alpha_n p'\alpha'_n} \right\} \mathcal{D}^{(v)}_{p'\alpha'_n p''\alpha''_n} C^{\nu_n}_{p''\alpha''_n} = 0, \tag{6}$$

where $\mathcal{V}^{(v)}_{p\alpha_n p'\alpha'_n}$ is the particle-phonon interaction whose expression can be found in Ref. [24].

Equation (6) is ill defined since the basis $\mid (p \times \alpha_n)^v\rangle$ is overcomplete. Following a procedure based on the Cholesky decomposition method, we extract a basis of linearly independent states and obtain a non-singular eigenvalue equation. Its iterative solution yields a basis of orthonormal states $\mid \nu_n\rangle$ $(n = 0, 1, ..n..)$ of the form (1). Such a basis is used to solve the final eigenvalue problem in the full multiphonon space

$$\sum_{\nu'_{n'}} \left\{ (E_{\nu_n} - \mathcal{E}_\nu)\delta_{\nu_n \nu'_{n'}} + \mathcal{V}^{(v)}_{\nu_n \nu'_{n'}} \right\} \mathcal{C}^{(\nu)}_{\nu'_{n'}} = 0, \tag{7}$$

where $\mathcal{V}^{(v)}_{\nu_n \nu'_{n'}}$ couples different subspaces and, therefore, is non vanishing only for $n' \neq n$. Eq. (7) yields the eigenfunctions $| \Psi_\nu \rangle = \sum_{\nu_n} \mathcal{C}^{\nu}_{\nu_n} \mid \nu_n \rangle$ which are used to derive the transition amplitudes

$$\langle \Psi_{\nu'} \parallel \mathcal{M}(\lambda) \parallel \Psi_\nu \rangle = \sum_{\nu_n \nu'_{n'}} \mathcal{C}^{\nu}_{\nu_n} \mathcal{C}^{\nu'}_{\nu'_{n'}} \langle \nu'_{n'} \parallel \mathcal{M}(\lambda) \parallel \nu_n \rangle. \quad (8)$$

The expression of $\langle \nu'_{n'} \parallel \mathcal{M}(\lambda) \parallel \nu_n \rangle$ can be found in Ref. [24].

For an odd nucleus with a valence hole the procedure remains the same with the hole-core states given by

$$| \nu_n \rangle = \sum_{h\alpha_n} C^{\nu}_{h\alpha_n} \mid (h^{-1} \times \alpha_n)^{v} \rangle = \sum_{h\alpha_n} C^{\nu}_{h\alpha_n} (b_h \times \mid \alpha_n \rangle)^{v}. \quad (9)$$

3. Calculations and results

The Hamiltonian we used is composed of an intrinsic kinetic operator T_{int} plus the optimized chiral two-body potential NNLO$_{opt}$ [28]. We generate a HF basis in a space including all harmonic oscillator major shells up to N$_{max}$ = 15 and derive the TDA phonons from a subset of HF states corresponding to N = 7. We checked that the inclusion of higher energy shells does not affect the results.

The TDA core states are free of center of mass (c.m.) spurious admixtures in virtue of the Gramm-Schmidt orthogonalization method outlined in Ref. [29]. We used all one-phonon particle(hole)-core states $| \ (p(h^{-1}) \times \lambda)^{\nu} \rangle$. The two-phonon particle(hole)-core subspace was spanned only by the states $| \ (p(h^{-1}) \times \alpha_2)^{\nu} \rangle$ which include only the two phonons α_2 built of TDA phonons having large overlap with $0 - \hbar\omega$ and $1 - \hbar\omega$ p-h subspaces.

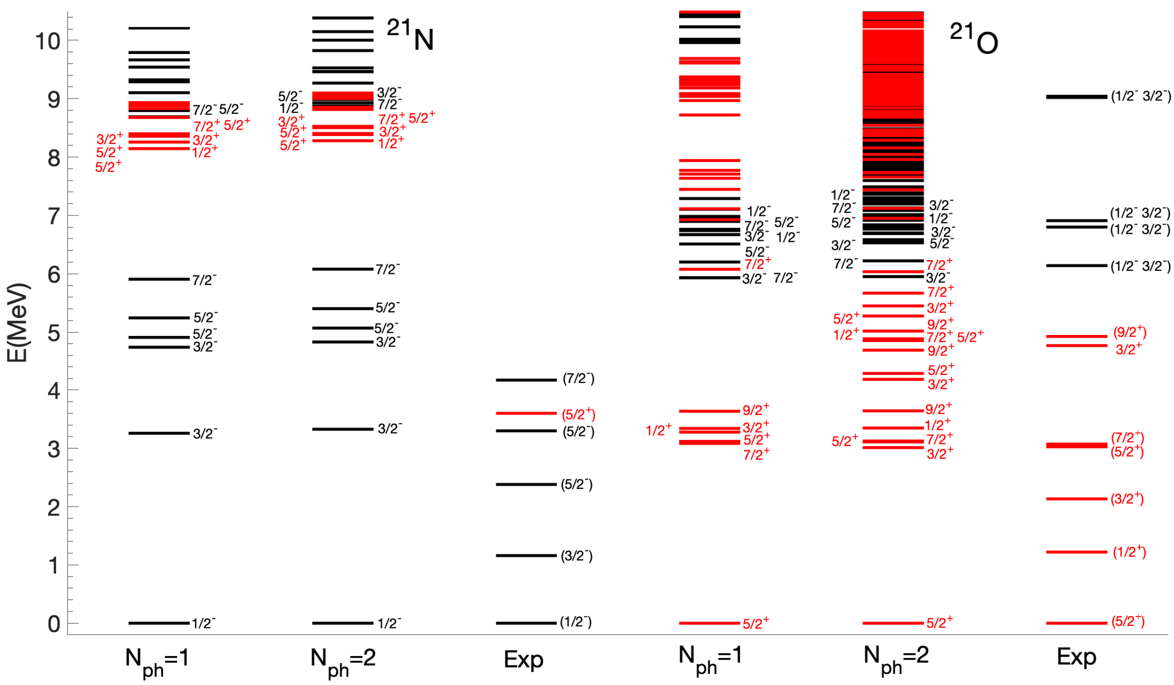

Figure 1. Theoretical versus experimental [30] spectra of ^{21}N and ^{21}O.

Theoretical and experimental spectra of ^{21}N and ^{21}O are shown in Fig.1. The ground state of ^{21}O has practically pure single particle nature accounting for 97%. The ground state of ^{21}N is also of single particle nature, $\sim$ 84%, but with an appreciable hole-phonon admixture. This

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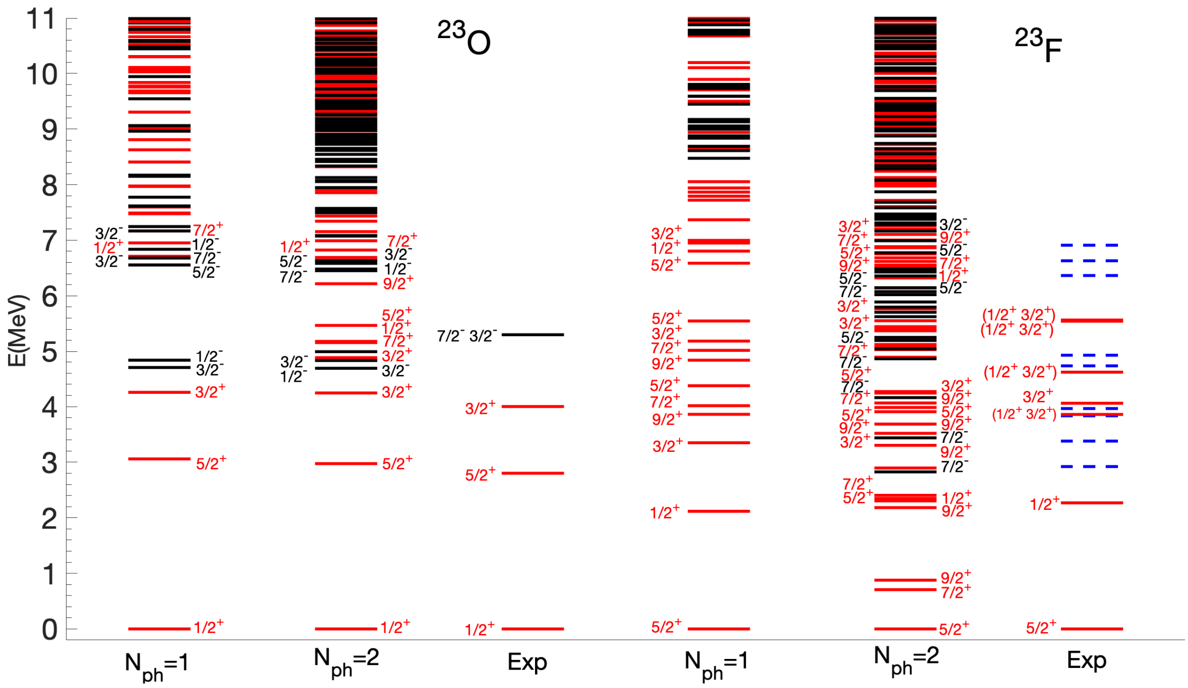

Figure 2. Theoretical versus experimental spectra [31, 32, 33] of ^{23}F and ^{23}O.

originates from the strong hole-phonon coupling induced by the strong interaction between the odd proton and the neutrons in excess.

The low-lying theoretical states of both nuclei have spins compatible with those attributed to the experimental ones but are higher in energy. They are characterized by the dominance of the low-lying 2^+ and 3^+ phonons. The only exception is the $3/2_1^-$ in the ^{21}N which has a dominant single particle nature. At high energy the theoretical spectrum of ^{21}O is very dense. This is not the case of ^{21}N due to the large gap between the excited and the ground states.

We have also investigated the β-decay transitions. The available experimental data [34] show that the states of ^{21}O populated by the decay of ^{21}N are in the energy interval $\sim 6-9$ MeV (Table 1). Their spins were not determined uniquely. In our calculation, the states which are populated with a rate comparable with the data are too high in energy. Theoretical and experimental spectra of ^{23}F and ^{23}O are shown in Fig.2. In analogy with the hole case, the ground state of ^{23}F has an appreciable one-phonon component. Its HF component accounts for $\sim 72\%$ to be compared with the 94% in the ^{23}O.

The low-lying experimental levels are well reproduced in ^{23}O but are poorly described in ^{23}F. In this latter nucleus, once the one-phonon components are included, several $3/2^+, 5/2^+, 7/2^+, 9/2^+$ levels occur in the region of experimental observation in addition to the low energy $1/2_1^+$ and $3/2_1^+$ levels which have an experimental counterpart. These levels were predicted also by shell model calculations using phenomenological two-body forces [32]. However, the inclusion of two phonons spoils the good agreement obtained at one-phonon level. These states, in fact, enhance dramatically the level density and push some of the high spin states very low in energy.

This unwanted effect is due to the strong interaction between the odd proton and the low-lying 2_1^+ and 3_1^+ ^{22}O TDA phonons of neutron nature. This interaction, in fact, induces a too strong coupling between the particle and the particle-phonon states as well as between the one-phonon and two-phonon particle-core states.

Table 1. Selected ground state β-decay of ^{21}N. The experimental data are taken from Ref. [34]. Some spins of the final states have not been determined experimentally.

	ν_f	E^f	$\log ft$	B(GT)
EMPM				
	$3/2^-$	5.95	7.14	0.00044
	$1/2^-$	7.30	7.55	0.00016
	$3/2^-$	10.02	5.60	0.01513
	$3/2^-$	10.43	6.30	0.00306
	$3/2^-$	14.54	5.32	0.02910
	$1/2^-$	14.70	5.57	0.00108
	$1/2^-$	18.84	5.77	0.00987
Exp				
	$(1/2^-, 3/2^-)$	6.14	5.44 ± 0.06	0.0224 ± 0.0032
	$(1/2^-, 3/2^-)$	6.80	5.19 ± 0.06	0.0399 ± 0.0056
	$(1/2^-, 3/2^-)$	6.91	5.44 ± 0.07	0.0224 ± 0.0035
	$(1/2^-, 3/2^-)$	9.02	4.78 ± 0.06	0.1015 ± 0.0145
	$(1/2^-, 3/2^-)$	9.04	4.62 ± 0.06	0.1462 ± 0.0206

Table 2. Selected ground state β-decay of ^{23}O. The experimental data are taken from Ref. [33]. Some spins of the final states have not been determined experimentally.

	ν_f	E^f	$\log ft$	B(GT)
EMPM				
	$1/2_1^+$	2.346	3.95	0.66
	$3/2_1^+$	3.302	5.20	0.04
	$3/2_2^+$	4.160	4.67	0.13
	$3/2_4^+$	5.776	3.61	1.48
	$1/2_2^+$	6.322	3.51	1.61
	$1/2_3^+$	7.454	4.52	0.15
	$3/2_7^+$	8.328	4.46	0.21
	$1/2_6^+$	9.413	3.86	0.77
	$1/2_8^+$	11.003	4.12	0.43
	ν_f	ω_f	$\log(ft)$	B(GT)
Exp				
	$1/2^+$	2.243	4.27	0.32
	$(1/2^+, 3/2^+)$	3.866	4.33	0.29
	$3/2^+$	4.066	4.24	0.36
	$(1/2^+, 3/2^+)$	4.604	4.82	0.09
	$(1/2^+, 3/2^+)$	5.553	4.68	0.13
	$(1/2^+, 3/2^+)$	5.559	4.28	0.32

The strengths of several GT transitions to the ^{23}F states of spin $3/2_i^+$ and $1/2_i^+$ are in fair agreement with the data. Few others are one order of magnitude larger (Table 2). Such a large contribution is due to the prominent single particle component of the initial state $1/2_1^+$ and to the large particle-phonon component of the final states.

4. Conclusions

In ^{21}N and ^{21}O the low-lying states are in one-to-one correspondence with the available experimental levels but lie at too high energy. These states, being of one-phonon nature, should be shifted down to the region of experimental observation by a stronger coupling to two phonons.

Such a strong coupling should shift downward also the one-phonon states at higher energy and, therefore, should fill the energy gap between computed and experimental β decay rates.

In ^{23}O, the spectrum as well as several β-transition rates are well reproduced. All the states have a dominant neutron character and have a pure single particle or phonon nature because of the weak neutron-neutron interaction.

Different is the case of ^{23}F. The odd proton of this nucleus, because of the strong proton-neutron interaction, couples strongly to the neutrons in excess thereby enhancing the density of states also at low energy. The coupling is, actually, too strong. In fact, several states of high spin without any experimental counterpart appear in this region.

More compressed spectra in ^{21}N and ^{21}O and weaker proton-neutron interaction may be obtained if the HF spectra get more compact thereby diminishing the neutron content of the TDA phonons in favor of the protons. The proton content, in fact, is negligible due to the large p-h proton energy gaps, ~ 22 MeV and ~ 28 MeV for negative and positive parity states, respectively.

We need, ultimately, a potential more performing than the NNLO$_{opt}$. A possible candidate is the NNLO$_{sat}$ [35] which includes explicitly the three-body contribution and describes properly the bulk properties of nuclei. According to our preliminary calculations, such a potential yields a considerably more compact HF spectrum and, therefore, smaller p-h energy gaps.

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