

# THE HYBRID CONFIGURATION MIXING MODEL AND THE SPECTROSCOPY OF ODD NUCLEI\*

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We introduce a new approach which is meant to be a step towards complete low-lying spectroscopy of odd nuclei. In the first applications, we limit ourselves to a magic core plus an extra neutron or proton. The model does not contain any free adjustable parameter, but is based on a Hartree–Fock (HF) description of particle states and Random Phase Approximation (RPA) calculations for core excitations. With respect to traditional particle-vibration coupling calculations, in which one can only address single-nucleon states and particle-vibration multiplets, we can also describe states of shell-model type like 2 particle–1 hole. The underlying spirit is, of course, related to filling the gap between shell-model-like approaches for low-lying spectroscopy, and the traditional HF+RPA approach to high-lying states like giant resonances.

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## 1. Introduction

There are many approaches to nuclear structure that try to deal with the many facets of the complex behaviour of atomic nuclei. While this is to some extent unavoidable, and the importance of the quest for a “universal” model should not be overemphasised, it is of clear interest to show connections between different approaches and learn about their pros and cons through confrontations.

In recent years, it has become clear that as an approach to nuclear structure, Density Functional Theory (DFT) has a very wide range of applicability [1]. It can be used for all nuclei except perhaps the lightest ones. It can

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explain ground state properties, but also collective excitations such as rotational bands of deformed systems, or vibrational states *i.e.* giant resonances. One main limitation, as pointed out by several authors [2], is that both in principle and in practice, the nuclear shell structure and thus the low-lying spectroscopy is not very satisfactorily accounted for.

Low-lying spectroscopy is the obvious playground for the nuclear shell model (SM) [3, 4]. Shell-model calculations are often too demanding as the size of the system under study increases. Even in systems of moderate size, model space limitations hinder the description of high-lying states. Therefore, even if the SM can be highly successful in the description of low-lying nuclear states, eventually the physics of other states like giant resonances is hard to be captured.

Our work goes along the line of filling such a gap, as it is mentioned in the abstract. We would like to use the typical implementations of DFT like HF and RPA as a starting basis, and introduce further couplings. Of course, we wish to benefit from our experience in implementing microscopic particle-vibration coupling (PVC) schemes [5–7] and go one step further.

The object of our study are low-lying spectra of odd nuclei consisting of one neutron or one proton outside a magic core. PVC models are based on the idea that these particles are significantly influenced by the low-lying core excitations, and a sound description of the odd nucleus should result from the treatment of the coupling between particles and core vibrations [8, 9]. A limitation of many “traditional” PVC calculations has been the use of purely phenomenological inputs while we stick to a fully microscopic, self-consistent description. We have started from Skyrme effective Hamiltonians or functionals, and we have already used this formalism to study the fragmentation of single-particle states around a magic core [10, 11] (similar calculations have been performed within the framework of Relativistic Mean Field in Refs. [12, 13]).

However, the low-lying spectra of odd nuclei are not simply characterised by the presence of fragmented single-particle strength. Some states have their largest component which is associated with the coupling of a particle with a core vibration, namely they are essentially members of a “particle-phonon multiplet” (we use here and below the word “phonon” meaning a collective vibration of the core). In such a case, the reduced decay transition probability from these states to the odd nucleus ground state is similar to the reduced transition probability of the phonon of the A-1 core (see *e.g.* [8]). On the other hand, if one tries to excite these states in transfer reactions, the spectroscopic factors turn out to be quite small, so that these states can be distinguished from “particle” states that, despite being not fully pure, have large spectroscopic factors instead.

One can also find in the low-lying nuclear spectra states that have, for instance, a main component of the type two particle–one hole (2p–1h), three particle–two hole (3p–2h), *etc.* These states do not fit at all a PVC model whereas they appear, naturally, in shell-model calculations. So, we may be driven to call them “shell-model-like” states. Mixed states, whose wave function does not have a dominant character, cannot be excluded; we will see some of them when discussing  $^{133}\text{Sb}$  in what follows.

All these considerations call for an appropriate hybrid model that we shall call Hybrid Configuration Mixing (HCM) model in this work. To take care of the various situations that we have outlined above, and to stick to the consistent use of Skyrme, in practice, we include in our model the occupied and unoccupied Skyrme–HF single-particle states, together with a number of states that for practical reasons emerge from self-consistent Random Phase Approximation (RPA) calculations but can have either collective character or pure p–h nature. We deal with the issue of the Pauli principle in the way that we shall describe below.

So, we describe briefly our formalism in Sec. 2 and we illustrate some preliminary results in Sec. 3. Finally, some conclusions and perspectives are discussed in Sec. 4.

## 2. Formalism

As said in Introduction, we start from a basis of states that are either pure particle states outside a core, or particles coupled with a core excitation (collective, or pure p–h) emerging from RPA.

The particle states have the usual quantum numbers  $n, l, j, m$  and we write  $jm$  in what follows for the sake of simplicity. The associated energies are written as  $\varepsilon$ , and we use the notation  $a$  and  $a^\dagger$  for the annihilation and creation operators of these fermionic states. For each spin and parity,  $J^\pi M$ , the core excitations will be labelled with an index  $N$  and we drop here the parity label. The associated energies, annihilation, and creation operators of these core excitations are denoted by  $\hbar\omega$ ,  $\Gamma$  and  $\Gamma^\dagger$ . Consequently, the basis states are either

$$|jm\rangle = a_{jm}^\dagger |0\rangle, \quad (1)$$

where  $|0\rangle$  is the even–even core, or

$$\left| [j' \otimes NJ]_{jm} \right\rangle = \sum_{m'M} \langle j'm'JM | jm \rangle a_{j'm'}^\dagger \Gamma_{JM}^\dagger |0\rangle. \quad (2)$$

On this basis we diagonalize, separately for each  $j$ , the Hamiltonian

$$\begin{aligned}
 H &= H_0 + V, \\
 H_0 &= \sum_{jm} \varepsilon_j a_{jm}^\dagger a_{jm} + \sum_{NJM} \hbar\omega_{NJ} \Gamma_{NJM}^\dagger \Gamma_{NJM}, \\
 V &= \sum_{jmj'm'} \sum_{NJM} h(jm; j'm', NJM) a_{jm} \left[ a_{j'}^\dagger \otimes \Gamma_{NJ}^\dagger \right]_{jm}, \quad (3)
 \end{aligned}$$

where  $H_0$  represents the HF states and RPA excitations and  $V$  their mutual coupling. The details of the HF plus RPA calculations can be found in Ref. [14]. The coupling matrix elements  $h$  can be calculated once the structure of the RPA states is known, and are defined in Eq. (A1) of Ref. [5]. The schematic structure of the Hamiltonian matrix for a given  $j$  is shown in Fig. 1.

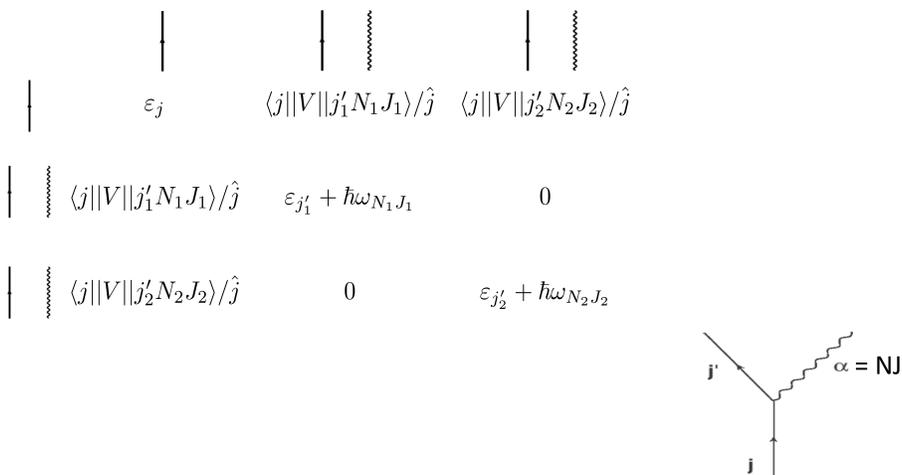


Fig. 1. The schematic structure of the Hamiltonian matrix (3) on a basis made up by one single-particle state of type (1) and by two states of type (2), is displayed in the upper-left corner of the figure. The matrix element coupling the states of the two types is diagrammatically shown in the lower-right corner.

Just using as a resulting physical spectrum the set of eigenvalues and eigenvectors resulting from the diagonalization of  $H$  would overlook the fact that the basis defined by Eqs. (1) and (2) is, in general, non-orthogonal and overcomplete. In particular, there exist non-trivial (*i.e.* not simply 0 or 1) overlaps between the different states (2): these overlaps can be calculated once the structure of the RPA states is known. If we define as  $N$  the overlap matrix in the sub-space of interest in which we solve  $H$ , the eigenvalue problem is solved by employing the technique described in Ref. [15].

Once the eigenvalue problem is solved, we can analyse the spectra but also calculate the electromagnetic transition probabilities between the states. The details of this calculations, as well as many details on this formalism that have been not discussed in this paper, will be reported in a forthcoming publication.

### 3. Results

In what follows, we discuss some results obtained for two nuclei, namely  $^{49}\text{Ca}$  (treated as  $^{48}\text{Ca}$  plus one neutron) and  $^{133}\text{Sb}$  (treated as  $^{132}\text{Sn}$  plus one proton).

The calculations are based on the use of two Skyrme interactions, namely SkX [16] and SLy5 [17]. The reasons for this choice are the following. While the latter is a standard Skyrme force with effective mass  $m^*$  around  $0.7m$ , so that it has been built without special attention to the single-particle shell structure around the Fermi energy, the former has been built by including in the fit protocol the single-particle energies of a few magic nuclei (as far as they are experimentally known), including  $^{48}\text{Ca}$  and  $^{132}\text{Sn}$ . The sensitivity of the final results to either choice will show up and will be briefly addressed.

The HF equations are solved in coordinate space by using a radial mesh that extends up to 15 fm in the case of  $^{48}\text{Ca}$ , and 20 fm in the case of  $^{132}\text{Sn}$ . The mesh size is 0.1 fm. Then, the RPA basis is built by considering all occupied states and unoccupied states that span 8 values of the radial quantum number  $n$  for each value of  $l$  and  $j$ . Unoccupied states in the continuum are solved by using box boundary conditions, and the box size is 15 fm and 20 fm, respectively, for  $^{48}\text{Ca}$  and  $^{132}\text{Sn}$ .

#### 3.1. $^{49}\text{Ca}$

We have selected the lowest unoccupied neutron orbitals of  $^{48}\text{Ca}$ , that is,  $2p_{3/2}$ ,  $2p_{1/2}$ ,  $1f_{5/2}$  and  $1g_{9/2}$ . As for the RPA core excitations, we have limited ourselves to those having angular momentum between  $J = 0$  and 8, either with positive and negative parity, and energy below 5.5 MeV.

The comparison of our theoretical results with the experimental findings is displayed in Table I. All excitation energies are with respect to the  $3/2^-$  ground state of  $^{49}\text{Ca}$  which is set at zero energy, both in experiment and theory. The reader should also note that we have chosen to display only the (few) lowest states of each multipolarity that appear between 0 and 5 MeV, provided an experimentally known state is found and its spin and parity are known without ambiguities.

By looking at the eigenvectors emerging from our calculation (that is, the wave functions of the states), we have checked that the  $3/2^-$  ground state has, as may be expected, mainly a particle character. The same is true

TABLE I

Results for the lowest states of  $^{49}\text{Ca}$ . See the text for the selection of experimental states to be shown. The experimental results are compared with the theoretical outcome in the case of the interaction SkX [16].

	Experiment [MeV]	Theory [MeV]
$1/2^-$	2.02	1.59
$7/2^-$	3.36	3.25
$5/2^-$	3.59	3.33
$9/2^+$	4.01	4.55

for the  $1/2^-$  state. On the other hand, the main component of the  $5/2^-$  state is  $1p_{3/2}$  coupled to the lowest  $2_1^+$  phonon of  $^{48}\text{Ca}$ , and the same can be said of the state  $7/2^-$ . Finally, the  $9/2^+$  state has the largest percentage in its wave function which is associated with the  $1p_{3/2} \otimes 3_1^-$  component, where  $3_1^-$  is the lowest (collective) octupole phonon of  $^{48}\text{Ca}$ .

Therefore, the model is able to reproduce states of different character that appear in the experimental spectrum. The details depend, of course, on the Skyrme interaction chosen. The theoretical spectrum is more stretched than the experimental one, yet this happens in a more pronounced manner for SLy5 than for SkX. The r.m.s. difference between experimental and theoretical energies is 0.429 MeV in the case of SkX. The results obtained with SLy5 are not shown in detail but such r.m.s. deviation increases to 0.661 MeV. The detailed mixing of the wave functions is also different for the two interactions.

### 3.2. $^{133}\text{Sb}$

The results obtained in this case by using the interaction SkX are shown in Table II. The ground state is  $7/2^+$  and its energy has been set at zero. The theoretical calculations have been performed by including in the model space the unoccupied proton orbitals  $1g_{7/2}$ ,  $2d_{5/2}$ ,  $2d_{3/2}$ ,  $1h_{11/2}$ ,  $3s_{1/2}$  of  $^{132}\text{Sn}$ . As for the core excitations obtained by means of the self-consistent RPA, we have considered the states having angular momentum between  $J = 0$  and  $J = 12$ , either with positive and negative parity, and energy below 5.5 MeV. As in the case of  $^{49}\text{Ca}$ , the theoretical spectrum is more stretched than the experimental one. The r.m.s. deviation between the experimental and theoretical energies is 0.869 MeV. As it is evident from the table, the negative parity states  $13/2^-$  and  $15/2^-$  are surprisingly too high with respect to experiment: one reason may lie in the fact that the  $3_1^-$  phonon of the  $^{132}\text{Sn}$  core is too high as well and both states are sensitive to this fact. If we compare theory and experiment for the other states than the  $13/2^-$  and  $15/2^-$ , the r.m.s. deviation decreases to 0.246 MeV.

TABLE II

The same as Table I in the case of  $^{133}\text{Sb}$ .

	Experiment [MeV]	Theory [MeV]
$5/2^+$	0.96	0.37
$3/2^+$	2.44	2.09
$11/2^-$	2.79	2.66
$11/2^+$	4.19	4.11
$13/2^-$	4.30	5.60
$13/2^+$	4.30	4.42
$15/2^-$	4.36	6.82
$15/2^+$	4.47	4.45
$17/2^+$	4.52	4.56
$21/2^+$	4.56	4.75

The  $7/2^+$  ground state, as well as the lowest  $5/2^+$ ,  $3/2^+$  and  $11/2^-$  states, have mainly single-particle character. The  $11/2^+$  state has a quite large percentage ( $\approx 77\%$ ) associated with the component  $1g_{7/2} \otimes 2_1^+$ , but its wave function shows also significant admixture of  $2p-1h$  states like  $\pi 1g_{7/2} \nu h_{11/2}^{-1} f_{7/2}$ . An evolution in the wave function composition can be observed with increasing spin, as the  $13/2^+$  and the  $15/2^+$  states show a quite mixed wave function, while the highest spin states  $17/2^+$  and  $21/2^+$  are markedly dominated by the valence proton coupled to the neutron  $h_{11/2}^{-1} f_{7/2}$  non-collective core excitation.

#### 4. Conclusions

In this work, we have introduced a model for odd nuclei. It is based on the coupling of single-particle states with core excitations, which are extracted from self-consistent RPA calculations but may correspond to either collective or non-collective states. The model does not have any adjustable parameter. A Skyrme force is used in the present case at each step. The problem is formulated in terms of a generalized eigenvalue problem: a norm matrix is introduced that corrects for the fact that states made up with one particle and one core excitation may not form an orthonormal basis.

We have applied this model to  $^{49}\text{Ca}$  and  $^{133}\text{Sb}$ . We have compared the energy of the states at low energy with the experimental findings. Our model can account well for the ordering and the absolute energy of the low-lying states, with discrepancies of the order of few hundreds of keV on the scale of 0–5 MeV. This refers, in particular, to results obtained with the Skyrme set SkX.

In general, the theoretical results provide a spectrum which is more stretched than the experimental one. While extensions of the model space are certainly to be envisaged, it is likely that these extensions will hit with some basic limitation of current density functionals.

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