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A self-consistent equation of motion multiphonon method for odd mass nuclei

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Abstract. An equation of motion phonon method, developed for even-even nuclear systems, is extended to odd nuclei and applied to $A = 17$ isobars. A calculation using a chiral potential is carried out in a space encompassing up to two phonons and, under some simplifying assumptions, three phonons. The low and high energy spectroscopic properties of ^{17}O and ^{17}F are thoroughly explored. The impact of the different phonon components on spectrum, transitions and dipole cross sections is discussed.

1. Introduction

Different methods have been developed to study the modifications of the single-particle states in odd nuclei induced by the core excitations. 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 random-phase approximation (RPA). Recently, PVC calculations were performed within the framework of energy density functionals deduced from Skyrme forces [3–5] or relativistic meson-nucleon Lagrangians [6, 7] or from the theory of finite Fermi systems [8].

Calculations using NN + 3N chiral forces were performed within the context of self-consistent Green's function theory [9], no-core shell model (NCSM) [10] and coupled cluster [11–13].

An equation of motion phonon method (EMPM), proposed [14, 15] for even nuclei and applied mainly to study the dipole response in neutron rich nuclei [16–18], has been extended recently to odd nuclei [19]. It consists in constructing and solving iteratively a set of equations of motion to generate an orthonormal basis of states composed of a valence particle coupled to n-phonon states ($n = 1, 2, ...n...$), also generated within the EMPM, describing the excitations of a doubly magic core. The basis is then adopted to diagonalize the full eigenvalue problem. The whole procedure does not rely on any approximations and preserves the Pauli principle.

We report here on the formulation of the method and its application to ^{17}O and ^{17}F. The calculations are fully self-consistent and make use of a nucleon-nucleon (NN) chiral potential $V_\chi = NNLO_{opt}$ optimized so as to minimize the effects of the three-body forces [20].

2. Outline of the EMPM method for odd nuclei

We use the second quantization formalism and denote the particle creation (annihilation) operators by $a_r^\dagger$ (b_r). We label the particle anf hole states by p and h, respectively.

The main goal of the method is to generate a basis of n-phonon states $\mid \nu_n\rangle$, of energies E_{ν_n}, having the form

$$|\nu_n >= \sum_{p\alpha_n} C^{\nu_n}_{p\alpha_n} \mid (p \times \alpha_n)^v\rangle = \sum_{p\alpha_n} C^{\nu_n}_{p\alpha_n} \Big\{ a_p^\dagger \times \mid \alpha_n > \Big\}^{\nu_n}, \tag{1}$$

where $a_p^\dagger$ creates a valence particle coupled to the n-phonon states

$$\mid \alpha_n >= \sum_{\lambda\alpha_{n-1}} C^{\alpha_n}_{\lambda\alpha_{n-1}} \Big\{ O_\lambda^\dagger \times \mid \alpha_{n-1}\rangle \Big\} \tag{2}$$

and $O_\lambda^\dagger = \sum_{ph} c^\lambda_{ph} (a_p^\dagger \times b_h)^\lambda$ is the TDA phonon operator. The $\mid \alpha_n >$ are generated iteratively within the EMPM starting from $n = 1$ (TDA phonons) and form an orthonormal basis.

We start with constructing the equations of motion in the n-phonon subspace

$$\langle \alpha \parallel [b_p, H]^p \parallel \nu\rangle = \Big(E_\nu - E_\alpha\Big) X^\nu_{p\alpha}, \tag{3}$$

where

$$X^\nu_{p\alpha} = \langle \alpha \parallel b_p \parallel \nu\rangle = \sum_{p'\alpha'} D^\nu(p\alpha, p'\alpha') C^\nu_{p'\alpha'} \tag{4}$$

and $\mathcal{D}^\nu(p\alpha, p'\alpha') = \langle (p \times \alpha)^v \mid (p' \times \alpha')^v\rangle$ is the metric or overlap matrix. We have omitted the subscript n for simplicity.

After expanding the commutator and making use of the relation (4) we obtain the generalized eigenvalue equations

$$\sum_{p_1\alpha_1 p'\alpha'} \Big[\mathcal{A}^\nu(p\alpha, p_1\alpha_1) - E_\nu \delta_{pp_1}\delta_{\alpha\alpha_1}\Big] \mathcal{D}^\nu(p_1\alpha_1, p'\alpha') C^\nu_{p'\alpha'} = 0. \tag{5}$$

$\mathcal{A}^\nu$ is a matrix of the simple structure

$$\mathcal{A}^\nu(p\alpha, p'\alpha') = (\epsilon_p + E_\alpha)\delta_{pp'}\delta_{\alpha\alpha'} + \mathcal{V}^\nu_{p\alpha,p'\alpha'}, \tag{6}$$

where $\mathcal{V}^\nu$ is the particle-phonon potential given by

$$\mathcal{V}^\nu_{p\alpha,p'\alpha'} = \sum_{\sigma tq} [2j_\sigma + 1]^{1/2} W(\alpha\sigma v p'; \alpha' p) F^\sigma_{pp'tq} \langle n; \alpha' \parallel \Big[a_t^\dagger \times b_q\Big]^\sigma \parallel n; \alpha\rangle. \tag{7}$$

Here, $\langle n; \alpha' \parallel \Big[a_t^\dagger \times b_q\Big]^\sigma \parallel n; \alpha\rangle$ is the n-phonon density matrix, W the Racah coefficients, and F the Pandya transform of the two-body potential.

Eq. (5) represents the eigenvalue equation in the overcomplete basis $\Big\{a_p^\dagger \times \mid \alpha >\Big\}^\beta$. The redundant states are eliminated by the procedure outlined in [14, 21], based on the Cholesky decomposition method. It is therefore possible to turn the singular eigenvalue equation (5) into a non singular one yielding only the physical states.

Since recursive formulas hold for all quantities entering $\mathcal{A}$ and $\mathcal{D}$, the eigenvalue equations are solved iteratively and, thereby, yield a basis of orthonormal multiphonon states $\{|\nu_0 >, |\nu_1 > , \ldots |\nu_n > \ldots\}$.

Represented in such a basis, the Hamiltonian matrix is composed of a sequence of diagonal blocks, one for each n, mutually coupled by off-diagonal terms $\langle \nu_{n'} \mid H \mid \nu_n \rangle$. These are non vanishing only for $n' = n \pm 1, n \pm 2$ and are computed by means of recursive formulas. A matrix of such a simple structure can be easily diagonalized yielding eigenfunctions of the form

$$\mid \Psi_\nu \rangle = \sum_{\nu_n} C^\nu_{\nu_n} \mid \nu_n \rangle. \tag{8}$$

These states can be used to evaluate the transition amplitudes of a multipole operator $\mathcal{M}(\lambda\mu)$. If the initial and/or final states have dominant single particle character, we have

$$\langle \psi_{\nu'} \parallel \mathcal{M}(\lambda) \parallel \psi_\nu \rangle \simeq \mathcal{M}^{(\nu\nu')}_{00}(\lambda) + \mathcal{M}^{(\nu\nu')}_{01}(\lambda) + \mathcal{M}^{(\nu\nu')}_{10}(\lambda), \tag{9}$$

where $\mathcal{M}^{(\nu\nu')}_{00}(\lambda)$, $\mathcal{M}^{(\nu\nu')}_{01}(\lambda)$, and $\mathcal{M}^{(\nu\nu')}_{10}(\lambda)$ are, respectively, the particle-particle, particle-phonon, and phonon-particle transition amplitudes, given by

$$\mathcal{M}^{(\nu\nu')}_{00}(\lambda) = \sum_{pp'} \mathcal{C}^\nu_p \mathcal{C}^{\nu'}_{p'} \langle p' \parallel \mathcal{M}_\lambda \parallel p \rangle, \tag{10}$$

and

$$\mathcal{M}^{(\nu\nu')}_{01}(\lambda) = (-)^{v-v'} \mathcal{M}^{\nu\nu'}_{10}(\lambda) = \sum_{pk} \mathcal{C}^\nu_p \mathcal{M}_{\lambda_k} P^{(\nu')}_{p\lambda_k}. \tag{11}$$

They are determined by the amplitudes of the transitions to the kth TDA state of spin $J_k = \lambda$

$$\mathcal{M}_{\lambda_k} = \langle k\lambda \parallel \mathcal{M}(\lambda) \parallel 0 \rangle = \frac{1}{[\lambda]^{1/2}} \sum_{ph} c^{(\lambda_k)}_{ph} \langle p \parallel \mathcal{M}_\lambda \parallel h \rangle \tag{12}$$

and by the weights $P^{(\nu')}_{p\lambda_k} = \sum_{\nu'_1} \mathcal{C}^{\nu'}_{\nu'_1} X^{\nu'_1}_{p\lambda_k}$ which incorporate the joint contributions of the one-phonon components $\mid \nu'_1 \rangle$ of the final states $\mid \Psi_{\nu'} \rangle$ and of the λ-multipole particle-phonon configurations $\mid [p \times \lambda_k]^{\nu_1} \rangle$ present in $\mid \nu'_1 \rangle$.

3. Calculations and results

The Hamiltonian we used is composed of an intrinsic kinetic operator T_{int} plus the optimized chiral two-body potential $V_\chi = NNLO_{opt}$ [20]. We generate a HF basis in a configuration space including up to the $N_{max} = 15$ harmonic oscillator major shell and derive the TDA phonons from a subset of HF states corresponding to $N = 12$.

The multiphonon particle-core basis is composed of all one-phonon states $\mid (p \times \alpha_1)^\nu \rangle$, the two-phonon $\mid (p \times \alpha_2)^\nu \rangle$ of energies $E_{\alpha_2} \leq 35$ MeV and the three-phonon $\mid (p \times \alpha_3)^\nu \rangle$ of energies $\epsilon_p + E_{\alpha_3} \leq 55$ MeV. The inclusion of the three-phonon particle-core states has required some approximations. We have neglected the phonon-phonon potential for the calculation of α_3 as well as the particle-core interaction $\mathcal{V}^\nu_{p\alpha_3,p'\alpha'_3}$ (diagonal approximation). We have also neglected the exchange terms between the odd particle and α_3 by putting $\mathcal{D}^\nu(p_1\alpha_3; p'\alpha'_3) = \delta_{p_1p'}\delta_{\alpha_3\alpha'_3}$.

The theoretical spectra of ^{17}O and ^{17}F are compared with experiments in Figs. 1 and 2, respectively. The one-phonon states alter appreciably the HF level scheme. They depress the lowest $5/2^+_1$ with respect to the other states thereby enhancing its distance from the other levels. This effect promotes the inversion between the $1/2^+_1$and $5/2^+_1$ in ^{17}F consistently with the experiments. Another important consequence is the occurrence of a large number of levels which enrich greatly the spectra. Unfortunately, these new states fall at too high energies ($\geq 11MeV$) with respect to the corresponding experimental levels. The inclusion of the two-phonon states enhances the level density only at high energy and, therefore, leaves the low-lying

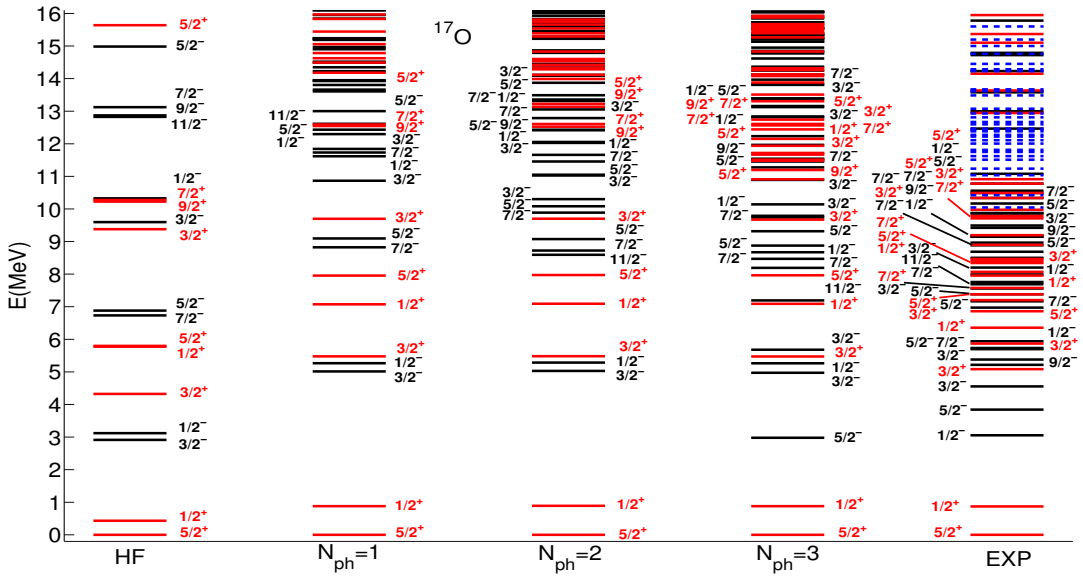

Figure 1. Theoretical versus experimental [22] spectra of ^{17}O. N_{ph} indicates the maximum phonon number. The dashed levels have unknown spin or parity or both.

sector unchanged. Only the three phonons, by pushing few negative parity states down in energy, enrich the low energy spectra but not sufficiently to reproduce the density of the experimental low-energy level schemes.

We use the intrinsic $E1$ operator referred to the CM coordinate which induces the effective charges $e_i = (N/A)e$ for protons and $e_i = (Z/A)e$ for neutrons. The E1 cross section is given by

$$\sigma_{int} = \int_{E_0}^{E} \sigma(\omega) d\omega = \frac{16\pi^3}{9\hbar c} \int_{E_0}^{E} \omega S(E1, \omega) d\omega, \tag{13}$$

where

$$S(E\lambda, \omega) = \sum_{\nu} B_\nu(E\lambda) \delta(\omega - \omega_\nu) \approx \sum_{\nu} B_\nu(E\lambda) \rho_\Delta(\omega - \omega_\nu) \tag{14}$$

is the strength function , ω is the energy variable, ω_ν the energy of the transition of multipolarity $E\lambda$ from the ground to the ν_{th} excited state of spin $J = \lambda$, and ρ_Δ is a Lorentzian of width Δ which replaces the δ function as a weight of the reduced transition probability

$$B_\nu(E\lambda) = \mid \langle \Psi_{\nu\lambda} \parallel \mathcal{M}(E\lambda\mu) \parallel \Psi_0 \rangle \mid^2 . \tag{15}$$

The one-phonon cross section in ^{17}O (Fig. 3(a)) is displaced upward by several MeV with respect to experiments and remains practically unchanged when we include the two phonons. It gets, instead, severely damped and down-shifted by the couplings to three phonons, though not sufficiently to reproduce the experimental main peak which remains ~ 2 MeV down. The unwanted secondary peak originates from a strong transition at ~ 20 MeV (Fig. 4(c)).

The phonon action in ^{17}F is analogous to the one exerted in ^{17}O. The cross section gets quenched and shifted mainly by the coupling to three phonons (Fig. 3(a)). Its behavior, however, is smoother than in ^{17}O. It exhibits a broad wiggly hump covering a wide energy range (20-40 MeV) arising from a huge numbers of closely packed small peaks. Unfortunately

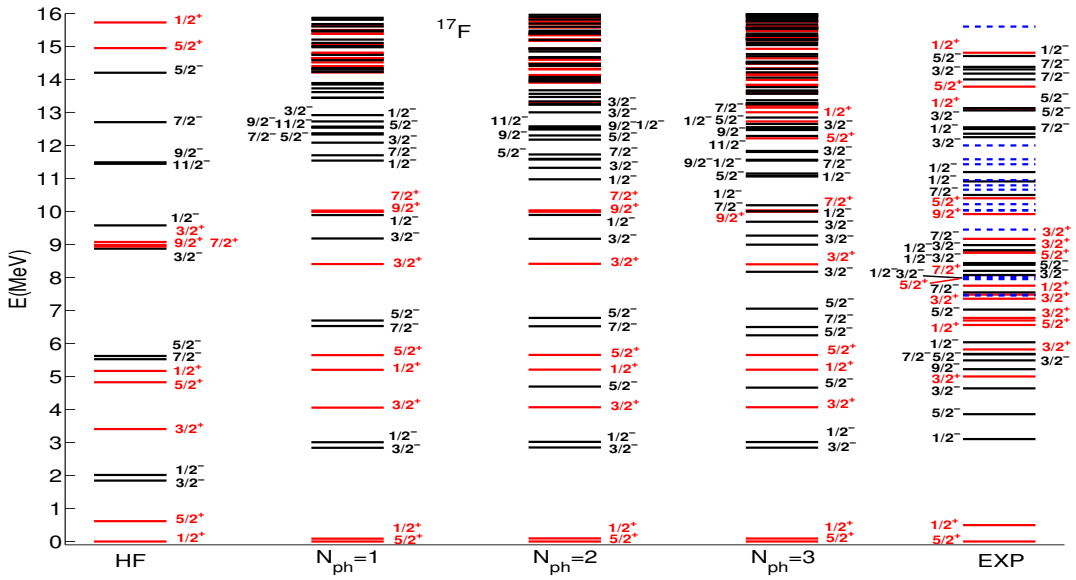

Figure 2. Level schemes of ^{17}F. The notations are the same as for ^{17}O

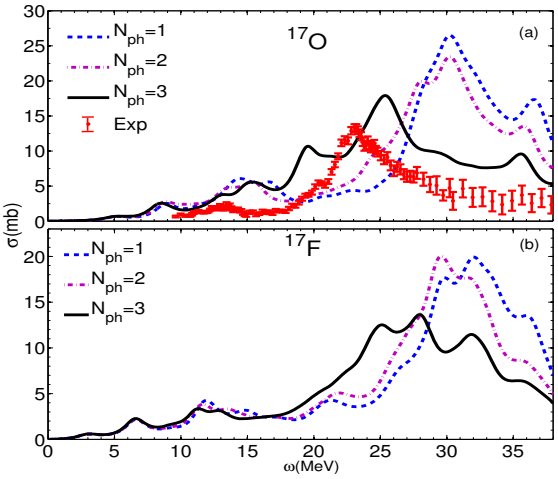

Figure 3. The theoretical E1 cross sections, computed in different multiphonon spaces, are compared in ^{17}F (b) and with the experimental ones [23] in and ^{17}O (a). A width of $\Delta = 2$ MeV have been used.

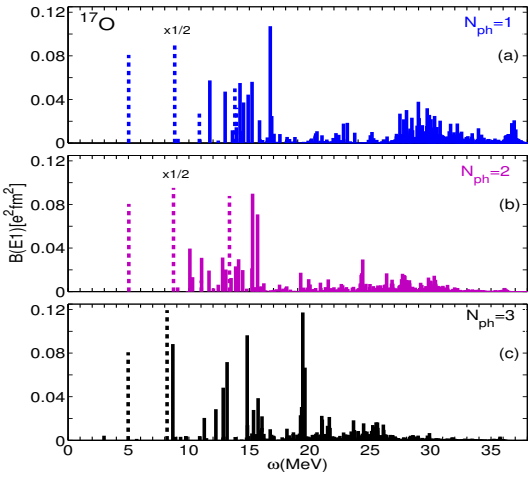

Figure 4. E1 strength distribution of ^{17}O computed in spaces including up to $N_{ph} = 1$ (a), $N_{ph} = 2$(b), and $N_{ph} = 3$(c) phonons.

no experimental data are available except for few low-lying transitions which we will discuss later.

The analysis of the $E1$ strength distribution in ^{17}O (Fig. 4) is helpful for clarifying the role of the different phonon subspaces. The coupling to two phonons induces an appreciable damping over the whole one-phonon spectrum, especially in the high-energy sector (Figs. 4 (a) and (b)). The three phonons deplete almost completely the high energy region and pack most of the strength in the range $5 - 25$ MeV. (Fig. 4(c)). This is the result of two actions. The three phonons shift the one-phonon energies downward and strengthen the amplitudes of several

one-phonon states at the expenses of the two phonons.

The small peaks at low energies should correspond to the pygmy resonance. This is the case of the hump in the $13-15$ MeV interval. This arises almost entirely from the $7/2^-$ excitations and is likely to correspond to the pygmy resonance, which, according to the experimental analysis of Ref. [22], is due to the excitation of two $7/2^-$ states.

4. Conclusions

The multiphonon states enhance enormously the density of levels and compress the whole spectrum, consistently with the data. In particular, the one-phonon states improve the description of low-lying states and enhance the density of levels only at high energy. The low-energy sector is enriched only by the three phonons which push down in energy few one-phonon states, through their strong coupling. The three phonons exert also a crucial quenching action on the $E1$ transitions which reduces substantially the gap between the theoretical and experimental $E1$ cross sections. Sizable discrepancies still remain. The damping and energy shift, though appreciable, are not sufficient to reproduce completely peak, shape and magnitude of the cross section in ^{17}O.

A possible recipe for bridging the gap with experimental data may consist in improving the HF description of the single particle spectra which amounts to improve the nucleon-nucleon potential. In fact, as shown in Figs. 1 and 2, the 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 NN interactions [24, 25]. These gaps are reduced substantially but not completely by the phonon coupling.

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