Collective Modes in Nuclei: An Exact Microscopic Multiphonon Approach

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Abstract. We report on an equation of motion method which generates a microscopic multiphonon basis by constructing and solving iteratively a set of equations of motion starting from the particle-hole vacuum up to a subspace spanned by states with an arbitrary number of Tamm-Dancoff phonons. In such a basis, the Hamiltonian takes a simple form and can be brought easily to diagonal form. We show how the method can be implemented to study the anharmonic features of few giant resonances in ^{16}O.

1 Introduction

Multiphonon excitations in nuclei, predicted since the original formulation of collective models [1], have been object of intensive experimental and theoretical studies in recent years. Low-energy experiments have detected quadrupole-quadrupole, octupole-octupole, and quadrupole-octupole excitations [2] and have provided conclusive evidence in favor of quadrupole proton-neutron mixed symmetry multiphonon states [3–5]. At high energy, the double giant dipole resonance has been detected [6–8].

The methods developed to study these multiphonon excitations are based on or inspired by the Fermion-Boson mapping technique [9–11].

A phenomenological realization of the Fermion-Boson mapping is the interacting boson model (IBM) [12], which has been adopted with great success to study the systematic of these excitations at low energy.

Among the microscopic approaches, the quasiparticle-phonon model (QPM) describes satisfactorily both low and high energy multiphonon excitations [13]. In the QPM, a Hamiltonian of generalized separable form is expressed in terms of RPA quasi-boson operators and then diagonalized in a severely truncated space which includes a selected set of two and three RPA phonons.

Other microscopic methods have tried to go beyond the quasi-boson approximation but with limited success [14, 15].

We report here on an iterative equation of motion method which we have proposed in order to generate a basis of TDA multiphonon states and, then, solve exactly the nuclear eigenvalue problem in the space spanned by such a correlated basis

using a general Hamiltonian. While a complete and detailed description of the approach can be found elsewhere [16], we will outline here the main steps of the method and illustrate how the procedure is implemented in the specific case of ^{16}O, which, because of its highly complex shell structure, represents a severe test for our multiphonon approach.

2 Brief Description of the Method

We intend to generate a set of multiphonon states $\mid n;\alpha\rangle = \mid \nu_1 \dots \nu_n\rangle$ which are the eigenstates of the Hamiltonian H with eigenvalues $E_\alpha^{(n)}$ within each separate subspace spanned by states with n phonons. The labels ν_i denote the quantum numbers of the i_{th} phonon.

To this purpose we have shown that, under the request that H be diagonal within each $n-$phonon subspace, it is possible to derive the equation

$$< n;\beta|\,[H, b_{ph}^\dagger]\,|n-1;\alpha> = (E_\beta^{(n)} - E_\alpha^{(n-1)}) < n;\beta|b_{ph}^\dagger|n-1;\alpha>, \qquad (1)$$

where $b_{ph}^\dagger = a_p^\dagger a_h$ is a bilinear form in the operators $a_p^\dagger$ and a_h which create respectively a particle (p) and a hole (h) with respect to the unperturbed ground state (ph vacuum).

We then write the Hamiltonian in second quantized form and expand the commutator $[H, a_p^\dagger a_h]$ on the left-hand side of the equation. After a linearization procedure, we obtain for the n-phonon subspace the eigenvalue equation

$$\sum_{\gamma p' h'} A_{\alpha\gamma}^{(n)}(ph\ ;\ p'h')\ X_{\gamma\beta}^{(n)}(p'h') = E_\beta^{(n)}\ X_{\alpha\beta}^{(n)}(ph), \qquad (2)$$

where

$$X_{\alpha\beta}^{(n)}(ph)\ \equiv < n;\beta|b_{ph}^\dagger|n-1;\alpha> \qquad (3)$$

and

$$\begin{aligned} A_{\alpha\gamma}^{(n)}(ph;p'h') = {} & \delta_{hh'}\delta_{pp'}\delta_{\alpha\gamma}^{(n-1)}\left[(\epsilon_p - \epsilon_h) + E_\alpha^{(n-1)}\right] \\ & + \sum_{h_1} V_{p'h_1h'p}\,\rho_{\alpha\gamma}^{(n-1)}(h_1h) \\ & - \sum_{p_1} V_{p'hh'p_1}\rho_{\alpha\gamma}^{(n-1)}(pp_1) \\ & + \frac{1}{2}\delta_{hh'}\sum_{p_1p_2} V_{p'p_1pp_2}\rho_{\alpha\gamma}^{(n-1)}(p_1p_2) \\ & - \frac{1}{2}\delta_{pp'}\sum_{h_1h_2} V_{hh_1h'h_2}\{\rho_{\alpha\gamma}^{(n-1)}(h_1h_2)\}. \end{aligned} \qquad (4)$$

The symbols ϵ_p (ϵ_h) are single particle (hole) energies, V_{ijkl} the matrix elements of the two-body potential, and

$$\rho^{(n)}_{\alpha\gamma}(kl) =< n;\ \gamma|a^{\dagger}_{k}a_{l}|n;\ \alpha > \tag{5}$$

defines the density matrix with $a^{\dagger}_{k}a_{l}$ written in normal order with respect to the ph vacuum.

The above system of equations represents a natural generalization of the Tamm-Dancoff equations of motion. These are recovered for $n = 1$.

It is easy to infer from the expression (3) of the vector amplitudes that the eigenvectors generated from solving such a system of equations are linear combinations of N_r states $b^{\dagger}_{ph}|n-1;\ \alpha >$. These are linearly dependent and, therefore, form an overcomplete set.

In order to extract a linear independent basis, we expand $|n;\ \beta >$ in terms of the redundant N_r states

$$|n;\ \beta >= \sum_{\alpha\, ph} C^{(n)}_{\alpha\beta}(ph)\, b^{\dagger}_{ph}\ |n-1;\ \alpha > . \tag{6}$$

Upon insertion in Eqs. (3) and (4), we get

$$X = \mathcal{D}C \tag{7}$$

$$A\,\mathcal{D}C = E\mathcal{D}C. \tag{8}$$

where $\mathcal{D}$ is the overlap or metric matrix

$$d^{(n-1)}_{\alpha\beta}(ph;p'h') = \langle n-1;\beta \mid b_{p'h'}b^{\dagger}_{ph} \mid n-1;\alpha\rangle. \tag{9}$$

Eq. (8) defines an eigenvalue equation of general form. It is, however, ill-defined. The matrix $\mathcal{D}$ is singular, since its determinant is necessarily vanishing.

The traditional methods adopted to overcome this problem are based on the straightforward diagonalization of $\mathcal{D}$ [17], which is time consuming. Moreover, the calculation of the metric matrix is a highly non trivial task. Elaborated diagrammatic techniques and complex iterative procedures have been envisaged to this purpose [14, 15, 18, 19].

Our equation of motion method provides the easiest and most natural solution to this latter problem by yielding the simple recursive formula

$$d^{(n-1)}_{\alpha\beta}(ph;p'h') = \sum_{\gamma}\left[\delta_{pp'}\delta_{\gamma\beta} - \rho^{(n-1)}_{\gamma\beta}(pp')\right]\rho^{(n-1)}_{\alpha\gamma}(hh'). \tag{10}$$

Moreover, we have avoided the direct diagonalization of $\mathcal{D}$ by adopting an alternative method based on the Choleski decomposition. This provides a fast and efficient prescription foe extracting a basis of linear independent states $b^{\dagger}_{ph}\ |n-1;\ \alpha >$ spanning the physical subspace of the correct dimensions $N_n < N_r$.

The additional prescription consists in solving the generalized eigenvalue problem (8) just in such a subspace. The basis for the n-phonon subspace is thereby generated.

We are now ready to face the $(n+1)$-phonon subspace. To this purpose we need to evaluate the amplitudes $X^{(n)}_{\alpha\beta}(ph)$ and the density matrix $\rho^{(n)}_{\alpha\beta}(kl)$ within the $n-$phonon subspace.

As for the $X^{(n)}_{\alpha\beta}(ph)$, we make use of Eq. (7), while for the density matrix we adopt the recursive relations

$$\rho^{(n)}_{\alpha\beta}(p_1p_2) = \sum_{ph\gamma\delta} C^{(n)}_{\alpha\gamma}(ph)\, X^{(n)}_{\delta\beta}(p_1h) \times \Big[\delta_{pp_2}\delta_{\gamma\delta} - \rho^{(n-1)}_{\gamma\delta}(pp_2)\Big], \tag{11}$$

$$\rho^{(n)}_{\alpha\beta}(h_1h_2) = \sum_{ph\gamma\delta} C^{(n)}_{\alpha\gamma}(ph)\Big[\delta_{hh_1}\delta_{\gamma\delta}X^{(n)}_{\gamma\beta}(ph_2) - X^{(n)}_{\delta\beta}(ph)\,\rho^{(n-1)}_{\gamma\delta}(h_1h_2)\Big]. \tag{12}$$

$X^{(n)}_{\alpha\beta}(ph)$ and $\rho^{(n)}_{\alpha\beta}(kl)$ are the new entries for the equations of motion in the $(n+1)$-phonon subspace.

The iterative procedure is clearly outlined at this stage. To implement it, we have just to start with the lowest trivial 0-phonon subspace, the ph vacuum, and, then, solve the equations of motion step by step up to a convenient n-phonon subspace.

The multiphonon basis is, thereby, generated. In such a basis, the Hamiltonian gets decomposed into diagonal blocks, mutually coupled by off-diagonal terms. These are given by recursive formulas and, therefore, easily computed. It remains now only to diagonalize the Hamiltonian matrix to get the exact nuclear eigenvalues and eigenvectors.

3 A Numerical Implementation of the Method

For illustrative purposes, we apply the method to ^{16}O. The low-lying excitations of this nucleus are known to have a highly complex ph structure since the pioneering work of Brown and Green [20]. The low- energy positive parity spectrum was studied in a shell model calculation which included up to $4p-4h$ and $4\hbar\omega$ configurations [21]. The same spectrum was studied very recently within a no-core shell model and an algebraic symplectic shell model [22]. In both approaches, the model space was enlarged so as to include all configurations up to $6\hbar\omega$.

At least at this preliminary stage, our method cannot compete with the shell model in describing the low-lying states of this nucleus. This might be possible only once we will be able to develop a reliable truncation procedure capable of selecting only the relevant states, no matter how large the number of phonons and of major shells, while rejecting the non relevant ones. Since the present numerical test intends to prove the exact nature of the method, we have to include all the states within a given $n-$phonon subspace. It is therefore unavoidable that the number of

multiphonon states becomes prohibitively large as soon as the number of phonons increases. In our case this happens for $n > 3$.

We have therefore included all ph configurations up to $3\hbar\omega$, which limits our phonon space up to $n = 3$. Such a space is considerably smaller than the one adopted in shell model. On the other hand, our method generates at once the whole spectrum of positive and negative parity states. This allows the study of low-lying as well as high energy spectroscopic properties and, in particular, the anharmonic features of the giant resonances. To this purpose, we used a Hamiltonian composed of a Nilsson unperturbed piece plus a bare G-matrix deduced from the Bonn-A potential [23].

We have adopted the method of Palumbo [24] to separate the intrinsic from the center of mass motion, obtaining states completely free of any spurious admixture.

Being the 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 ph vacuum.

The structure of the shell model ground state as determined in Ref. [21] is quite different. According to this calculation, in fact, the ph vacuum and the $2p - 2h$ configurations contribute with comparable weight, a bit more than 40%. The rest, about 13%, comes from the $4p - 4h$ configurations. On the other hand, the more consistent no-core and symplectic shell model calculations, performed in a space which includes up to 6 $\hbar\omega$ configurations, give numbers somewhat closer to our estimates: About 60% for the $0p - 0h$, 20% for $2p - 2h$ and 20% for the other more complex configurations [22].

Let us now investigate the anharmonicities induced by the multiphonon configurations on some selected giant resonances. We have studied isoscalar and isovector dipole and quadrupole transitions. To this purpose, we have computed the strength function

$$\mathcal{S}(\omega; F^{(n)}_\lambda, J^\pi) \approx \mathcal{S}_\Delta(\omega; F^{(n)}_\lambda, J^\pi) = \sum_\nu B_\nu(F^{(n)}_\lambda; gr \to J^\pi)\, \rho_\Delta(\omega - \omega_\nu), \quad (13)$$

where

$$\rho_\Delta(x) = \frac{\Delta}{2\pi} \frac{1}{x^2 + (\frac{\Delta}{2})^2} \quad (14)$$

is a Lorentzian weight for the reduced transition probability

$$B_\nu(F^{(n)}_\lambda, J^\pi) = \left| \langle \Phi_{\nu J^\pi} \| F^{(n)}_\lambda \| 0 \rangle \right|^2 . \quad (15)$$

The field $F^{(n)}_\lambda$ is

$$F^{(n=\lambda)}_\lambda = \mathcal{M}(E\lambda, \mu) = \frac{e}{2} \begin{pmatrix} 1 \\ \tau_3 \end{pmatrix} r^\lambda Y_{\lambda\mu}(\hat{r}) \quad (16)$$

for the quadrupole and the isovector dipole transitions and

$$F^{(n=3)}_{\lambda=1\mu} = r^3 Y_{1\mu}(\hat{r}) \quad (17)$$

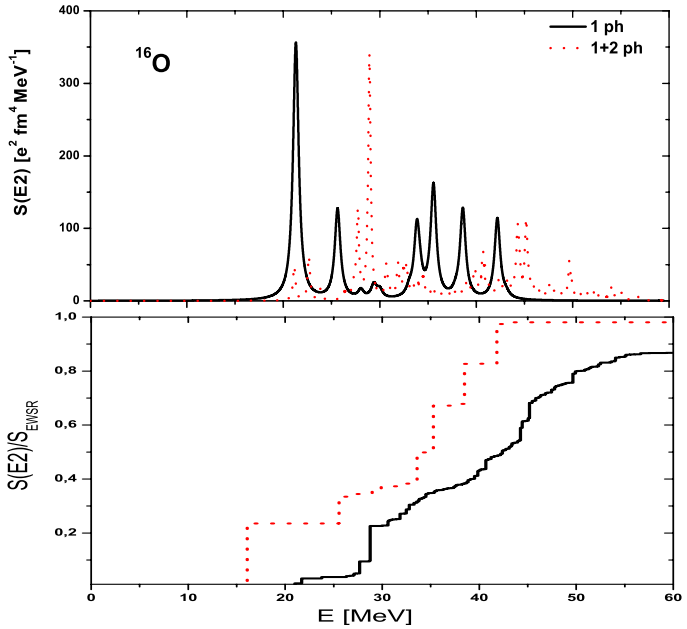

Figure **1.** $E2$ strength distribution and running sum in ^{16}O.

for the isoscalar dipole excitations (squeezed dipole mode). It is important to notice the absence of any corrective term in this latter operator. This is generally included in order to eliminate the spurious contribution due to the center of mass excitation. Such a term is not necessary in our approach which guarantees a complete separation of the center of mass from the intrinsic motion.

Figure 1 shows the distribution of the $E2$ strength over a very large energy interval. The two-phonon configurations have a damping and spreading effect. One may notice that the agreement with experiments gets worse as the two-phonon configurations are included. The $E2$ strength of the lowest 2^+ is quenched and pushed at too high energy with respect to the experiments.

These features appear more clearly in the second panel of Figure 1. This shows that, because of the two-phonon coupling, some strength is pushed so high in energy as to deplete the EWSR. This discrepancy is an indication that the multiphonon space considered here is too restricted.

The negative parity states take full advantage of the configurations included in the space up to 3-$\hbar\omega$. As shown in Figure 2, the isovector $E1$ response is only slightly affected by the complex configurations, an indication that the isovector giant dipole resonance (IVGDR) mode is basically harmonic.

More dramatic is the effect of the multiphonon excitations on the isoscalar $E1$ response. The strength gets spread over a much larger energy range as we include the multiphonon configurations (Figure 3). Such a spreading was expected. Indeed, the isoscalar giant dipole resonance (ISGDR) is due to ph excitations of $3\hbar\omega$. This

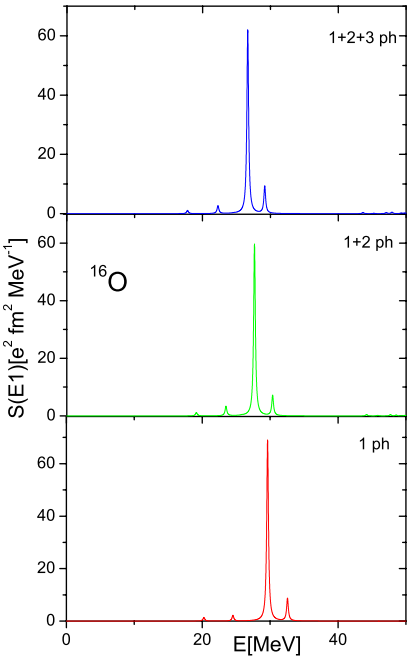

Figure **2.** Isovector $E1$ strength distributions in ^{16}O.

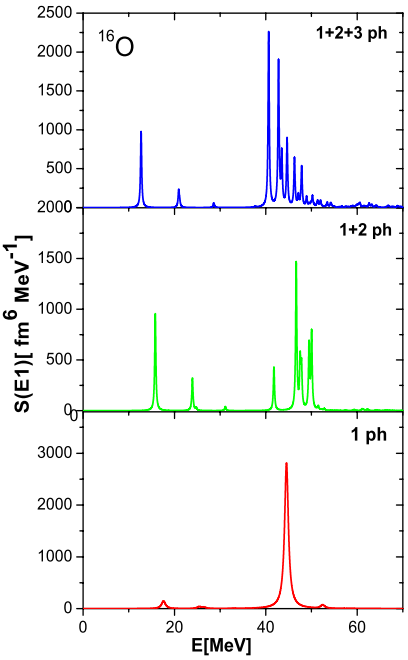

Figure **3.** Isoscalar $E1$ strength distributions in ^{16}O.

is also the energy of many $2p-2h$ and $3p-3h$ configurations which are therefore to be included in a consistent description of the mode.

Both the isovector and isoscalar $E1$ strengths are at too high energies with respect to experiments or mean field estimates. The peak of the IVGDR is about 5 MeV above the experimental one, while the ISGDR is pushed by about 6 MeV with respect to experiments [25]. These discrepancies are to be ascribed only partly to the complex configurations excluded by our space. Since the ph vacuum is the main component of the ground state, the $E1$ response is expected to be mainly a one-phonon excitation which couples to two and three phonons at most. Such a response is affected by the complex configurations only through the $np-nh$ components present in the ground state with considerably smaller amplitudes. The mentioned upward shifts of the strengths may be due, to a large extent, to the Nilsson potential adopted here which induces a too large gap between major shells.

4 Concluding Remarks

The method we have proposed leads to eigenvalue equations of simple structure in any n-phonon subspace. It is, therefore, not only exact but also of easy implementation for a Hamiltonian of general form. Moreover, it generates at once the whole

nuclear spectrum. It is therefore suitable for studying the low-lying spectroscopic properties as well as the high energy giant resonances.

Its exact numerical implementation in ^{16}O was confined to a space which includes up to three-phonons and 3 $\hbar\omega$, sufficient for our illustrative purposes, but too restricted to describe exhaustively all spectroscopic properties of this complex nucleus.

Extending the calculation to a larger space is not straightforward. Indeed, the number of density matrices to be computed increases so rapidly with the number of phonons as to render the procedure unbearably slow.

The method, however, generates a basis of correlated states. It is therefore conceivable that most of them are non collective and unnecessary. The selection of the relevant basis states may be done efficiently by an importance sampling algorithm developed recently [26], which allows a severe truncation while monitoring the accuracy of the solutions. Such a procedure should render manageable the eigenvalue problem up to at least four phonons and 4 $\hbar\omega$ in ^{16}O .

We believe, however, that enlarging further the space will affect modestly the $E1$ giant resonances investigated here. Indeed, since our phonon Hamiltonian couples states differing by two-phonons, at most, the anharmonicities on the $E1$ one phonon states come almost entirely from the coupling with two and three phonons, accounted here. It remains, therefore, to exploit the sensitivity of the $E1$ response to the single particle energies in order to improve the agreement with experiments.

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