New spin assignments in the odd-odd N = Z nucleus ⁴²Sc and the breaking of the ⁴⁰Ca core

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Using the ⁴⁰Ca(³He, *p*) reaction at $E_{3He} = 9$ MeV and the multidetector array HORUS, angular correlations of coincident pairs of γ transitions in the odd-odd N = Z nucleus ⁴²Sc have been measured at the FN tandem Van de Graaff accelerator of the University of Cologne. The analysis of the data allowed nine new spin assignments and the determination of a series of new multipole mixing ratios. In particular, the spin and parity of the 5⁺ and 7⁺ levels belonging to the lowest $T = 0\pi f_{7/2} v f_{7/2}$ multiplet have been determined and the (6⁺) level from the T = 1 multiplet has been tentatively assigned. In this way, all T = 1 states up to an excitation energy of 3.2 MeV now have known spins as well as the lowest T = 0 quadruplet ($J^{\pi} = 1^+, 3^+, 5^+, 7^+$) and many other T = 0 states of unknown structure. The comparison with shell-model calculations reveals that a breaking of the ⁴⁰Ca core has to be invoked to describe the level structure of ⁴²Sc.

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I. INTRODUCTION

The doubly magic nuclei and their nearest neighbors are particularly interesting for nuclear structure studies. With Z = 21 protons and N = 21 neutrons, the nucleus ⁴²Sc lies on the N = Z line and differs from the doubly magic nucleus ⁴⁰Ca by two nucleons, having one proton and one neutron more. In 42 Sc, the $f_{7/2}$ orbital starts to be filled and the two lowest families of excitations, i.e., the T = 0 ($J^{\pi} = 1^{+}, 3^{+}, 5^{+}, 7^{+}$) and the T = 1 $(J^{\pi} = 0^+, 2^+, 4^+, 6^+)$ multiplets, are expected to be based on the $\pi f_{7/2} \nu f_{7/2}$ configuration. Indeed, the spectroscopy of ⁴²Sc (cf. Ref. [1] and references therein) reveals the existence of these multiplets as well as of many other states at excitation energies up to about 4 MeV. These circumstances make this nucleus a very attractive testing ground for shell-model calculations (especially with respect to the validity of the Z = 20 proton shell closure that has been questioned, e.g., for ^{44,46}Ca [2,3] and ^{46,48}Ti [4], which are rather mid-neutron-shell nuclei) and for a test of the validity of the isospin symmetry. Despite the great interest in this nucleus, many spins of low lying levels in ⁴²Sc were still not well known, calling for a new experiment. The aim of the present work is, by performing angular correlation measurements, to determine new spins of states in ⁴²Sc and thus facilitate further theoretical studies. A number of articles on low-spin states in odd-odd N = Z nuclei in the *pf* shells have been published by coworkers of the Institut für Kernphysik of the

Cologne University (⁴⁶V [5–8], ⁵⁰Mn [7–12], ⁵⁴Co [7,9,13,14], ⁵⁸Cu [15,16]). The present study is also a continuation of these investigations. So far, they revealed that large-scale shell-model calculations, as, e.g., in the case of ⁵⁸Cu, are needed to describe the experimental data. Such calculations would also have to be invoked if it turns out that Z = 20 needs to be broken, which we will discuss at the end of this article.

II. EXPERIMENTS

Excited states in ⁴²Sc were populated using the fusion reaction ⁴⁰Ca(³He, *p*) at an incident energy of $E_{^{3}He} = 9$ MeV. The ³He beam was provided by the FN Tandem Van de Graaff accelerator of the Cologne University. The target consisted of 1.1 mg/cm² nat Ca sandwiched between a 0.2 mg/cm² gold foil to prevent oxidisation facing the beam and another 2 mg/cm^2 gold foil serving as a backing to stop the recoiling nuclei. Deexciting γ rays were registered by the multidetector array HORUS, on which more details can be found in Ref. [17]. The spectrometer was equipped with nine HPGe single crystal detectors and one Euroball cluster detector [18]. Here we mention only some main features that are important for the analysis: The cluster detector and five HPGe detectors were positioned in a plane that is perpendicular to the beam direction and contains the target. Two of the remaining HPGe detectors were positioned at angles of 45° with respect to the beam axis, whereas the two other detectors were positioned at angles of 135°. About $8.4 \times 10^8 \gamma \gamma$ coincidence events were recorded at an average coincidence event rate of 9 kHz. They were subsequently sorted, after corrections for gain shifts,

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TABLE I. The angular correlation groups of the multidetector setup of HORUS used in the analysis. θ_1 and θ_2 are the angles between the target-detector axis and the beam axis, and ϕ is the relative angle between the two planes formed by the beam axis and the respective target-detector axes. The number of detector pairs involved in each group is also given.

Group number	θ_1	θ_2	ϕ	Detector pairs
1	90°	90°	55°	16
2	90 °	90°	180°	6
3	90 °	90°	70°	8
4	135°	90°	-270°	8
5	135°	90°	-215°	16
6	135°	45°	0°	8
7	135°	45°	-180°	4

into matrices corresponding to independent angular correlation groups of Horus (as listed in Table I). An energy and efficiency calibration was performed with a ²²⁶Ra source placed at the target position. An example of a γ -ray spectrum measured in coincidence with the 894-keV transition is shown in Fig. 1.

III. DATA ANALYSIS

The angular correlation function $W(\theta_1, \theta_2, \phi)$ for two successive transitions from oriented states is derived and given in Refs. [19,20]. This function mainly depends on the spins of the initial, intermediate, and final levels as well as on the two multipole (L + 1)/L mixing ratios $\delta[(L + 1)/L]$ of the two coincident γ transitions. The first γ transition is detected at angle θ_1 with respect to the beam axis, the second γ transition at angle θ_2 , and ϕ is the angle between the two planes



FIG. 1. Spectrum of γ rays measured in coincidence with the 894-keV transition connecting the 5⁺ level at 1510 keV and the 7⁺ level at 616 keV, observed with the detectors of correlation group 1 (see Table I).

containing the detection axes and the beam axis ($\phi = \phi_2 - \phi_1$ where ϕ_2 and ϕ_1 are the azimuthal angles of the corresponding detectors). The symmetries of the coincident radiation event of the two γ rays lead to symmetries [21] of the function W. They can be used to establish the independent angular correlation groups of a given setup. For a given group of detector pairs, the values of the W function are the same and for the calculation of the detected coincident area only the sum of the coincident efficiencies of the participating detector pairs is of importance. The coincidence efficiency can be represented to a good approximation as a product of the efficiencies of the two detectors. For the angular correlation analysis, we used the code CORLEONE [22–24].

The relative efficiencies of the detector groups were adjusted by requiring a reasonable reproduction of the properties of a known γ cascade in ⁴²Sc, namely the $3_1^+ \rightarrow 1_1^+ \rightarrow 0_1^+$ one, consisting of a pure *E*2 transition of 880 keV and a pure M1 transition of 611 keV, where the spins of the initial, intermediate, and final states are known. The data analysis was performed using the seven angular correlation groups shown in Table I. For a given spin hypothesis, the data analysis consists of fitting the intensity of the cascade by adjusting the parameter σ characterizing the distribution of the magnetic substates m of the spin of the first oriented level and the multipole mixing ratios δ_1 and δ_2 of the two successive transitions. This is done via a least-squares fit comparing the experimental value of the W function with the expected theoretical value as a function of the possible free parameters (the spin values, the multipole mixing ratios and the σ parameter). In most cases, this analysis is simplified by the fact that one or two spins in the cascade are already known, leaving only a few hypotheses to test. In most of the cases the value of δ_2 could also be fixed, leaving only the parameters σ and δ_1 to be varied to optimise the χ^2 value for a given spin hypothesis. Some preliminary results of this experiment have already been published [25]

The $3_1^+ \rightarrow 1_1^+ \rightarrow 0_1^+$ cascade is a good testing ground for the analysis as the multipolarity of both transitions in the cascade is pure. Trying to fit the experimental data to the theoretical function with alternative spin hypotheses always leads to much worse χ^2 values. The angular correlation pattern of this cascade is shown among others in Fig. 2 together with the theoretical fit using different spin hypotheses to demonstrate the power of the technique.

IV. RESULTS

In Figs. 2, 3, and 4, the results of the correlation analysis are illustrated by the experimental angular correlation patterns and the best fits corresponding to different spin hypotheses. The analysis of the 975- to 611-keV cascade of γ -ray transitions confirms the spin assignment $J^{\pi} = 2^+$ of Ref. [1] for the level at 1586 keV. A new and significantly lower value of the multipole mixing ratio $\delta = 0.000(21)$ was derived for the 975-keV $2^+ \rightarrow 1^+$ transition (the value from the literature [26] is 0.05(3)). This value was used as a fixed parameter for the analysis of the angular correlation data of other cascades in which the 975-keV transition participates to reduce the number of free parameters. Similarly, the E2/M1 mixing ratio δ of the 1875-keV transition was determined in the analysis of the



FIG. 2. Angular correlation patterns for the cascades involving either the 611- and/or 1875-keV transitions. For each spin hypothesis, the best fit is shown. The pattern of the adopted spin hypothesis is marked with a solid black line. The excitation energy is assigned to each J^{π} level as a subscript for better identification.

1875- to 611-keV cascade to be $\delta = 0.031(29)$ and can be kept fixed in the analysis of the 905- to 1875-keV cascade from the level at 3393 keV. The transitions of 611 and 880 keV used in other two-step cascades are characterized by a pure multipolarity ($\delta = 0$). The results of the correlation analysis are summarized in Table II.

In total, nine new spins have been unambiguously determined from the angular correlation analysis. Seven spins known from the literature have been confirmed by our experiment and for three levels the range of possible spins has been narrowed.

The 616 (7⁺)- and 1510 (5⁺)-keV levels require special attention. The 616-keV state is a long-living isomer that β decays to the 6⁺ level (3189 keV) in ⁴²Ca. This transition has a log *ft* value of 4.163(19) [27], suggesting it is a Gamow-Teller transition. Therefore the allowed J^{π} values are 5⁺, 6⁺, and 7⁺. Furthermore the $J^{\pi} = 5^+$ assignment for the level at 1510 keV was uncertain, which means that in all cascades involving transitions coincident to the 894-keV transition at least two spins would be unknown. Using the known $J^{\pi} = 4^+$ of the T = 1 state at 2815 keV, depopulated by the 894-1305 cascade leading to the 616-keV level via the 1510-keV level, all possible spin hypotheses were tested. The only hypotheses leading to an acceptable χ^2 value with a reasonable σ parameter were the 4-3-5 and 4-5-7 hypotheses.

The 4-3-5 hypothesis, however, leads to an E2/M1 multipole mixing ratio value for the first (isovector) transition of





FIG. 3. Angular correlation patterns for the cascades involving the 880-keV transitions and one involving the 975-keV transition. For each spin hypothesis, the best fit is shown. The pattern of the adopted spin hypothesis is marked with a solid black line. The excitation energy is assigned to each J^{π} level as a subscript for better identification.

 $\delta_1 \approx 20$, implying an *E*2 transition character. The 1305-keV transition has, however, previously been determined to be an *M*1 transition, with B(M1) = 0.17(7) W.u. [1]. The $T = 1, 4^+$ level at 2815 keV has $T_{1/2} = 35(14)$ fs [1], and about 61% of the deexiting γ rays decay to the 1510 (5⁺)-keV level. If the transition were of mixed multipolarity, then $\lambda(E2 + M1) = (1 + \delta^2)\lambda(M1)$ would imply a *E*2/*M*1 multipole mixing ratio of about $\delta \approx 0.1$, which cannot be reproduced by the 4-3-5 hypothesis. However, the 4-5-7 hypothesis is well in line with this ratio and has a low χ^2 value (see Table II). Other cascades involving the 894-keV transition connecting the two levels also confirm this hypothesis (see Fig. 5 and Table III).

The only remaining question concerns the parity of the 1510-keV level, the positive parity of the 7⁺, 616-keV level having already been established [1]. The negative-parity option $(4^+ \rightarrow 5^- \rightarrow 7^+)$ can be excluded by the lifetime and the multipole mixing ratio of the 894-keV $5 \rightarrow 7$ transition. From the results of the angular correlation analysis we get an average multipole mixing ratio for the 894-keV transition of $\delta = -0.12$. If the transition were to involve a parity change it would be predominantly of M2 character. The 1510-keV level has $T_{1/2} = 45(7)$ ps [28,29]. Using the Weisskopf estimates for the total transition probability of the 894-keV decay and supposing M2 character of this decay one gets a $B(M2, E_x = 1510 \rightarrow E_x = 616)$ value of 1998(311) μ^2 fm² or 100(16) W.u., which can be ruled out. However, the

E _{level} (keV)	J^{π} NDS	J^{π} (present work)	Т	$J_1 - J_2 - J_3$	$\begin{array}{c} E_{\gamma_2} - E_{\gamma_1} \\ (\text{keV}) \end{array}$	χ^2	σ	δ_1 (present work)	δ_2 (present work)
0	0^{+}	0^{+}	1	2-1-0 ^g	611–975	1.3	2.12(18)	0.000(21)	0.00
611	1^{+i}	1^{+}	0	2-1-0 ^a	611-975	1.3	2.12(18)	0.000(21)	0.00
616	$(7)^{+}$	7 ^{+b}	0	4-5-7	894-923	0.2	1.51(26)	0.398(86)	-0.068(53)
				4-5-7	894-1305	0.8	2.89(77)	-0.060(36)	-0.16(12)
				4-5-7	894-1513	1.0	2.65(1.03)	-0.032(78)	-0.07
1490	3+	3+	0	3-1-0 ^{c,d}	611-880	0.9	2.46(29)	-0.011(28)	0.00
1510	(5^{+})	5 ^{+b}	0	4-5-7	894-1305	0.8	2.89(77)	-0.060(36)	-0.16(12)
1586	2+	2^{+}	1	2-1-0 ^c	611-975	1.3	2.12(18)	0.000(21)	0.00
1845	(3 ⁺)	3(+)	0	3-1-0 ^e	611-1235	0.4	2.03(87)	-0.122(148)	0.00
1874	0^{+}		1						
1889	1^{+i}		0						
2187	$(2,3)^+$	3+	0	3-2-1	975-601	5.5	1.99(21)	-0.234(41)	0.00
2269	$(1,2^+)$	2^{+}	0	2-1-0	611-1658	0.7	1.77(61)	-0.057(63)	0.00
2295	n/a	(1,2)	0	(1,2)-2-1	975-709	0.6	4(16)	-196(197)	0.00
				(1,2)-2-1	975-709	0.5	2.42(2.15)	-2.69(77)	0.00
2433	$(3,4,5)^+$	4^{+}	0	4-3-1 ^f	880-943	0.4	2.95(50)	-0.476(112)	0.00
2486	2+	2^{+}	1	2-1-0	611-1875	2.2	2.22(23)	-0.010(31)	0.00
				2-3-1	880-996	1.4	2.07(67)	-0.016(40)	0.00
2587	$(1^+ \text{ to } 5^+)$	$(2^+, 4^+)$	0	(2,4)-3-1	880-1096	1.2	1.74(24)	-0.012(43)	0.00
				(2, 4) - 3 - 1	880-1096	0.7	3.50(94)	-0.102(55)	0.00
2815	4+	4^{+}	1	4-3-1 ^f	880-1325	0.2	2.63(39)	-0.001(42)	0.00
2910	$(3,4,5)^+$	$(2,4)^+$	0	(2,4)-3-1	880-1420	0.6	2.60(1.55)	-0.002(51)	0.00
				(2,4)-3-1	880-1420	0.5	5.23(2.84)	-0.136(66)	0.00
3023	$(4)^{-}$	4^{-h}	0	4-5-7	894-1513	1.0	2.65(1.03)	-0.032(78)	-0.07
3393	$(1,2,3)^+$	3+	0	3-2-1	1875-905	4.1	2.03(26)	-0.111(50)	-0.01
3688	1^{+i}	1^{+}	0	1-2-1	975-2101	3.3	1.54(1.09)	-0.070(37)	0.00
3933	$(1,2,3)^+$	3+	0	3-2-1	975-2347	1.3	2.12(29)	1.23(52)	0.00

^aA total of 16 cascades where this level participates has been analyzed.

^bFor detailed description of the arguments leading to the assignments of the 616 and 1510 levels, see discussions in text.

^cA total of six cascades where this level participates has been analyzed.

^dThe cascade described in the table is the one used for the correction of the efficiency calibration.

^eThe 975- to 258-keV cascade has also been analyzed but gives no clear result. However it rules out the I = 4 hypothesis. ^fSee also the cascade leading to the 616-keV level.

^gA total of five cascades where this level participates has been analyzed.

^hLowest known negative-parity state in ⁴²Sc.

ⁱThese states have also been observed in a recent ${}^{42}Ca({}^{3}He, t)$ experiment at RCNP, Osaka [30].

positive-parity assumption for the 1510-keV level gives a reasonable $B(E2, E_x = 1510 \rightarrow E_x = 616)$ value of 22.11(344) $e^2 \text{fm}^4$ or 2.55(40) W.u., which compares to the $B(E2, 2_1^+ \rightarrow 0_1^+)$ value of 8(3) W.u.

Thus $J^{\pi} = 5^+$ is firmly assigned to the 1510-keV level and $J^{\pi} = 7^+$ is firmly assigned to the 616-keV level.

V. DISCUSSION

Isospin assignments in ⁴²Sc can be made by a comparison with the T = 1 levels in the isobaric analog nuclei ⁴²Ti and

⁴²Ca. This is done graphically in Fig. 6. An upward shift of 61.7 keV of the energies of the ⁴²Ca levels leads to a very good correspondence between the T = 1 levels in the two nuclei (with exception of the ground state). The other levels in ⁴²Sc below $E_x = 3.3$ MeV have T = 0 character as expected from the minimal value of the isospin corresponding to the projection $T_z = (N - Z)/2 = 0$. The levels in ⁴²Ti can similarly be shifted by 30.3 keV.

The energy differences in every triplet of levels is presumably mainly due to the differences of the Coulomb energies [31-34] of the three nuclei. We note that the level at 3242 keV

$\frac{E_{\gamma_2} - E_{\gamma_1}}{\text{(keV)}}$	Spin cascade hypothesis	χ^2	σ	δ_1	δ_2
894–923	4-5-7 4-3-5	0.2	1.51(26) 2.03(22)	0.398(86) -0.402(85)	-0.068(53) -0.268(114)
894–1305	4-5-7	0.8	2.89(77)	-0.060(36)	-0.16(12)
	4-3-5	0.9	2.65(66)	$20.43^{+85.62}_{-9.15}$	$-1.41\substack{+0.33\\-0.48}$
894–1513	4-5-7	0.7	3.44(141)	-0.071(49)	$-0.98\substack{+0.85\\-5.58}$
	4-5-7	1.0	2.65(103)	-0.032(78)	-0.07(fix)
	4-3-5	0.8	2.12(65)	$19.84^{+85.23}_{-11.26}$	$-1.31\substack{+0.44\\-0.76}$

TABLE III. Detailed information on the fit results of cascades involving the 616and 1510-keV levels with focus on the 4-3-5 and 4-5-7 cascade alternatives.

in ⁴²Sc has been previously assigned [1] as $J^{\pi} = (5, 6, 7)^+$. The good correspondence with the 6⁺ level in ⁴²Ca (and to a lesser extent with the 6⁺ level in ⁴²Ti) strongly favors an assignment of $J^{\pi} = (6)^+$ for this level. Thus, a complete set of T = 1 states below $E_x = 3.3$ MeV could be established in the isobaric triplet.

One might expect that the lowest state for a $T_z = 0$ nucleus has an isospin of T = 0, as the deuteron. This is not fulfilled in ⁴²Sc where the ground-state is a T = 1, $J^{\pi} = 0^+$ state, and in other $T_z = 0$ *fp*-shell nuclei with the exception of ⁵⁸Cu [15,35,36]. Thus, a theoretical description of both the



FIG. 4. Angular correlation patterns for the cascades involving the 894- or 975-keV transitions. For each spin hypothesis, the best fit is shown. The pattern of the adopted spin hypothesis is marked with a solid black line. The excitation energy is assigned to each J^{π} level as a subscript for better identification.

T = 0 and T = 1 multiplets would be a stringent test for the nuclear shell model (cf., e.g., Ref. [37]). We note that an interesting aspect of the present work is the determination of the spins of all levels of the $f_{7/2}^2$ multiplets. In the nucleus 54 Co, which has a neutron and a proton hole in the $f_{7/2}$ subshells and thus is an analog of ⁴²Sc which has neutron and proton particles in these subshells, the shell model gives a reasonable description of the multiplets [38]. Similarly, shell-model calculations available in the literature reproduce the levels of the multiplets in ⁴²Sc. The good agreement with the shell model was found already in 1967 by J. J. Schwartz et al. [39]. However, the exact reproduction of other states, including those with spins assigned firmly in the present work, remains a problem for shell-model calculations. As a reason for this, the softness of the ⁴⁰Ca core is pointed out, expressed, for example, by the existence of a low-lying deformed 0^+ state at $E_x = 3.353$ MeV, implying a breaking of the core leading to the appearance of states with more complicated wave functions.

Within such an approach Flowers and Skouras [37] were able to reproduce the levels known at the time of their study in addition to those of the first multiplets. In addition to states from the *fp* shells, these authors used also deformed 4p-2h states appearing from the breaking of the ⁴⁰Ca core. Examples of T = 1 deformed states in ⁴²Sc are provided by the first



FIG. 5. Detailed view of the decay scheme of 42 Sc involving the 1510-keV (5⁺) and 616-keV (7⁺) levels. The analyzed transitions feeding the 1510-keV level are shown (see also Fig. 1) with the respective energies of the γ rays as well as the spins of the originating levels.



FIG. 6. T = 1 isospin multiplets in ⁴²Ti, ⁴²Sc, and ⁴²Ca up to an excitation energy of 3.3 MeV. The levels in ⁴²Ti and ⁴²Ca are shifted relative to the ⁴²Sc levels by 30.3 and 61.7 keV, respectively, to match the excitation energy of the first 2⁺ (T = 1) levels. The lowest T = 0 states in ⁴²Sc up to 1.5 MeV are also shown in the left part of the figure.

excited 0^+ state at 1873.6 keV and the excited 2^+ state at 2486.6 keV. Thus, below 3.3 MeV the calculations of Flowers and Skouras describe all T = 1 states with isospin assigned by analogy with ⁴²Ca. Below 1.5 MeV, they describe the lowest $T = 0 f_{7/2}^2$ multiplet and many other T = 0 states above 1.5 MeV. In the same spirit, Sherr et al. [40] employed a weak coupling model for 4p-2h states that yielded a reasonable agreement with the data. These authors also pointed out that negative-parity states should be observed in ⁴²Sc, starting from an excitation energy of 1.9 MeV as suggested by the spectrum of neighboring ⁴¹Sc. Such states have not been identified so far, with the exception of the $J^{\pi} = 4^{-}$ level at 3022.8 keV, which is firmly assigned by our data. However, further experimental work (cf. Ref. [1] and references therein) using particle and γ spectroscopy led to the identification of additional states, also in the region below 4 MeV. It is possible that some of these have negative parity.

An interesting result of our work is that some isovector transitions (transitions between T = 1 and T = 0 levels) have been observed in ⁴²Sc. These isovector transitions with $\Delta I = 1$ are predicted to be predominantly of M1 character [41–44] and should thus exhibit a multipole mixing ratio (δ) close to zero. Table IV gives a summary of the δ values extracted from the $\gamma\gamma$ -coincidence angular correlation analysis of cascades involving isovector transitions. Indeed all the δ values in the table are small and thus confirm the expectations of the theory.

The description of the other levels in ⁴²Sc lying below 4 MeV remains a task for the future development of nuclear theory and in particular of the nuclear shell model. For large-scale shell-model calculations, such as those developed by

TABLE IV. Multipolarity mixing ratios of isovector transitions determined by angular correlation analysis, and comparison with the results obtained by shell-model calculations.

T = 1 level		T = 0 level		E_{γ} keV	δ		
$E_{\rm keV}$	J^{π}	$\overline{E_{\rm keV}}$	J^{π}		Present work	Th2	
1586	2+	611	1^{+}	975	0.000(21)	0.01	
		2187	3+	601	-0.234(41)	0.01	
2486	2^{+}	611	1^{+}	1875	-0.010(31)	0.04	
		1490	3+	996	-0.016(40)	0.04	
		3393	3+	905	-0.111(50)	0.15	
2815	4+	1490	3+	1325	-0.001(42)	0.02	
		1510	5^{+}	1305	-0.060(36)	0.04	

the Strasbourg (cf. Ref. [45]) and Tokyo (cf. Ref. [46] and references therein) groups, this problem is a challenge.

VI. SHELL-MODEL CALCULATIONS

To get more quantitative insight into the problem of ⁴⁰Ca core breaking, we have performed two sets of shell-model calculations for ⁴²Sc. The first one (Th1) is in the full *pf* shell with the KB3G effective interaction [47] assuming ⁴⁰Ca as an inert core. The results of the calculation for the low-energy part of the spectrum are compared to the experimental set of firmly assigned levels in Fig. 7. The figure includes, on the experimental side, all 20 levels that now have firmly assigned spin and parity. Levels with uncertain spin or parity have been left out. The only exception is the $T = 1.6^+$ level for which we know from the Coulomb energy differences that it must lie in the $E_x = 3240$ keV region. Although the level is not firmly



FIG. 7. Comparison of the results of the full *pf*-shell calculation with KB3G effective interaction assuming ⁴⁰Ca as inert core (right part) to the assigned experimental levels (left part). All T = 1 levels are marked with the exception of the ground state, which is also a T = 1 state.

assigned, we included it in the picture to be able to compare the experimental and calculated levels.

Although the yrast states are pretty well reproduced (within about 200 keV systematic underprediction), all other states are at much higher energy. Furthermore, the yrast states have very different decay properties, e.g., calculated M1 transition rates of quasideuteron origin for the 2_1^+ , T = 1 and the 4_2^+ , T = 1 states are an order of magnitude larger than the experimental ones (see Table V).

The only way to introduce new degrees of freedom capable of changing the picture is to excite particles from the *sd* shell to the *pf* shell. Recent studies [48] indicate, however, that one has to deal with *n*-particle-*n*-hole excitations across the *sd-pf* shell closure with large n ($n \ge 6$), i.e., the 4p-2h approach of the 70s mentioned above is still not sufficient. Therefore, we have performed a second calculation mixing *sd* and *pf* shells using a recently constructed effective interaction [48]. Similar calculations have been applied successfully to explain isocalar matrix elements from the first 2^+ excited states in the A =42 isobaric triplet [49].

The interaction has been designed for the configurational space spanned by $s_{1/2}$, $d_{3/2}$, $f_{7/2}$ and $p_{3/2}$ orbitals, i.e., assuming a ²⁸Si inert core. However, the derived interaction [48] does not properly take into account the relative monopole shifts of T = 0 and T = 1 parts of the interaction: all the T = 0 states in ⁴²Sc are predicted to be more than 1 MeV above the T = 1 states. We have corrected this problem by adding -1.2 and 0.3 MeV to all diagonal T = 0 and T = 1 two-body matrix elements (tbme), respectively. This does not effect the structure of the states but just shifts all the T = 0 states relative to the T = 1 states by a constant. Another important modification is found to be required for the diagonal $f_{7/2,(J,T=0)}^2$ tbme's. We have added -0.8, 0.3, and 0.5 MeV to the above mentioned thme's with J = 1, 3. and 5, respectively. This is just a rough renormalization of the interaction giving an idea about the fine tuning that needs to be done, but it leads to correct tendencies for the fragmentation of strong M1 strength associated with the $f_{7/2}^2$ structures. We have performed the shell-model calculations with this renormalized interaction using the shell-model code ANTOINE [50,51].

TABLE V. Comparison of calculated and experimental transition rates. The results of shell model calculations in *pf* and *sdpf* shells are shown in columns Th1 and Th2, respectively. The quadrupole effective charges $e_p = 1.5$ and $e_n = 0.5$ have been used in the *E*2 transition operator. The quenching factor q = 0.75 has been used for the spin part of the *M*1 operator. The experimental *B*(*E*2) and *B*(*M*1) quoted in the column labeled NNDC are taken from Ref. [1]. The last columnn contains the values we obtained calculating transition rates using branching ratios and lifetimes from Ref. [1] and our determined multipole mixing ratios.

E_{level1} J_{level1}^{π}		E_{level2}	$J^{\pi}_{ ext{level2}}$	E_{γ}	ΔT	πλ		B(7	τλ), (W.u.)	
ĸev		keV		keV	keV		NNDC	Th1	Th2	Exp.
611	1+	0	0^+	611	1	<i>M</i> 1	[1.9(8) ^a]	2.52	1.68	3.5(18)
1490	3+	611	1^{+}	879	0	E2	4.0(7)	4.38	1.27	4.0(7)
1510	5^{+}	616	7+	894	0	E2		5.40	8.90	2.5(4)
1586	2^{+}	611	1^{+}	975	1	M1	0.31(10)	1.28	0.51	0.31(10)
		0	0^+	1586	0	E2	8(3)	3.3	13.3	8(3)
1874	0^+	611	1^{+}	1263	1	M1	>0.16	0.001	0.12	
1889	1^{+}	0	0^+	1889	1	M1	>0.078	0.03	0.02	
2187	3+	1586	2^{+}	601	1	M1	0.18(8)	0.27	0.36	0.17(10)
						E2		0.01	0.002	76(51)
		611	1^{+}	1576	0	E2		0.03	2.01	12(10)
2223	$(2^+, 3^+)$	1586	2^{+}	637	1	M1	0.13(8)	0.0	0.04	
2269	2^{+}	611	1^{+}	1658	0	M1		0.0	0.0003	< 0.07(1)
						E2		3.80	0.40	< 0.2(6)
2433	4+	1490	3+	943	0	M1		0.0	0.0	< 0.15(3)
						E2		0.14	9.82	<115(53)
2486	2^{+}	1490	3+	996	1	M1	>0.10	0.09	0.10	>0.21(2)
		611	1^{+}	1875	1	M1	>0.051	0.0001	0.09	>0.035(3)
2815	4+	1846	3+	969	1	M1	0.03(3)	0.49	0.008	
		1510	5^{+}	1305	1	M1	0.17(7)	1.82	0.26	0.18(6)
						E2		0.64	0.05	1(1)
		1490	3+	1325	1	M1	0.09(4)	1.27	0.37	0.10(5)
3688	1^{+}	1586	2^{+}	2101	1	M1		1.54	0.01	>0.084(2)
						E2		0.33	0.01	>0.3(3)
3933	3+	1586	2^{+}	2347	1	M1	>0.033	0.0	0.038	>0.013(8)
						<i>E</i> 2		0.002	0.02	>11(5)

^aThe value quoted in Ref. [1] is the transition rate for for the "up" transition $0^+ \rightarrow 1^+$, thus the value has to be multiplied by $\sqrt{3}$ to get the usual "down" transition rate.

We find that for the case of 42 Sc the convergence of the energies for the low-lying states is achieved at the level of 10 nucleons promoted from the *sd* shell to the *pf* shell. This truncation leads to a very high dimension of the Hilbert space, e.g., it is 4×10^7 for the M = 0 state in the m-scheme approach.

Recent studies of the M1 properties of ³⁸Ar in sd-pf shell-model space [52] indicate that one-particle-one-hole excitations from the $d_{5/2}$ orbital to the rest of the sd space strongly couple to the cross-shell excitations from the $s_{1/2}d_{3/2}$ subspace to the $f_{7/2}p_{3/2}$ subspace. This drastically affects the M1 strength at high energy around 10 MeV. However, there is only a minor change for the spectra of the low-lying states and the M1 transitions between low-lying states below 4 MeV in ³⁸Ar. Taking into account that in the case of ⁴²Sc we have already two particles in the pf shell at the 0-particle 0-hole approximation we expect that the effect of the $d_{5/2}$ orbital will be small for the low-energy spectra. Unfortunately, the intractable dimension of the ⁴²Sc configurational space that includes $d_{5/2}$ orbital excitations hinders the direct test of the $d_{5/2}$ orbital effects.

The results of our large-scale calculation of the spectrum are compared to the experimental spectrum in Fig. 8. Here, like in Fig. 7, only the 20 experimental levels with firmly assigned spin and parity have been included, with the exception of the $T = 1, 6^+$ state. To calculate transition rates (see Table V), the quadrupole effective charges $e_p = 1.5$ and $e_n = 0.5$ have been used in the *E*2 transition operator. The quenching factor q = 0.75 has been used for the spin part of the *M*1 operator.

With this new fit one obtains a fairly good description of many experimental levels below 4 MeV with one-to-one matching for most of them, whereas in Th1 the excitation energies of most yrare states show strong deviations from the experimental energies (see Table VI). In particular the 0_2^+ state would have 5.6 MeV excitation energy, whereas the experimental one only has 1.8 MeV. The core-breaking Th2 is thus justified. However, the density of the states is



TABLE VI. Comparison of experimental excitation energies with the corresponding states of the shell-model calculations. All energies are given in keV. We only give the lowest and next lowest levels in J^{π} where Th1 deviates a lot, which clearly establishes that a breaking of the ⁴⁰Ca core is needed.

J_i^{π}	$E_{\rm th1}$	$E_{\rm ex.}$	E_{th2}	J_i^{π}	$E_{\rm th1}$	$E_{\rm ex.}$	$E_{\rm th2}$
0_{2}^{+}	5657	1874	2049	3_{1}^{+}	1074	1490	1450.80
1_{1}^{+}	342	611	845	3^{+}_{2}	3123	2187	1856
1_{2}^{+}	4111	1889	1542	5^{+}_{1}	1117	1510	1300
2_{1}^{+}	1370	1586	1635	6_{1}^{+}	2782	(3242)	3621
2_{2}^{+}	3271	2269	2288	7^{+}_{1}	242	616	544

considerably larger now than in the case of pure pf shell especially if one takes into account a bulk of negative-parity states, most of which are not assigned yet (see Fig. 9). The comparison indicates that a sizable fraction of the unassigned experimental states should have negative parity. The theory, however, also predicts a too-low excitation energy value for the lowest negative-parity states.

We notice that there is a strong mixing between different *n*-particle-*n*-hole configurations leading to the substantial fragmentation of the quasideuteron *M*1 strength with only a small fraction of it distributed to yrast states (see Table V). There is also considerable enhancement of the *E*2 strength for the decay of the 2_1^+ , T = 1 state, indicating a large fraction of deformed configurations in its wave function originating from the breaking of ⁴⁰Ca core.

Going from the *fp* to the *sdpf* picture and adopting an appropriate interaction the structure of the low-energy states changes dramatically. Predominantly collective states, like the 0_2^+ , T = 1 state, are lowered in excitation energy.



FIG. 8. Comparison of the results of the shell-model calculation with the new effective interaction using ²⁸Si as inert core (right part) to the assigned experimental levels (left part). All T = 1 levels are marked with the exception of the ground state, which is also a T = 1 state.

FIG. 9. Unassigned and negative-parity levels compared. The left side of the picture contains the experimental levels of ⁴²Sc with unassigned spin and/or parity, as well as the known 4⁻ state at 3023 keV. The right side of the picture shows the negative-parity levels obtained by the shell-model calculation using the new effective interaction and ²⁸Si as inert core.

Furthermore, we notice a considerable enhancement of pairing correlations in the ground state in the *sdpf* space. This causes a lowering of the 0_1^+ , T = 1 state and, consequently, an increase in the excitation energy of noncollective and weakly collective states. Th2 does not give much better overall agreement with the experiment in respect to reduced transition probabilities; however, it is worthwhile emphasizing that the calcuations presented in this article help to identify the origin of the experimentally observed strong fragmentation of the quasideuteron low-energy M1 strength that has not been explored theoretically so far.

VII. SUMMARY AND CONCLUSIONS

Angular correlations in ⁴²Sc have been measured using the reaction ⁴⁰Ca(³He, p) at E_{3He} = 9 MeV at the HORUS spectrometer in Cologne. Nine new spins of levels and 20 new multipole mixing ratios (including seven δ values for

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 $\Delta T = 1$ transitions) have been determined. All T = 1 states below 3.3 MeV and all T = 0 states below 1.5 MeV now have firmly assigned spins. The comparison with previous shell-model calculations [37] and new calculations with the KB3G interaction reveals that a breaking of the doubly magic ⁴⁰Ca core has to be invoked to describe the T = 0 level structure below 4 MeV in ⁴²Sc.

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