APPLICATION OF SHELL MODEL WITH THE MODIFIED SURFACE DELTA INTERACTION TO ^{42}Ca AND ^{42}Sc NUCLEI

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The shell model with MSDI residual interaction is used to investigate properties of levels in the ^{42}Ca and ^{42}Sc nuclei. The ^{40}Ca core with two active outer nucleons is assumed. The interaction between two outer nucleons is given. The numerical values of 196 two-particle antisymmetrized matrix elements were calculated. Two different ways were used in the construction of the interaction term: a) The parametrs A_0 and A_1 were considered to be state independent, thus being constant in the configuration space, b) The parameters A_0 and A_1 were allowed to vary in the dependence of the combination of j values. In order to simulate this dependence three values for A_0 and A_1 were fitted. The reasons of this assumption are discussed. In the calculations performed in these two versions the parameters A_0 and A_1 were adjusted to produce the best agreement with the experimental level schemes. The energy matrices were diagonalized and the calculated level schemes for both ^{42}Ca and ^{42}Sc nuclei are presented. In the both nuclei the density of the calculated levels is significantly less than of the observed levels. This fact leads to the conclusion that some core excitation models play an important role in the formation of low-lying states in the ^{42}Ca and ^{42}Sc nuclei.

1. Introduction

Many observed properties of nuclei can be successfully described in the framework of the classical shell model. This model uses two principal assumptions:

1. There exists an innert core, made of closed shells, which acts with central forces on valence nucleons, and

2. there exists a residual interaction caused by two-body forces acting between the valence nucleons.

This latter interaction, in contrast to the interaction between electrons in the atom, is not weak and thus cannot be treated as perturbation. Because neither of these forces is well known, it is necessary to make simplified assumption concerning them both.

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The simplest and somewhat idealized form of residual interaction is the surface delta interaction (SDI). This form was proposed in 1966 by Moszkowski and co-workers [1] and developed by Glaudemans [2–4] who introduced the isospin dependence in the matrix elements of the two-body interaction. This method, called the modified surface delta interaction (MSDI), has proved in several studied [5–14] to be successful in reproducing many nuclear observables.

In the work presented in this paper the MSDI method was applied to the investigation of states of the ^{42}Ca and ^{42}Sc nuclei. According to the simple shell model picture, these nuclei are described in terms of two valence nucleons outside the doubly closed $1d$–$2s$ shell — considered in the following as an innert core.

The energy levels of these nuclei were often utilized [15–18] for extraction of effective two-body interaction parameters then being used in calculations of energies of heavier nuclei belonging to the $1f$–$2p$ shell.

Several investigations have been undertaken to describe the states of ^{42}Ca and ^{42}Sc in terms of the simple shell model [19–30]. Various forms of two-body interaction were employed. However, neither the empirical two-body interaction parameters found by least squares fit to the known levels of Ca isotopes (Engerland [19], Dieperink [31]), nor that realistic calculated by Kuo and Brown [30], were able to reproduce the experimental level scheme. It appears that some core excitation effects play here an important role.

We decided to perform the shell model calculations on the full basis of Pauli allowed states for two-valence nucleons distributed in the $1f_{7/2}$. $2p_{3/2}$, $2p_{1/2}$, and $1f_{5/2}$ orbits outside the ^{40}Ca core. The existing studies on the lighter [5–11] as well as on the heavier nuclei [12–14] have shown that the shell model with MSDI is able to predict all observed phenomena such as energy levels, spectroscopic factors, multipole moments, and electromagnetic transition rates. It appears from these studies that this form of interaction is no less valuable than other, more complicated forms of interaction. In particular the microscopic calculations performed in a large model space are able, as was shown in a few recent works [6–8, 10, 32–34], to account for the core excited phenomena. Some structure properties of nuclei, belonging to $1d$–$2s$ shell and known as deformed nuclei, have been predicted in this way.

The purpose of our work was:

(*i*) to check whether the MSDI two-body matrix-elements are correlated to the empirical and realistic ones as was done in the case of the $1d$–$2s$ shell [6, 7, 9]. Hitherto, nobody has proved that this correlation persists also in the case of the $1f$–$2p$ shell;

(*ii*) to prove the validity of MSDI residual interaction in describing the properties of nuclei belonging to the $1j$–$2p$ shell when the configuration space is extended to a larger number of orbits.

2. *The surface delta interaction*

Residual nucleon-nucleon interaction is that part of the interaction which is not included in the central average potential. In consequence of the Pauli principle, most inelastic collisions inside the nucleus are prohibited. Therefore the nucleons move almost

freely in the nuclear matter and the effective interaction between the nucleons occurs mainly in the nuclear surface. Using this assumption, Moszkowski and co-workers [1] have proposed a simple model, able to describe the interaction between the valence nucleons. This model of interaction assumes that

1. The residual interaction V_{ab} between particles a and b takes place at the nuclear surface only;

2. The two-body forces are delta forces, i. e. the interaction takes place only if the two nucleons are in the same place:

$$V_{ab} = -4\pi A\delta(\Omega_{ab}) \tag{1}$$

where A represents the interaction strength and Ω_{ab} is the angular distance between the interacting particles. The factor 4π is introduced for normalization purposes;

3. The radial one-particle wave functions of the active shell have the same absolute value at the nuclear surface, i. e. V_{ab} does not depend on l.

Interaction defined in this way possesses all the features of pairing interaction. It is short-ranging and allows only symmetric spatial states. It should be pointed out that the SDI exists not only between particles coupled to $J = 0$, $T = 1$, but also between particles coupled to $J \neq 0$. Unlike pairing, SDI interaction acts also in states with $T = 0$. Therefore the SDI should be a better approximation then a pure pairing one. Following the work of Glaudemans [3] where the isospin dependence of the interaction was taken into account, the interaction may be written in the form

$$V_{ab}[\mathrm{MSDI}] = -4\pi A_T\delta(\Omega_{ab})\delta(\hat{r}_a-\hat{R})\delta(\hat{r}_b-\hat{R})+B\tau_a\cdot\tau_b, \tag{2}$$

where $\hat{r}_a$, $\hat{r}_b$ are the position vectors of interacting particles, $\hat{R}$ is the nuclear radius, τ are isospin operators. The strength of interaction A_T, where $T = t_a+t_b$, depends on the isospin of interacting particles. The correction term $B\tau_a\cdot\tau_b$ is introduced to account for the splitting between the groups of levels with different isospin. The eigenvalue of the operator product $\tau_a\cdot\tau_b$ is found from the relation

$$T^2 = t_a^2+t_b^2+2t_at_b.$$

Taking into account that $t = 1/2\,\tau$ and $t_a = t_b = 1/2$, one obtains

$$t_at_b = \frac{T(T+1)-t_a(t_a+1)-t_b(t_b+1)}{2} = \frac{2T(T+1)-3}{4} \tag{3}$$

and

$$\tau_a\cdot\tau_b = 2T(T+1)-3.$$

Such a form of interaction is called Modified Surface Delta Interaction [MSDI].

In the simple case of two valence nucleons outside the closed shell the Hamiltonian is given by

$$H = H_{\mathrm{core}}+E(j_a)+E(j_b)+\langle j_aj_b|V_{ab}|j_cj_d\rangle, \tag{4}$$

where $E(j)$ are the single particle energies. The antisymmetrized matrix element of V_{ab}

is given (see Ref. [3]) by

$$\langle j_a j_b|V_{ab}|j_c j_d\rangle_{JT} = -\frac{A_T}{2(2J+1)}\left\{\frac{(2j_a+1)(2j_b+1)(2j_c+1)(2j_d+1)}{(1+\delta_{ab})(1+\delta_{cd})}\right\}^{1/2}$$

$$\times[(-1)^{l_a+l_b+j_c+j_d}\times\langle j_a\tfrac{1}{2}\, j_b-\tfrac{1}{2}|J0\rangle\langle j_c\tfrac{1}{2}\, j_d-\tfrac{1}{2}|J0\rangle\{1-(-1)^{l_c+l_d+J+T}\}$$

$$-\langle j_a\tfrac{1}{2}\, j_b-\tfrac{1}{2}|J1\rangle\langle j_c\tfrac{1}{2}\, j_d-\tfrac{1}{2}|J1\rangle\{1+(-1)^T\}]+[2T(T+1)-3]B\delta_{ac}\delta_{bd}, \qquad (5)$$

where $\langle j_a\frac{1}{2}\, j_b-\frac{1}{2}|JM\rangle$ are the Clebsh-Gordon coefficients and $j_a j_b j_c j_d$ are the spin states of particles. Correspondingly, J and T indicate the spin and isospin of a two particle state. The diagonal matrix elements with $j_a = j_c$ and $j_b = j_d$ correspond to pure states.

In the case of pure states, the excitation energies are given by the difference between the binding energy of the i-th level and the binding energy of the ground state. When configuration mixing is considered the energies are obtained by carrying out the diagonalization of energy matrices.

3. *Calculations and results*

The numerical values of 196 two-particle matrix elements were calculated according to the formula (5) for both the $T = 0$ and $T = 1$ states. The parameters $E(j_a)$ and $E(j_b)$ were taken from single particle states of ^{41}Ca and ^{41}Sc nuclei. They are equal to those used by Kuo and Brown [30].

Two different ways were used in the construction of the interaction term (5) in the Hamiltonian (4):

a) The parameters A_0 and A_1 were considered to be state independent, thus being constant in the configuration space. This is an essential postulate of the pure MSDI model.

b) The parameters A_0 and A_1 were allowed to vary in going from state to state.

In calculations performed according to the first way the parameters A_0 and A_1 were adjusted to produce the best agreement with the experimental level schemes. The energy matrices were diagonalized and the calculated level schemes for both ^{42}Ca and ^{42}Sc nuclei are presented in the second column on Figure 1. In the case of the ^{42}Ca nucleus the sequence of levels (except for the second and third excited states at 1.84 and 2.42 MeV, which are known to arise from core excitation) is satisfactory. The energy lowering of the first 2^+ experimental state may be due to its interaction with the core excited second 2^+ state at 2.42 MeV. The calculated level scheme of the ^{42}Sc nucleus roughly reproduce the observed level sequence and is less successful in reproducing the energies. The first 3^+ state lies below the well-known 7^+ state, which together with the first 1^+ state forms a close energy doublet at 0.6 MeV in the experimental scheme.

In the calculations performed in the second way the state dependence of the interaction was taken into account by changing the parameters A_0 and A_1.

The nuclei belonging to the $1f-2p$ shell may be more deformed than those belonging to the $1d$—$2s$ shell. A coefficient resulting from this dependence may be for the former nuclei different from that for the latter, which is equal ± 1.

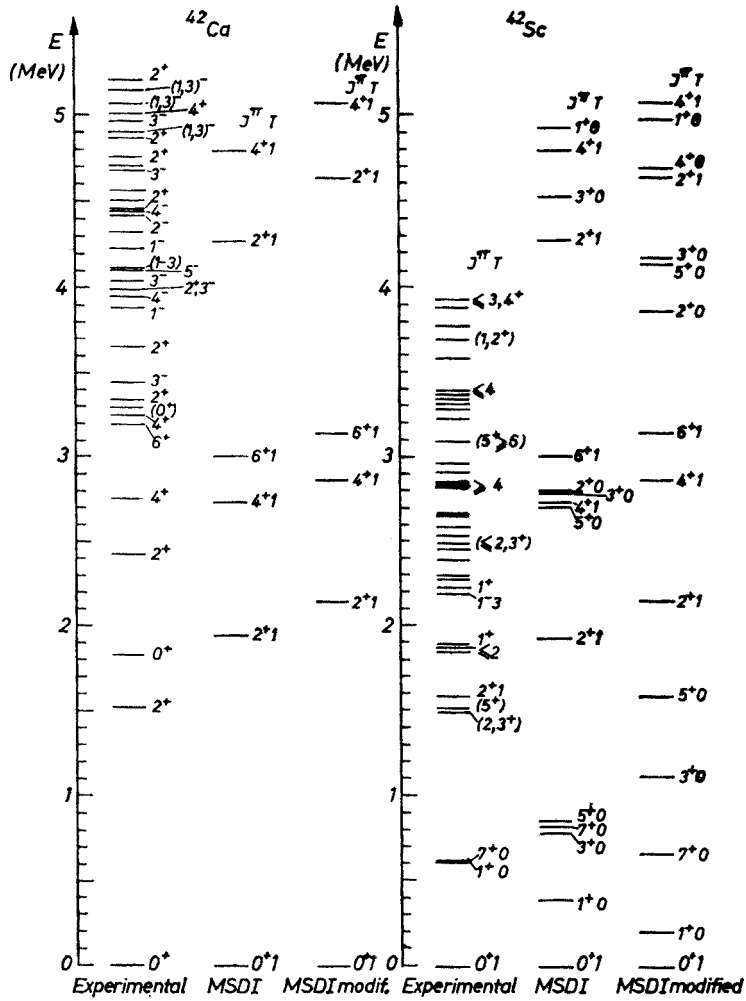

Fig. 1

In order to account for this effect the overlaps of four single particle wave functions, $I = \int R_a(r)R_b(r)R_c(r)R_d(r)dr$ appearing in the matrix elements $\langle j_a j_b|V|j_c j_d\rangle$ were calculated. The Saxon–Woods potential with parameters

U[MeV]	W[MeV]	r_u [f]	r_w [f]	a_u [f]	a_w [f]	r_c [f]
51	13	1.250	1.250	0.650	0.470	1.250

was utilized to generate the radial functions.

The numerical values of these overlaps exhibit three distinct groups depending on the combination of j-values (Figure 2). In order to simulate this geometrical effect, three corresponding values of A_T for both $T = 0$ and $T = 1$ were fitted by varying the parameters A_T between 0.35–0.95 MeV. The best results were obtained with the values $A_1 = 0.65$ —

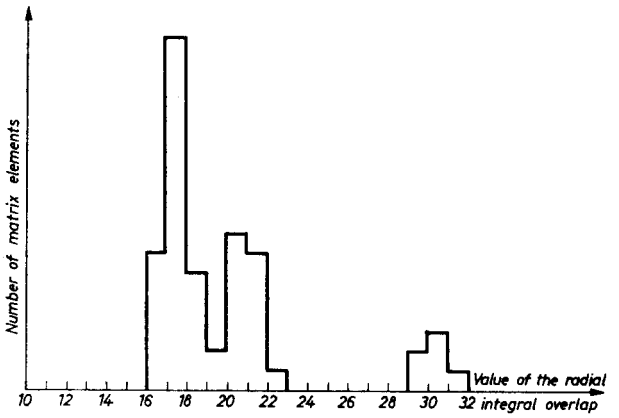

Fig. 2. Distribution of the integrals of radial overlaps

	$\langle 7/2\ 7/2\rangle$	$\langle 7/2\ 5/2\rangle$	$\langle 7/2\ 3/2\rangle$	$\langle 7/2\ 1/2\rangle$	$\langle 5/2\ 5/2\rangle$	$\langle 5/2\ 3/2\rangle$	$\langle 5/2\ 1/2\rangle$	$\langle 3/2\ 3/2\rangle$	$\langle 3/2\ 1/2\rangle$	$\langle 1/2\ 1/2\rangle$
$\langle 7/2\ 7/2\rangle$	0.31									
$\langle 7/2\ 5/2\rangle$	0.31	0.30								
$\langle 7/2\ 3/2\rangle$	0.21	0.20	0.18							
$\langle 7/2\ 1/2\rangle$	0.21	0.21	0.18	0.19↑						
$\langle 5/2\ 5/2\rangle$	0.30	0.30	0.19↑	0.20	0.30					
$\langle 5/2\ 3/2\rangle$	0.20	0.19↑	0.17	0.17	0.19↑	0.16↑				
$\langle 5/2\ 1/2\rangle$	0.21	0.20↑	0.17↑	0.18↑	0.17↑	0.17↑	0.17↑			
$\langle 3/2\ 3/2\rangle$	0.18↑	0.17	0.18↑	0.18↑	0.17↑	0.17	0.17	0.22		
$\langle 3/2\ 1/2\rangle$	0.18	0.17↑	0.18↑	0.18↑	0.17↑	0.17	0.22	0.22	0.21↑	
$\langle 1/2\ 1/2\rangle$	0.19	0.18↑	0.18↑	0.18	0.17↑	0.22↑	0.20↑	0.21↑	0.20	0.21

0.31 $A_1 = 0.65$ MeV $A_0 = 0.70$ MeV

0.20 $A_1 = 0.55$ MeV $A_0 = 0.60$ MeV

0.18 $A_1 = 0.45$ MeV $A_0 = 0.40$ MeV

Fig. 3. Diagram of the values of the overlap $I = \int R_a(r)R_b(r)R_c(r)R_d(r)dr$

$-0.55 - 0.45$ MeV and $A_0 = 0.70 - 0.60 - 0.40$ MeV. The method of fitting the parameters A_T to the single particle matrix elements is shown in Figure 3. Parameter B is chosen to be equal 0.20 MeV. The parameters $E(j_a)$ and $E(j_b)$ were taken to be the same as in the method a). The results are shown in the third column of Fig. 1.

4. *Discussion*

In both nuclei the density of calculated levels is significantly less than that of observed levels. This fact leads to the conclusion that some core excitation modes play an important role in the formation of low-lying states of the nuclei ^{42}Ca and ^{42}Sc. In particular, the states 0^+ at 1.84 MeV and 2^+ at 2.42 MeV in ^{42}Ca must be predominantly core excited and therefore they cannot be described by the model used here. The radiative transition 0^+ 1.84 $\rightarrow$ 2^+ 1.52 MeV in ^{42}Ca is larger than that given by the single particle estimate by a factor of 15 (Bertsch [35]). The ^{42}Sc nucleus is an unstable nucleus. It is strongly deformed, hence many so-called "intruder states" appear in its energy level scheme.

One of the most probable modes of core excitations is the formation of the $4p-2h$ configuration in which two nucleons are promoted from the $1d_{3/2}$ or $2s_{1/2}$ orbit to the $1f_{7/2}$ orbit. In the particular case $T = 0$ a weakly bound alpha cluster is created [37]. This model, applied by the authors of Refs [25, 36, 42], has led to excellent reproduction of the low-lying states of ^{42}Ca and ^{42}Sc nuclei.

We have made a careful comparison of the MSDI two-body matrix elements with those obtained in another way. We have found that the deviations of the MSDI matrix elements of the $1f-2p$ shell from the empirical or realistic one is much larger than in the case of the $1d-2s$ shell discussed in [6, 7, 9]. The reason lies in the fact that the empirical and realistic two-body interaction parameters absorb the core excitation effects and thus can better reproduce the experimental states.

On the other hand, the MSDI calculations can give a good agreement for the pure single-particle states. The MSDI parameters are derived on the assumption of a pure shell model and do not absorb the core excitation effects. Therefore they cannot reproduce states in which the core excitation phenomena play an important role. The introduction of the variable A_T parameters leads to the correct level sequence in the ^{42}Sc nucleus. The fact that the deviations from the experimental results of the MSDI calculations in the case of the ^{42}Ca and ^{42}Sc nuclei are much greater than in that of the $1d-2s$ shell, leads to the conclusion that the core excitation admixture in both $A = 42$ nuclei is more important than in the nuclei belonging to the $1d-2s$ orbit.

The MSDI method can be used as a good instrument for reproducing the single-particle levels in the $1f-2p$ shell. From the range of deviation we can also estimate the dimension of the core excitation admixtures.

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