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Spectra of $N = Z$ nuclei in a formalism of quartets

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Summary. — We describe the spectra of even-even $N = Z$ nuclei in a formalism of quartets. Quartets are α-like four-body structures characterized by an isospin $T = 0$. The structure of the quartets is fixed by resorting to the use of proper intrinsic states. Various types of intrinsic states are introduced which generate different sets of quartets for a given nucleus. Energy spectra are constructed via configuration-interaction calculations in the spaces built with these quartets. Some applications of this formalism are discussed for nuclei in the *sd* and *pf* shells. A good description of the low-lying spectra of these nuclei is achieved.

1. – Introduction

The study of $N = Z$ nuclei, *i.e.*, nuclei with an equal number of neutrons and protons, is an issue of great interest in contemporary nuclear structure physics. What makes $N = Z$ nuclei particularly interesting is the appearance of new types of correlations induced by the proton-neutron (pn) pairing interaction. This interaction is expected to play a relevant role in these nuclei owing to the fact that protons and neutrons share the same orbitals [1].

Understanding the type of correlations induced by the pn pairing force in the wave function of $N = Z$ nuclei has proved to be a not trivial task. Following the seminal work by Belyaev *et al.* [2], in most studies the ground state of a pn pairing Hamiltonian has been described in the Hartree-Fock-Bogoliubov (HFB) approximation. However, this approximation which does not conserve the particle number, the spin and the isospin does not provide a sufficiently accurate description of the ground state of a pn pairing Hamiltonian.

An unambiguous indication of the type of correlations that are generated by the pn pairing in $N = Z$ nuclei can be provided by the study of exactly solvable Hamiltonians. In a recent work [3], we have derived the exact solutions of the isovector pairing and evidenced a peculiar aspect of these solutions which had escaped previous investigations [4, 5] We have shown on an analytic basis that what characterizes the eigenstates of an isovector pairing Hamiltonian in $N = Z$ systems is the occurrence of correlated α-like structures ("quartets").

One needs to remark that, well before the exact treatment just discussed the essential role played by four-body correlations in $N = Z$ systems subject to an isovector pairing force, but limited to the special case of degenerate single-particle levels (the so-called SO(5) model), had already been emphasized in ref. [6]. More generally, quartets have definitely a long history in nuclear structure physics [7-10], but their complexity has undoubtedly represented a hindrance to the development of quartet models.

In a recent past, $T = 0$ quartets have been introduced to build an approximation scheme for the ground state of the isovector pairing Hamiltonian [11]. This approach, known as Quartet Condensation Model (QCM), assumes this ground state to be a condensate of $T = 0$ quartets, each quartet consisting of two collective isovector pairs coupled to $T = 0$. The QCM approach has turned out to be very accurate both in the case of deformed and spherical mean fields. In the latter case the quartets are also characterized by an angular momentum $J = 0$ [12]. The QCM formalism has been later on extended to a more general form of *pn* pairing which also included an isoscalar component [13-15] as well as to quite general Hamiltonians [16].

The use of quartets has not been limited to the analysis of the ground state only. A more elaborate quartet formalism, involving quartets other than the single $J = 0, T = 0$ one of the QCM approach, has been developed to describe the spectra of $N = Z$ systems [17-19]. In this approach, simply referred to as Quartet Model (QM), spectra (of both positive and negative parity states) have been generated by carrying out configuration-interaction calculations in a space of states formulated as products of collective $T = 0$ quartets of various J.

A crucial aspect of the QM approach consists in the definition of the quartets to involve in the calculations. In the early applications of this quartet formalism we have adopted the criterion of assuming as $T = 0$ quartets those defining the low-lying eigenstates of the nearest $T = 0$ one-quartet systems [17-19]. While having the advantage of being straightforward, this "static" definition of the quartets is clearly not the most appropriate one since it fully neglects the effect of the Pauli principle on the amplitudes of the quartets when two or more of these quartets have to coexist in the same nucleus. Finding the most appropriate quartets to be employed in a QM calculation is a matter of primary importance. The approach which will be illustrated in this contribution resorts to the use of special quartet-based intrinsic states [20]. Quartets will result from the minimization of these intrinsic states for each $N = Z$ nucleus. In this sense, this approach provides a "dynamical" definition of the quartets. Energy spectra will be then constructed via configuration-interaction calculations in the spaces built with these quartets.

In sect. 2, we will describe our formalism. In sect. 3 we will show some applications and, finally, in sect. 3, we will summarize the results and draw the conclusions.

2. – Formalism

We work in a spherically symmetric mean field and, using the standard notation, we introduce the label $i \equiv \{n_i, l_i, j_i\}$ to identify the orbital quantum numbers. We define the $T = 0$ quartet creation operator as

$$q^+_{JM} = \sum_{i_1 j_1 J_1} \sum_{i_2 j_2 J_2} \sum_{T'} q_{i_1 j_1 J_1, i_2 j_2 J_2, T'} [[a^+_{i_1} a^+_{j_1}]^{J_1 T'} [a^+_{i_2} a^+_{j_2}]^{J_2 T'}]^{JT=0}_M, \tag{1}$$

where $a^+_{i\tau}$ creates either a proton or a neutron (depending on the isospin projection τ) on the orbital i and M stands for the projection of J. No restrictions on the intermediate

couplings J_1T' and J_2T' are introduced and the amplitudes $q_{i_1j_1J_1,i_2j_2J_2,T'}$ are supposed to guarantee the normalization of the operator. We shall focus on systems of N_π protons and N_ν neutrons such that $N_\pi = N_\nu$ and $N_\pi + N_\nu = 4n$ $(n = 2, 3)$ and assume axially symmetry of these systems.

In the representation spanned by the quartets (1) we construct a set of intrinsic states. As a starting point, we introduce the "ground" intrinsic state

$$|\Theta_g\rangle = \mathcal{N}_g(Q_g^+)^n|0\rangle, \tag{2}$$

where by n is denoted the number of quartets which can be formed with the valence nucleons outside the closed core, denoted by $|0\rangle$. As can be noticed, $|\Theta_g\rangle$ is a condensate of the intrinsic quartet Q_g^+ defined by

$$Q_g^+ = \sum_J \alpha_J^{(g)}(q_g^+)_{J0}, \tag{3}$$

where

$$(q_g^+)_{J0} = \sum_{i_1j_1J_1}\sum_{i_2j_2J_2}\sum_{T'} q^{(g)}_{i_1j_1J_1,i_2j_2J_2,T'}[[a_{i_1}^+a_{j_1}^+]^{J_1T'}[a_{i_2}^+a_{j_2}^+]^{J_2T'}]_0^{JT=0} \tag{4}$$

In order to fix Q_g^+, we minimize the energy of the state $|\Theta_g\rangle$ with respect to the coefficients $q^{(g)}_{i_1j_1J_1,i_2j_2J_2,T'}$ and $\alpha_{g,J}$.

In addition to the ground intrinsic state, we introduce a family of "excited" intrinsic states which are generated by promoting one of the quartets Q_g^+ of $|\Theta_g\rangle$ to an excited $T = 0$ configuration. These states have the general form

$$|\Theta_k\rangle = \mathcal{N}_kQ_k^\dagger(Q_g^\dagger)^{(n-1)}|0\rangle, \tag{5}$$

with

$$Q_k^\dagger = \sum_J \alpha_J^{(k)}(q_k^\dagger)_{Jk}, \tag{6}$$

$$(q_k^+)_{Jk} = \sum_{i_1j_1J_1}\sum_{i_2j_2J_2}\sum_{T'} q^{(k)}_{i_1j_1J_1,i_2j_2J_2,T'}[[a_{i_1}^+a_{j_1}^+]^{J_1T'}[a_{i_2}^+a_{j_2}^+]^{J_2T'}]_k^{JT=0} \tag{7}$$

Assuming that the quartet Q_g^+ has already been fixed, we construct the new quartet Q_k^+ by minimizing the energy of $|\Theta_k\rangle$ with respect to the coefficients $q^{(k)}_{i_1j_1J_1,i_2j_2J_2,T'}$ and $\alpha_J^{(k)}$ (under the constraint of orthogonality when various states with the same k are involved). The states (5) will be identified with the value of the quantum number k and, in particular, we shall refer to β and γ intrinsic states for $k = 0$ and 2, respectively. It can be seen that these states, as well as the state (2), have an undefined angular momentum.

Once the quartets have been fixed, we generate the energy spectra by carrying out configuration-interaction calculations. To this purpose we define the set of states (we work in the m-scheme)

$$|\Psi^{(n)}_M, \{N_{JM}\}\rangle = \prod_{J\in(0,J_{max});M\in(-J,J)} (q_{JM}^+)^{N_{JM}}|0\rangle \tag{8}$$

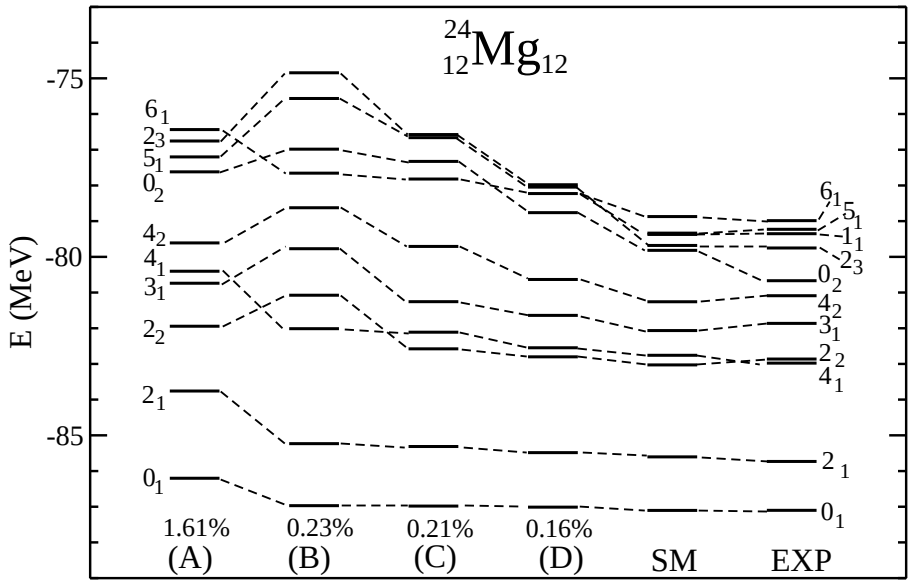

Fig. 1. – Spectra of ^{24}Mg obtained by performing configuration-interaction calculations in spaces built with various sets of $T = 0$ quartets (see text): (A), $J = 0, 2, 4$ static quartets from ^{20}Ne; (B), $J = 0, 2, 4$ dynamical quartets from the ground intrinsic state (2); (C), the same set as in (B) plus $J = 2, 3, 4$ quartets from the γ intrinsic state ((5) for $k = 2$); (D), the same sets as in (C) plus $J = 0, 2, 4$ quartets from the β intrinsic state ((5) for $k = 0$). SM, shell model results; EXP, experimental spectrum. The numbers above the symbols (A)-(D) are the relative errors in the ground state correlation energy with respect to the shell model value.

with the conditions

$$\sum_{JM} N_{JM} = n, \qquad \sum_{JM} M N_{JM} = \overline{M}. \tag{9}$$

We then orthonormalize the states (8) and diagonalize the Hamiltonian in this new basis for the various $\overline{M}$.

3. – Applications

Calculations have been carried out in the *sd* and *pf* shells by adopting the USDB [21] and KB3G [22] interactions, respectively. The vacuum state $|0\rangle$ in the equations of sect. 2 stands for the nucleus ^{16}O for *sd* shell nuclei and for ^{40}Ca for *pf* shell nuclei.

In figs. 1, 2 and 3 we plot the spectra of ^{24}Mg, ^{28}Si and ^{48}Cr, rispectively, generated with various sets of quartets. The spectrum (A) of each figure has been obtained by adopting static quartets, namely the quartets describing the lowest J=0,2,4 states of ^{20}Ne for the *sd* shell nuclei and the lowest J=0,2,4,6 of ^{44}Ti for ^{48}Cr. In spite of the quite good results for the ground state correlation energy (defined as the difference between the ground state energies with and in absence of interaction) in all cases the spectra show significant differences with respect to the shell model results. For the spectra (B) of the same figures, instead, we have adopted the dynamical quartets with the same J's as the previous ones, obtained from the minimization of the ground intrinsic states. In all three

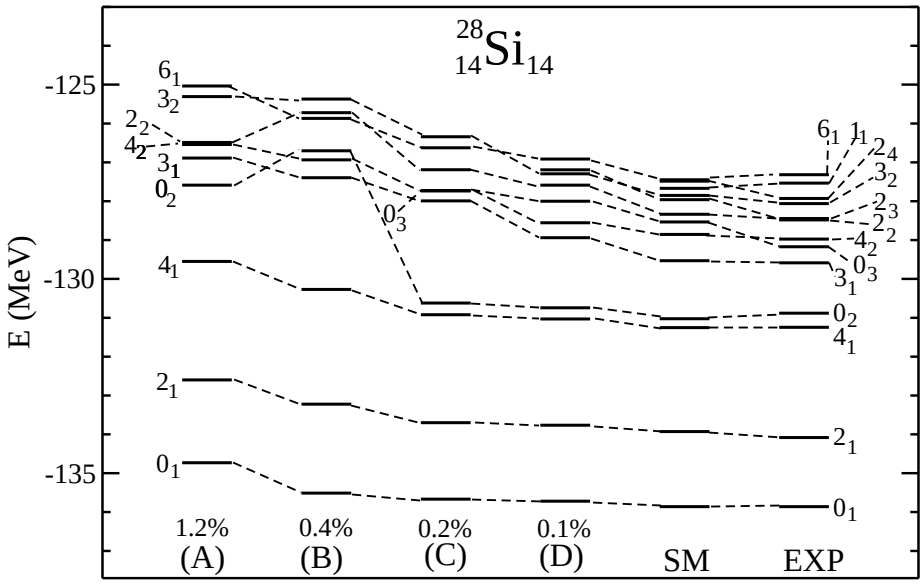

Fig. 2. – Spectra of ^{28}Si obtained by performing configuration-interaction calculations in spaces built with various sets of $T = 0$ quartets (see text): (A), $J = 0, 2, 4$ static quartets from ^{20}Ne; (B), $J = 0, 2, 4$ dynamical quartets from the ground intrinsic state (2); (C), the same set as in (B) plus $J = 0, 2, 4$ quartets from the β intrinsic state ((5) for $k = 0$); (D), the same sets as in (C) plus $J = 3, 4$ quartets from the $k = 3$ intrinsic state (5). SM, shell model results; EXP, experimental spectrum. The numbers above the symbols (A)-(D) are the relative errors in the ground state correlation energy with respect to the shell model value.

nuclei one observes a lowering of the yrast states $J = 0, 2, 4, 6$ forming the ground state bands while most of the remaining states are pushed up in energy. The new ground state bands are all closer in energy to the shell model ones and a considerable improvement is observed also in the accuracy of the ground state correlation energies. Thus adopting the quartets $(q_g^+)_{J0}$ associated with $|\Theta_g\rangle$ has had a positive effect only on the ground state bands of the nuclei under study.

In the remaining spectra of the above figures we show the effect of introducing further quartets generated from the excited intrinsic states (5) in the configuration interaction calculations. In the following we shall examine this effect case by case. In ^{24}Mg, fig. 1(B), one notices that a band formed by the $J_k = 2_2, 3_1, 4_2, 5_1$ states has been shifted higher in energy when passing from static to dynamical quartets. By making use of the definition of the γ intrinsic state ((5) for $k = 2$), we construct new quartets with $J = 2, 3, 4$ and perform a configuration-interaction calculation that includes these new quartets in addition to those already used for the calculation of fig. 1(B). The new result is shown in fig. 1(C). We observe a clear lowering of the energies of the states $J_k = 2_2, 3_1, 4_2, 5_1$ while the states of the ground state band have remained basically unmodified with respect to those of column (B). The inclusion of the quartets derived with the help of the γ intrinsic state has therefore essentially affected only those states which can be associated to a γ band of ^{24}Mg (and, in addition, the state 2_3). As a final step, we have explored the effect on this spectrum of the inclusion of a set of quartets with $J = 0, 2, 4$ built from the β intrinsic state ((5) for $k = 0$). The basic effect which

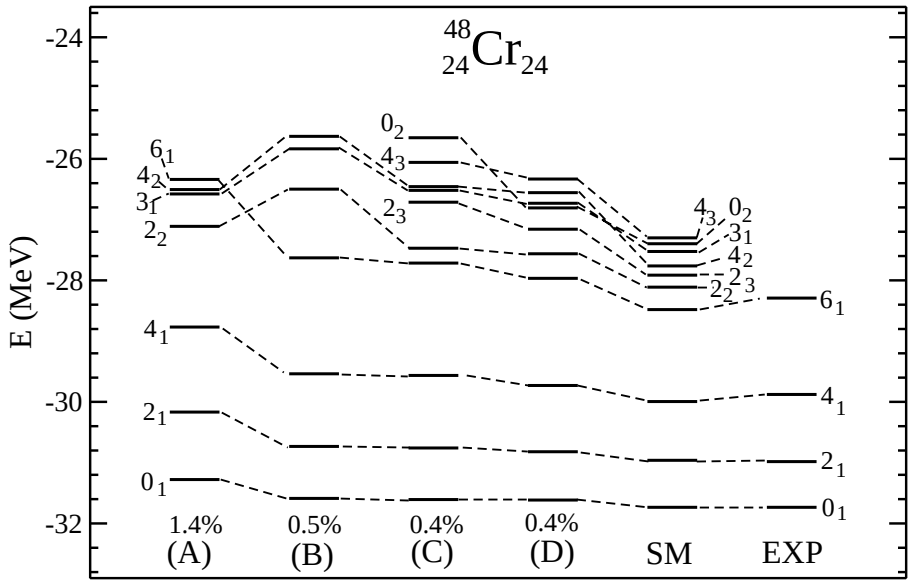

Fig. 3. – Spectra of ^{48}Cr obtained by performing configuration-interaction calculations in spaces built with various sets of $T = 0$ quartets (see text): (A), $J = 0, 2, 4, 6$ static quartets from ^{44}Ti; (B), $J = 0, 2, 4, 6$ dynamical quartets from the ground intrinsic state (2); (C), the same set as in (B) plus $J = 2, 3, 4$ quartets from the γ intrinsic state ((5) for $k = 2$); (D), the same sets as in (C) plus $J = 0, 2, 4$ quartets from the β intrinsic state ((5) for $k = 0$). SM, shell model results; EXP, experimental spectrum. The numbers above the symbols (A)-(D) are the relative errors in the ground state correlation energy with respect to the shell model value.

can be observed in fig. 1(D) is a lowering the states $J = 0_2, 2_3$ which can be associated to a β band of ^{24}Mg. As a result of the new diagonalization, also the 5_1 state is lowered in energy. The final spectrum shows a good agreement with the shell model one.

For what concerns ^{28}Si, what is most striking in the spectrum of fig. 2(B) is the absence of a state 0_2 close to the state 4_1 as observed in both the shell model and the experimental spectrum. By interpreting this state 0_2 as the head of a β band, as a next step, we enlarge the model space by also including the quartets with $J = 0, 2, 4$ associated with the β intrinsic state. The result of the new configuration calculation can be seen in fig.2(C). The inclusion of the new quartets mostly affects the yrare $J = 0, 2$ states by giving rise, in particular, to a surprising lowering of the 0_2 state which positions itself immediately above the 4_1 state, where it is expected to be. In spite of the fact that a reasonably good agreement with the shell model spectrum has already been achieved, we perform an additional calculation which also includes the quartets $(q_3^\dagger)_{J3}$, with $J = 3, 4$, associated with the $k = 3$ intrinsic state (5). As it can be seen in fig. 2(D), the new calculation essentially lowers the energy of the 3_1 and 4_2 states and, in addition, that of the 3_2 state. This new calculation further improves the quality of the QM spectrum which compares well with the shell model one.

The last case under investigation, ^{48}Cr, shares some analogies with the corresponding one of ^{24}Mg. Indeed one observes in fig. 3(B) that, also in this case, the states $2_2, 3_1, 4_2$ have been shifted higher in energy when replacing the static quartets with the corresponding dynamical ones associated with the ground intrinsic state. These states

reminding those of a γ band, we proceed as for ^{24}Mg by introducing the quartets associated with the γ intrinsic state, with $J = 2, 3, 4$. The new calculation, fig. 3(C), leaves unaffected the states of the ground rotational band (as for ^{24}Mg) while it lowers significantly the states $2_2, 3_1, 4_2$. The new calculation also leads to the appearance of new states $(2_3, 4_3, 0_2)$ in the highest part of the spectrum. These states have a correspondence with the shell model ones but with a 0_2 still too high in energy. By interpreting this state as a possible head of a β band and wishing to lower its energy, we perform a final calculation which includes also the quartets with $J = 0, 2, 4$ associated with the β intrinsic state. This calculation leads to a significant lowering of the 0_2 state (fig. 3(D)) which improves the agreement between exact and approximate spectra.

As a final comment, we like to remark that the high quality of the ground states reached in these calculations, with errors in the correlation energies confined within the 0.4% (figs. 1, 2, 3) depends almost entirely on the low-J quartets of the ground intrinsic state. Indeed, by performing configuration-interaction calculations which include only the quartets $(q_g^+)_J$ with $J = 0, 2$ these errors remain confined within 0.7% for ^{24}Mg and ^{28}Si while, for ^{48}Cr, one finds 1.6%. In the latter case, however, it is sufficient to add the J=4 quartet to reduce this error to 0.6%. As already evident from the comparisons between the columns (A) and (B) of the same figures, these errors increase considerably if static quartets are used instead of the dynamical ones.

4. – Summary and conclusions

In this contribution we have provided a description of deformed $N = Z$ nuclei in a formalism of α-like quartets. Quartets have been constructed variationally by resorting to the use of proper intrinsic states. Spectra have been obtained by carrying out configuration-interaction calculations in spaces built with these quartets. For each nucleus more sets of quartets have been used in correspondence with the various types of intrinsic states introduced. The intriguing aspect of these calculations has been the observation of band-like structures associated with the various sets of quartets. The procedure has been applied to ^{24}Mg, ^{28}Si and ^{48}Cr nuclei and it has provided a good description of the low-lying spectra in all three cases. A merit of this description is that of relying on only a few degrees of freedom. For what concerns the ground states, in particular, we have shown that already the $T = 0$ quartets with $J = 0$ and $J = 2$ can guarantee an accurate approximation of these states. As a general conclusion, the results achieved in this work promote the new method proposed for the definition of the quartets as well as the use of the latter as basic structures for an effective description of the ground and excited states of deformed $N = Z$ nuclei.

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