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DESCRIPTION OF $A = 22$ NUCLEI IN THE COLLECTIVE PAIR APPROXIMATION

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The structure of $A = 22$ nuclei has been studied in the framework of the collective pair approximation. The collective pairs determined by diagonalizing the Hamiltonian in the space of two nucleons with respect to the closed core of ^{16}O have been considered as building blocks to expand the truncated shell-model space in terms of three pairs. It is shown that the low-lying, shell-model spectrum can be described by considering only a selected subset of all possible $T = 0$, 1 pairs.

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1. Introduction

Fifty years after the pioneering work of Haxel, Jensen and Suess [1] and Goeppert–Mayer [2], the Shell Model (SM) still plays a crucial role in the study of nuclear properties. While well suited to describe nuclei with a small number of nucleons outside the closed shells, however, it is well known that its application to more complex systems is problematic. On the one hand, the huge dimensionality of the SM space makes the calculations very difficult. On the other hand, even when, thanks to the new computational techniques, this description becomes possible, it is all but "transparent". These aspects of the SM have favoured the development of less refined but easier-to-apply SM related methods for describing those nuclear systems which are outside the natural range of applicability of the model. We quote, for instance, the Broken Pair Approximation [3, 4], the Generalized Seniority Scheme [5, 6] and the Chain-Calculation Method [7].

In two previous publications [8, 9], a description of $1s0d$ and $1p0f$-shell nuclei has been provided in terms of the Collective Pair Approximation (CPA) [10, 11]. The essence of such an approximation consists in singling out a set of collective pairs in terms of which a subspace of the full SM space is constructed, and then in diagonalizing the Hamiltonian of the system in such a subspace. The structure of the collective pairs is fixed by diagonalizing the Hamiltonian in the space of two active nucleons outside the closed shell core. The calculations of Refs. [8, 9] have referred to systems having up to five particles outside the closed shells. This limited number of particles has also allowed to perform full SM calculations. The comparison between SM and CPA calculations has provided an excellent testing ground for this approximation.

A crucial point within the CPA approach is represented by the choice of the collective pairs. In the just mentioned calculations, we have followed the simplest possible procedure, namely we have diagonalized the SM Hamiltonian in the space of two particles outside the closed shells and we have selected the pairs whose energy was below a given threshold. These pairs have then been used to describe systems with three, four and five active particles.

From the comparison with the exact results, *i.e.* the SM results, we have observed that it was possible to reproduce to a good extent the low-lying levels of A=19–21 and A=43–45 [8, 9] nuclei remaining in spaces considerably reduced with respect to the SM ones.

In the present paper we extend the previous calculations to $A = 22$ even-even and odd–odd $1s0d$-shell nuclei. Also in this case SM calculations are possible and they will help us to judge the quality of the approximate results.

The paper is organised as follows. In Section 2, we will describe the basic formalism of CPA. In Section 3, we will present the method adopted to fix the structure of the pairs. Finally, in Section 4, we will discuss the results of our calculations and give some conclusions.

2. Formalism

In this section we illustrate the CPA formalism to describe spectra of nuclei with $2n (n = 3)$ nucleons outside the closed shells.

The operator $\hat{A}^{\dagger}_{\nu\Gamma\Gamma'}$ creating a collective pair of multipolarity $\Gamma(=JT)$ and projection $\Gamma'(=J'T')$ is defined as

$$\hat{A}^{\dagger}_{\nu\Gamma\Gamma'} = \sum_{\lambda_1\lambda_2} C^{\nu}_{\Gamma}(\lambda_1\lambda_2)\hat{Z}^{\dagger}_{\Gamma\Gamma'}(\lambda_1\lambda_2)\,, \tag{1}$$

where

$$\hat{Z}^{\dagger}_{\Gamma\Gamma'}(\lambda_1\lambda_2) = (1+\delta_{\lambda_1\lambda_2})^{-1/2}\left[a^{\dagger}_{\lambda_1}\times a^{\dagger}_{\lambda_2}\right]_{\Gamma\Gamma'} \tag{2}$$

creates a two-nucleon state with nucleons occupying orbitals λ_1 and λ_2 and coupled to total spin-isospin angular momenta $\Gamma(J,T)$ and their projection $\Gamma'(=J',T')$. The index ν denotes different collective pairs with the same quantum numbers $\Gamma\Gamma'$. The coefficients $C^{\nu}_{\Gamma}(\lambda_1\lambda_2)$ determine the structure of the collective pairs. Detailed procedures to find these coefficients are described in Section 3. The collective pairs defined by Eq. (1) are used as building blocks to construct a truncated SM basis which can be used to expand the wavefunctions of $A = 22$ nuclei. The basis states can be expressed as

$$|i\rangle \equiv |\nu_1\Gamma_1\nu_2\Gamma_2\{\Gamma_{12}\}\nu_3\Gamma_3;\Gamma\Gamma'\rangle = \left[\left[\hat{A}^{\dagger}_{\nu_1\Gamma_1}\times\hat{A}^{\dagger}_{\nu_2\Gamma_2}\right]_{\Gamma_{12}}\times\hat{A}^{\dagger}_{\nu_3\Gamma_3}\right]_{\Gamma\Gamma'}|0\rangle\,, \tag{3}$$

where square brackets indicate the order of spin-isospin angular momenta couplings, the intermediate spin-isospin angular momenta are specified by Γ_{12}, while the total spin-isospin angular momenta and their projections are indicated by Γ and Γ'. In the case of two identical pairs, *i.e.* $\nu_1 = \nu_2$ and $\Gamma_1 = \Gamma_2$, the spin and isospin angular momenta $\Gamma_{12} = (J_{12}T_{12})$ have to fulfil the condition $(-)^{\Gamma_1+\Gamma_2-\Gamma_{12}} = 1$.

Taking into account the completeness of the basis states $|2n\beta\Lambda\Lambda'\rangle$ spanning the full SM space of nuclei with nucleons in active orbits, the identity operator can be defined

$$\hat{I}(2n) = \sum_{\beta\Lambda\Lambda'}|2n\beta\Lambda\Lambda'\rangle\langle 2n\beta\Lambda\Lambda'|\,, \tag{4}$$

where the quantum numbers $\Lambda\Lambda'$ define the total spin-isospin angular momenta and their projections and β give a set of additional quantum numbers to distinguish states with the same $\Lambda\Lambda'$. By inserting the $\hat{I}(2n=4)$ and $\hat{I}(2n=6)$ into Eq. (3), employing the Wigner–Eckart theorem and utilizing the orthonormality conditions of the Clebsch–Gordan coefficients, Eq. (3) can be expressed as

$$|i\rangle \equiv |\nu_1\Gamma_1\nu_2\Gamma_2\{\Gamma_{12}\}\nu_3\Gamma_3;\Gamma\Gamma'\rangle = \sum_{\beta} C_{i\beta}|2n=6\beta\Gamma\Gamma'\rangle\,, \tag{5}$$

where

$$C_{i\beta} = \sum_{\lambda_1\lambda_2\lambda_3\lambda_4\lambda_5\lambda_6\beta_1\Lambda} C^{\nu_1}_{\Gamma_1}(\lambda_1\lambda_2)C^{\nu_2}_{\Gamma_2}(\lambda_3\lambda_4)C^{\nu_3}_{\Gamma_3}(\lambda_5\lambda_6)\left(\frac{2\Gamma_{12}+1}{2\Gamma+1}\right)^{1/2}$$
$$\times \begin{Bmatrix} \Gamma_1\Gamma_2\Gamma_{12} \\ \Gamma_3\Gamma\Lambda \end{Bmatrix} \langle 6\beta\Gamma||\hat{Z}^\dagger_{\Gamma_1}(\lambda_1\lambda_2)||4\beta_1\Lambda\rangle\langle 4\beta_1\Lambda||\hat{Z}^\dagger_{\Gamma_2}(\lambda_3\lambda_4)||2\Gamma_3(\lambda_5\lambda_6)\rangle\,. \tag{6}$$

In Eq. (6) the symbol $\{\ \}$ stands for the product of the spin and isospin $6j$ coefficients and the coefficients $\langle\ldots||\hat{Z}^\dagger_\Gamma||\ldots\rangle$ are the reduced matrix elements of the two-nucleon transfer operator $\hat{Z}^\dagger_\Gamma$ defined by Eq. (2).

States of Eq. (5) are neither normalised nor linearly independent. By constructing the overlap matrix $\langle i|j\rangle$ and diagonalizing it, we find a new set of orthonormal states

$$|\Phi_{\gamma\Gamma\Gamma'}\rangle = (N_\gamma)^{-1/2}\sum_{i=1}^{N} f_{i\gamma}|i\rangle\,, \qquad \gamma = 1,2,\ldots,\bar{N}\,. \tag{7}$$

The number $\bar{N}$ of states (7) whose norm $N_\gamma > 0$, in general, is less than the number N of states $|i\rangle$. Due to Eq. (5), these states can be expanded in terms of the complete SM basis states $|2n = 6\beta\Gamma\Gamma'\rangle$ as follows

$$|\Phi_{\gamma\Gamma\Gamma'}\rangle = (N_\gamma)^{-1/2}\sum_{i,\beta} f_{i\gamma}C_{i\beta}|2n = 6\beta\Gamma\Gamma'\rangle\,. \tag{8}$$

Thus, the matrix representation of the SM Hamiltonian in the CPA space spanned by the states (8) can be written as

$$\begin{aligned}\langle\Phi_{\gamma\Gamma}||\hat{H}||\Phi_{\gamma'\Gamma'}\rangle &= (N_\gamma N_{\gamma'})^{-1/2}\sum_{ii'\beta\beta'} f_{i\gamma}C_{i\beta}\langle 2n = 6\beta\Gamma||\hat{H}||2n \\ &= 6\beta'\Gamma'\rangle C_{i'\beta'}f_{i'\gamma'}\,.\end{aligned} \tag{9}$$

Looking at Eqs (6) and (9) one sees that in order to solve the eigenvalue problem of the Hamiltonian in the CPA space spanned by states (8) the matrix elements of the two-nucleon transfer operator (Eqs (2) and (6)) and matrix elements of the Hamiltonian expressed in the complete SM basis have to be known. Both these matrix elements can be calculated with the aid of standard SM programs [12].

3. Structure of collective pairs

The notation which we will adopt in this paper is the same of previous works [8–9]. Therefore, s, d, g pairs will stand for $T = 1$, $J = 0, 2, 4$ pairs while Θ_1, Θ_3, Θ_5 for $T = 0$, $J = 1, 3, 5$ pairs, respectively. The structure of the collective pairs has been fixed by simply diagonalizing the Hamiltonian of the system in the space of two nucleons moving in the orbitals $0d_{5/2}$, $1s_{1/2}$ and $0d_{3/2}$ outside the closed $0s0p$ shells, *i.e.* the space of states

$$\{\hat{Z}^{\dagger}_{\Gamma\Gamma'}(\lambda_1\lambda_2)|0\rangle\} \tag{10}$$

and using the Wildenthal's interaction [13]. The $T = 0$ and 1 spectra which result from this diagonalization are shown in Table I. As in Refs [8–9], we have selected the lowest five $T = 1$ pairs, *i.e.* the s, d, g, s' and d' pairs, and the lowest three $T = 0$ pairs, *i.e.* the Θ_1, Θ_3, and Θ_5 pairs. Such a choice has been guided by the presence of small gaps in the energy spectra which separate these pairs from the remaining ones (see Table I).

TABLE I

The energies of the $T = 0$ and $T = 1$ pairs. For details see text.

$T = 0$			$T = 1$		
pair	J	E(MeV)	pair	J	E(MeV)
Θ_1	1	-13.583	s	0	-12.171
Θ_3	3	-12.212	d	2	-9.991
Θ_5	5	-12.121	g	4	-8.389
Θ_2	2	-9.277	s'	0	-7.851
Θ'_3	3	-9.076	d'	2	-7.732
Θ'_1	1	-8.671	f	3	-6.445
Θ''_1	1	-6.872	d''	4	-3.421
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4. Results and discussion

The calculations we are going to discuss in this section refer to $A = 22$, $T = 0$–2 systems. Their results are displayed in Figs 1–3 where in the columns denoted by (SM) and (CPA) we report the SM levels and the results obtained within CPA, respectively. We compre our results with the SM ones, whose quality with respect to the experimental data has been widely discussed in several papers (see for instance Ref. [13]). For each level we show the angular momentum and, in parenthesis, the overlap between corresponding CPA and SM states. In Table II, we also show the dimensionalities of

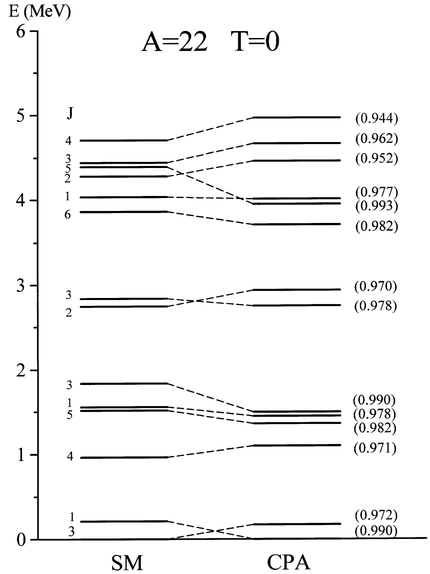

Fig. 1. Comparison between the shell model (SM) and the collective pair approximation (CPA) spectra of the $T = 0$ states of $A = 22$ nuclei. The CPA spectra are calculated in terms of the set of pairs ss' dd' $g\Theta_1$ $\Theta_3\Theta_5$. For details see text.

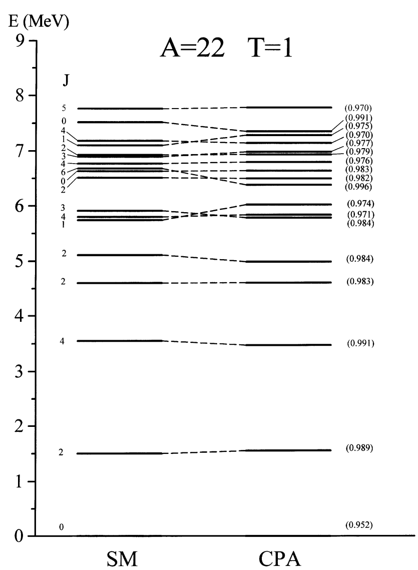

Fig. 2. The same as in Fig. 1 but for the $T = 1$ states of $A = 22$ nuclei.

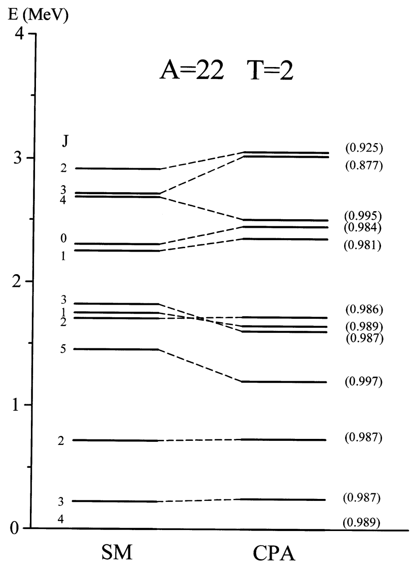

Fig. 3. The same as in Fig. 1 but for the $T = 2$ states of $A = 22$ nuclei.

the SM and CPA spaces. As we see, in the case $T = 3$ the CPA dimensionalities coincide in most of the cases with the SM ones. Therefore, the two calculations give almost identical results and we do not present them. The overall agreement is reasonably good for all T values and particularly good for $T = 1$. In this case all the overlaps of the 18 states lying below 8 MeV excitation energy are larger than 0.95. One can observe a few inversions in the order of the levels with respect to the SM spectrum. We stress, however, that the difference in energy is never larger than $\sim$ 200 KeV. For $T = 0$ and $T = 2$, the quality of the overlaps remains basically the same while the discrepancy in the energies is a bit larger in the average, the maximum being, however, only $\sim$ 250 KeV. As shown in Table II the CPA dimensionalities for the $T = 0$–2 systems are considerably reduced with respect to the SM ones.

These calculations confirm that CPA can be considered as an effective tool for the study of the low-lying spectra of nuclei with several nucleons outside closed shells and that a further extension of the CPA method to nuclei with more than three collective pairs is feasible. Adequate candidates for such studies are the medium weight nuclei with active nucleons in the $1p0f$ shell above the closed $A = 40$ core as well as heavier nuclei. Although for these nuclei the large-scale SM calculations are already feasible [14–15], it is undoubtedly not very useful to look at several hundred thousands if not several million expansion coefficients of an eigenstate [16–17]. Therefore

TABLE II

Comparison between the shell model (SM) and collective pair approximation (CPA) dimension for the $T = 1$–3 states of $A = 22$ nuclei. In the columns we report: the spin (J) of the state, the shell model dimension (SM) and the collective pair approximation dimensions (CPA) for the set of pairs ss' dd' $g\Theta_1$ $\Theta_3\Theta_5$.

	$T=0$		$T=1$		$T=2$		$T=3$	
J	SM	CPA	SM	CPA	SM	CPA	SM	CPA
0	71	9	148	76	54	26	14	14
1	243	88	351	107	164	85	19	10
2	307	84	525	221	219	118	33	33
3	366	138	537	203	232	137	29	25
4	311	106	502	241	195	129	26	26
5	259	117	369	178	144	116	12	12
6	169	77	255	163	82	80	8	8
7	107	68	135	95	41	41	1	1
8	47	31	67	66	14	14		
9	24	24	21	21	3	3		
10	5	5	6	6				
11	1	1						

for an instructive understanding of the structure of the individual states and the relation between them, irrespective of whether the large-scale SM calculations are feasible or not, realistic truncations of the SM space have to be found. The calculations presented in this paper show that the CPA can give the answer to the question on how to truncate the huge SM space to a manageable subspace without loosing the fundamental philosophy of the SM.

Work on the extension of the CPA to nuclei with a larger number of collective pairs is in progress.

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