Role of multiphonon configurations in nuclear spectra and responses: a new approach

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Abstract. A basis of multiphonon states is generated by constructing and solving iteratively a set of equations of motion. Represented in this basis, the Hamiltonian has a simple structure and can be easily brought to diagonal form. The method is adopted to compute the energy levels and the electromagnetic responses in ¹⁶O, chosen as test ground because of its complex structure.

1. Introduction
The role of the multiphonon configurations in determining the properties of the low-lying nuclear spectra and in shaping the high-energy giant resonances is becoming more and more manifest. In fact, the experimental evidence of multiphonon collective mode at low-energy and of multiple giant resonance at high energy has grown rapidly in recent years [1, 2, 3, 4]. Moreover, multiphonon configurations affect crucially the width and damping of the giant resonances [5].

Tamm-Dancoff (TDA) and random-phase approximations (RPA) can only describe the global features of collective modes and explain in part their fine structure by accounting for their decay to single-particle excitations (Landau damping). These approaches, however, are not suited to the study of the anharmonicities of the many low-lying multiphonon spectra and of the high-energy multiple resonances. They are not even able to account for the full fragmentation of the giant resonances.

It is therefore necessary to go from the particle-hole (p − h) to a larger space that includes more complex np − nh configurations and account properly for the couplings between them.

Several theoretical approaches have been devoted to the achievement of such a task. A notable one is the nuclear field theory [6], where the p − h space is coupled to 2p − 2h configurations and to the continuum. Such a method is clearly well suited for describing the damping of the giant resonances.

Of considerable interest is also a method that extends Migdal’s theory and exploits the Green function techniques to enlarge the configuration space beyond the TDA and RPA [7]. The method was applied with considerable success to the study of collective modes and giant resonances.

The most widely adopted approach is the quasiparticle-phonon model (QPM) [8], that effectively diagonalizes a separable Hamiltonian of general form in a space spanned by states.
with a number of phonons up to \( n = 3 \), the phonons being generated in the quasiparticle RPA. The QPM has been adopted systematically in heavy spherical and deformed nuclei. Among the most recent investigations, we may mention the study of double giant resonances [9] and, at low energy, the investigation of the mixed symmetry states in spherical nuclei [10, 11]. In deformed nuclei, the QPM has been successfully adopted to study the \( 0^{+} \) states discovered in large abundance in the rare earth region and the actinides [12] and to investigate the controversial nature of the \( 4^{+} \) states in transitional nuclei [13].

Recently, we have formulated an equation of motion phonon method (EMPM) [14], that moves along the lines drawn within the multistep shell model [15, 16]. The method generates iteratively a basis of multiphonon states built of phonons obtained in the Tamm-Dancoff approximation (TDA). Such a basis greatly simplifies the structure of the Hamiltonian matrix, which can be easily brought to diagonal form yielding exact eigenvalues and eigenvectors. A numerical implementation was carried out on \(^{16}O\). A space spanned by all states up to three phonons and \( 3h\Omega \) was adopted to compute spectra and nuclear responses [17]. The most meaningful results of this calculation will be discussed here.

2. The method

We consider [14] a two-body Hamiltonian \( H \) of general form

\[
H = \sum_i \epsilon_i a_i^\dagger a_i + \frac{1}{4} \sum_{ijkl} V_{ijkl} a_i^\dagger a_j^\dagger a_i a_k^\dagger ,
\]

where \( \epsilon_i \) are the single-particle energies, \( V_{ijkl} \) the antisymmetrized matrix elements of the nucleon-nucleon interaction, \( a_i^\dagger \) \( (a_i) \) the creation (annihilation) particle operators with respect to the physical vacuum.

We intend to generate a basis of \( n \)-phonon states \( |n; \beta > \), having the structure

\[
|n; \beta > = \sum_{\alpha \phi h} C_{\alpha \beta}^{(n)} (\phi h) b_{\phi h}|n - 1; \alpha > ,
\]

where \( b_{\phi h} = a_{\phi h}^\dagger a_{\phi h} \) creates a \( \phi h \) state out of the unperturbed Hartree-Fock vacuum and \( |n - 1; \alpha > \) are states with \( (n-1) \) phonons.

In order to construct such a basis we extend a well established equation of motion method. Indeed, under the request that the Hamiltonian be diagonal within each \( n \)-phonon subspace, spanned by the states \( |n; \alpha > \), the following equations of motion hold

\[
< n; \beta | H, b_{\phi h}^\dagger | n - 1; \alpha > = (E_{\beta}^{(n)} - E_{\alpha}^{(n-1)}) X_{\alpha \beta}^{(n)} (\phi h),
\]

where

\[
X_{\alpha \beta}^{(n)} (\phi h) \equiv < n; \beta b_{\phi h}^\dagger | n - 1; \alpha > .
\]

Upon expansion and linearization of the commutator \([H, b_{\phi h}^\dagger]\), one obtains for the \( n \)-phonon subspace the eigenvalue equations

\[
\sum_{\gamma \gamma'} A_{\alpha \gamma}^{(n)} (\phi h; p'h') X_{\gamma \beta}^{(n)} (p'h') = E_{\beta}^{(n)} X_{\alpha \beta}^{(n)} (\phi h).
\]

The matrix \( A^{(n)} \) has the simple structure

\[
A_{\alpha \gamma}^{(n)} (\phi h; p'h') = \delta^{(n)}_{\alpha \gamma} \left[ \delta_{hh'} \delta_{pp'} (\epsilon_p - \epsilon_h + E_{\alpha}^{(n-1)}) + V_{ph'hp'} \right] + \delta_{hh'} W_{\alpha \gamma}^{(n-1)} (pp') - \delta_{pp'} W_{\alpha \gamma}^{(n-1)} (hh'),
\]

where

\[
\delta^{(n)}_{\alpha \gamma} = \begin{cases} 1 & \text{if } \alpha \rightarrow \gamma, \\ 0 & \text{otherwise}, \end{cases}
\]

and

\[
W^{(n-1)}_{\alpha \gamma} (pp') = \frac{1}{2} \sum_{ijkl} \frac{1}{2} \epsilon_i \epsilon_j \frac{V_{ijkl}}{2} X_{\alpha \gamma}(n-1)(pp').
\]

The last term on the right-hand side is the result of the linearization of the commutator which is given by

\[
\left[ H, b_{\phi h}^\dagger \right] = \frac{1}{2} \sum_{ijkl} V_{ijkl} \left( a_i^\dagger a_j^\dagger a_k a_l - a_i a_j a_k^\dagger a_l^\dagger \right).
\]
where

\[ W^{(n)}_{\alpha\gamma} (pp') = \sum_{h_1h_2} V_{p'h_1h_2}^{(n-1)} (h_1h_2) + \frac{1}{2} \sum_{p_1p_2} V_{p'p_1p_2}^{(n-1)} (p_1p_2) \]

\[ W^{(n)}_{\alpha\gamma} (hh') = \sum_{p_1p_2} V_{hp_1h'_2p_2}^{(n-1)} (p_1p_2) + \frac{1}{2} \sum_{h_1h_2} V_{hh_1h'_2h_2}^{(n-1)} (h_1h_2). \] (7)

Here

\[ \rho^{(n)}_{\alpha\gamma} (kl) = \langle n; \gamma|a_k^\dagger a_l|n; \alpha \rangle \] (8)

is the density matrix.

We now insert the expansion (2) of \(| n; \beta \rangle \) into Eq. (4) obtaining

\[ X^{(n)} = D^{(n)} C^{(n)}, \] (9)

where \( D^{(n)} \) is the overlap or metric matrix. In virtue of Eq. (9), the equation of motion (5) becomes the eigenvalue equation of general form

\[ A^{(n)} D^{(n)} C^{(n)} = E^{(n)} D^{(n)} C^{(n)}, \] (10)

where \( A^{(n)} \) is still given by Eq. (6) and the overlap matrix \( D^{(n)} \) has the expression

\[ D^{(n)}_{\alpha\beta} (pp'; hh') = \sum_{\gamma} \left[ \delta_{pp'} \delta_{\gamma\beta} - \rho_{\gamma\beta}^{(n-1)} (pp') \right] \rho_{\alpha\gamma}^{(n-1)} (hh'). \]

The density matrices can be computed by the recursive relations

\[ \rho^{(n)}_{\alpha\beta} (p_1p_2) = \sum_{ph\gamma} C^{(n)}_{\alpha\gamma} (ph) X^{(n)}_{\delta\beta} (p_1h) \left[ \delta_{pp_2} \delta_{\gamma\delta} - \rho_{\gamma\delta}^{(n-1)} (pp_2) \right], \]

\[ \rho^{(n)}_{\alpha\beta} (h_1h_2) = \sum_{ph\gamma\delta} C^{(n)}_{\alpha\gamma} (ph) X^{(n)}_{\delta\beta} (ph_2) \left[ \delta_{hh_1} \delta_{\gamma\delta} - \rho_{\gamma\delta}^{(n-1)} (h_1h) \right]. \] (12)

Once the redundancy of the basis states is eliminated by the the Choleski decomposition method, the recursive formulas of \( A^{(n)} \), \( D^{(n)} \) and \( \rho^{(n)} \) allow to solve the generalized eigenvalue problem iteratively starting from \( n = 0 \), namely the \( p - h \) vacuum, up to a \( n \)-phonon subspace. A basis of linearly independent multiphonon states, \( \{| >, |1, \lambda >, \ldots, |n, \alpha > \} \), is thereby generated.

This basis greatly simplifies the structure of the Hamiltonian matrix and makes its diagonalization much easier. The eigenvectors so obtained are exact and have the structure

\[ | \Psi_{\nu} \rangle = \sum_{n, \beta} C^{(n)}_{\beta} (n, \beta). \] (13)

Using these wave functions, we obtain for the transition amplitudes of the one-body operator

\[ M = \sum_{kl} M_{kl} a_k^\dagger a_l \] (14)

the formula

\[ M(i \rightarrow f) = \langle \Psi_f | M | \Psi_i \rangle = \sum_{kln_i, \alpha_i, \beta_f} M_{kl} C^{(n_i)}_{\alpha_i, \alpha} C_{\alpha_f}^{(n_f)} \left[ \rho_{\alpha_i\beta_f}^{(n_i, n_f)} (kl) \right]. \] (15)
These amplitudes involve the density matrix, which can be computed through Eqs. (12) when \( n_i = n_f \). When \( n_i \neq n_f \), \( \rho_{ij}(kl) \) is nothing but \( X_{ij}(ph) \) (Eq. 4) or its complex conjugate.

The composite structure of the transition amplitudes deserves few words of comment. Let us look, for instance, at the wave functions considered in the present calculation. The ground state |\( \Psi_0 \rangle \rangle is a linear combination of the vacuum |\( \Psi_0 \rangle \rangle, a very small one-phonon piece and a set of two-phonon states, while the excited states |\( \Psi_\nu \rangle \rangle contain up to three phonons. It follows that the transition amplitude can be written schematically

\[
M(0 \rightarrow \nu) \sim p_{01} < 1|M|1 > + p_{11} < 1|M|1 > + p_{12} < 2|M|1 > + p_{21} < 1|M|2 > + p_{22} < 2|M|2 > + p_{23} < 3|M|2 >, \]

(16)

where \( i = 1, 2, 3 \) indicates the number of phonons and \( |p_{ij}| < 1 \) the weights. The above equation makes clear that, within the EMPM, the transition amplitudes contain the Tam-Dancoff piece (one-phonon), quenched by a factor \( |p_{01}| < 1 \), plus many other corrective terms coming from the coupling, promoted by the operator \( M \), between states with \( i = j \) or \( i = j \pm 1 \).

3. A numerical test ground: \( ^{16}\text{O} \)

We have chosen \( ^{16}\text{O} \) as bench mark for our method. Its low-energy positive parity spectrum, well known for its complex structure, was studied in large scale shell model calculations which included up to 4p−4h and 4h\( \omega \) configurations [18] and, more recently, up to 6h\( \omega \) [19].

For our illustrative purposes, we have included all \( p−h \) configurations up to \( n = 3 \) and 3h\( \omega \) and used a Hamiltonian composed of a Nilsson unperturbed piece plus a bare G-matrix deduced from the Bonn-A potential.

In order to get a complete separation of the intrinsic from the center of mass motion, we have

![Figure 1](image-url)
Figure 2. $E\lambda$ strength distributions in $^{16}\text{O}$, computed in TDA, RPA and EMPM.

Figure 3. $E\lambda$ strength distributions computed for $^{16}\text{O}$ in the EMPM with and without c.m. spurious admixtures.
adopted the method of Palumbo [20, 21], which separates the center of mass spurious mode from the intrinsic states and pushes such a spurious state high up in energy.

Being our space confined to $3 \hbar \omega$, the ground state contains correlations up to 2-phonons only. These account for about 20% of the state, while the remaining 80% pertains to the $p-h$ vacuum. A no-core shell model calculation [19] yields about 60% for the $0p-0h$, 20% for $2p-2h$ and 20% for the other more complex configurations, excluded from our restricted space.

As shown in Fig. 1, the deviations of the computed spectra from the experimental ones, while reasonably small for negative parity levels, are dramatic for positive parity. This was largely expected, since one has to include four-phonon states, at least, in order to hope to approach the positive parity experimental levels [18, 19]. It might be worth pointing out the importance of removing the CM motion. If this is not removed, the spurious $1^-$ becomes the ground state!

As shown in Fig. 2, the multiphonon configurations have a very strong impact on the nuclear response. Only the isovector giant dipole resonance is not strongly altered, an indication of the basically harmonic character of this mode. The $E1$ spectrum is slightly shifted downward and keeps its shape while the prominent peak is considerably quenched with respect to the TDA or RPA. The strength distribution is compatible with the experimental dipole cross section [22, 23]. It is concentrated in the domain of the experimental cross section and has the main peaks in close correspondence with the observed ones. The nature of those peaks changes little with respect to TDA. They are described by states with dominant $J^\pi = 1^-, T = 1$ one-phonon components.

Strong is the impact on the $E3$ response. Because of the the strong coupling between one and three-phonon configurations, the dominantly one-phonon peaks are pushed down in energy, while the states contributing to the high energy broad hump acquire large two and, especially, three-phonon components, which become dominant in several instances.

Dramatic are the changes brought into the other two $E\lambda$ spectra. The $E2$ peaks are severely damped and the full strength strongly fragmented. Such a large effect is to be ascribed to the nature of the $2^+$ states. These are dominated by low-energy two-phonon components like $|3^- \otimes 3^-|_{2^+}^>$. Similarly, the strength of the isoscalar $E1$ response gets spread and its peaks severely reduced in magnitude as the multiphonon components come into play. The sensitivity of the isoscalar giant dipole resonance to multiphonon configurations was largely expected. Indeed, once the c.m. spurious mode is removed, most of the $p-h$ excitations entering the isoscalar $1^-$ states have an excitation energy of $3\hbar \omega$. For a consistent treatment of the mode, one has to include the huge number of $2p-2h$ and $3p-3h$ configurations of the same energy. In the EMPM, all these configurations are treated on the same footing of the $p-h$ states through the two- and three-phonon components.

In all cases, the multiphonon coupling has the effect of severely damping and strongly fragmenting the $E\lambda$ strengths. Once again, it is worth to point out the dramatic effect of removing the CM motion (Fig. 3).

4. Conclusions
The comparative analysis outlined in the previous section shows that, at least in $^{16}$O, the multiphonon (or $np-nh$) configurations are important ingredients of the negative parity states and crucial constituents of the positive parity ones. They affect strongly the nuclear response for most $E\lambda$ transitions by inducing a severe damping and fragmentation of the strengths.

In computing the $E\lambda$ transitions, it becomes more and more compelling to remove the c.m. motion as the number of phonons increases. Otherwise, the c.m. admixtures would completely alter the strength distribution, at least for some multipolarities $E\lambda$.

Our calculation, though performed with no approximations, was carried out using a multiphonon basis composed of states with a maximum number of three TDA phonons. Because of these restrictions, the present calculation is far from reproducing the observed spectroscopic
properties of this nucleus, especially those concerning the positive parity states. We need to include the \((n = 4)\)-phonon subspace at least.

This extension is made possible by a new formulation of the method. This consists in replacing the basis states \(a_p^\dagger a_h|n - 1\alpha >\) with the more correlated ones \(O^\dagger_{\lambda}|n - 1\alpha >\), where \(O^\dagger_{\lambda}\) is the TDA phonon operator. By so doing, a large number of \(p - h\) states, with no restrictions on their energy, can be incorporated into the correlated TDA phonons. Moreover, it is possible to select the phonon states that are collective and discard the others thereby achieving a substantial truncation of each multiphonon subspace. Such a truncation should enable us to enlarge the phonon space by reaching subspaces with a large number of phonons \((n \geq 4)\) and, on the other hand, to apply the method to heavy nuclei. The upgrade of the method is being completed and its numerical implementation in progress.

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