Level Structure of Sc⁴³ and Odd-Mass Ca Isotopes with Reaction Matrix Elements

H. %. Kung, R. P. Singh, R. Raj, and M. I. Rustgi

Physics Department, State University of New York, Buffalo, New York 14214

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Employing Ca 40 as the core, the odd-parity states of Sc 43 and Ca 43 are calculated within the shell-model framework using the reaction matrix elements of the Hamada-Johnston nucleonnucleon potential as calculated by Kuo and Brown. The three extracore particles are considered to occupy the $0f-1p$ orbitals. The effect of including the additional $0g_{9/2}$ orbital is also investigated. The odd-mass calcium isotopes (Ca^{43}, Ca^{45}) and Ca^{47}) are then described by the modified Tamm-Dancoff approximation (MTDA) method and the results are compared with the shell-model calculations of Federman and Talmi and of Engeland and Osnes that had been carried out in a much more restricted configuration space. The MTDA calculations are also performed with the reaction matrix elements of the Tabakin interaction for comparison with the Hamada-Johnston results.

1. INTRODUCTION

In the last few years there has been considerable progress in devising improved techniques to calculate the Brueckner G matrix for realistic nucleon-nucleon interactions with hard core, in order to explain the properties of finite nuclei. In an excellent series of papers, employing the Hamada- Johnston nucleon-nucleon potential, Kuo and Brown¹⁻³ have derived these G matrices for use in the shell-model calculations in various regions of the Periodic Table. Their matrix elements are found to give rather satisfactory results for some standard nuclear structure calculations involving the interaction of two valance nucleons. These calculations have the obvious advantage over the conventional shell-model approach in that they do not have any adjustable parameters and the nature of the residual interaction does not remain obscure. This approach is also preferable to that pioneered by Talmi,⁴ in which the interac tion matrix elements are treated as adjustables, and where one has to decide beforehand on the number of configurations necessary to provide an adequate description of the nuclear states under consideration.

In a previous publication by Barman Roy, Raj, and Rustgi,⁵ the Kuo and Brown matrix elements⁸ were employed to perform shell-model calculawere employed to perform shell-model calcula-
tions to study the level structure of Cr^{52} and Ni^{60} .
Quasiparticle calculations for even Ni isotopes were also made. It was found that for Ni^{60} , the quasiparticle results showed tremendous improvements over the shell-model results in describing the vibrational characteristic of the second excited 2⁺ state and the branching ratio $B(E2: 3^+_1 \rightarrow 2^+_1)/$ $B(E2: 3₁⁺ + 2₂⁺)$. This has encouraged us to perform shell-model calculations to study the level structure of Sc⁴³ and Ca⁴³ assuming Ca⁴⁰ as the core,

and then the quasiparticle calculations for the oddmass Ca isotopes (Ca⁴³, Ca⁴⁵, and Ca⁴⁷).

Recently the energy-level structure of $Sc⁴³$ has been investigated by Manthuruthil, Poirier, and Walinga, 7^8 who have made unique spin assignments to a number of levels. Earlier measurements are to a number of level<mark>s. Earlier measurements ar</mark>e
reported in previous works.⁹⁻¹⁵ Theoretically the level spectrum of Sc⁴³ arising from $f_{7/2}^3$ configu ration was first calculated by McCullen, Bayman, and Zamick¹⁶ employing an effective interaction deduced from the Sc^{42} spectrum. Their approach was not very successful since it gave no low-spin level below 3-MeV excitation. Other shell-model studies have been made by Raz and Soga¹⁷ and Flowers and Johnstone.¹⁸ Malik and Scholz¹⁹ have applied the strong- coupling symmetric-rotator model, including the coriolis coupling between bands. They obtain very poor agreement for the negative-parity states, though it is good for the positive-parity states. More successful calculations have been reported by Johnstone and Payne.^{20,21} The present calculation is similar to the shell-model calculations mentioned above, though we have considered many more configurations and used the two-body reaction matrix elements reported in Ref. 3. Our calculation therefore does not have any adjustable parameters. These calculations are reported in Sec. 2.

Similar calculations are also performed for $Ca⁴³$. The resulting energy spectrum, reported in Sec. 3, agrees reasonably well with the observed one. In Sec. 4, the quasiparticle calculations for $Ca⁴³$, $Ca⁴⁵$, and $Ca⁴⁷$ are carried out in the framework of the modified Tamm-Dancoff approximation (MTDA) method. This method describes the lowlying states of odd nuclei as a superposition of one- and three-quasiparticle states, and uses a complete set of orthonormal and nonredundant quasiparticle basis states. All the working formu-

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las required for this part of the calculation are contained in an earlier work.²²

SHELL-MODEL CALCULATION OF Sc⁴³ $2.$

The two-body shell-model reaction elements. which go as the primary input data in the present shell-model calculation, are listed by Kuo and Brown.³ In deriving these matrix elements, the authors of Ref. 3 have assumed Ca⁴⁰ as the core with $0f_{7/2}$, $0f_{5/2}$, $1p_{3/2}$, $1p_{1/2}$, and $0g_{9/2}$ as the single-particle orbitals available to the nucleons outside the core, the unperturbed energies of which are listed in that paper. We have performed our calculation for two different cases. In the first case, the three extracore nucleons were distributed in all possible ways amongst the $0f_{7/2}$, $0f_{5/2}$, $1p_{3/2}$, and $1p_{1/2}$ orbitals. The dimensions of the various matrices for $J^{\pi} = \frac{1}{2}$, $\frac{3}{2}$, $\frac{5}{2}$, $\frac{7}{2}$, $\frac{9}{2}$, $\frac{11}{2}$, $\frac{13}{2}$, $\frac{15}{2}$, $\frac{17}{2}$, and $\frac{19}{2}$ are 30×30, 49×49, 61×61, 61×61, 49×49, 36×36, 23×23, 11×11, 5×5, and 2×2 , respectively. In the second case, the orbital $0g_{9/2}$ was also included, and the extracore particles were now distributed amongst $0f_{7/2}$, $0f_{5/2}$, $1p_{3/2}$, $1p_{1/2}$, and $0g_{9/2}$ orbitals in all possible ways. The dimensions of the matrices are now increased to 38×38 , 63×63 , 79×79 , 81×81 , 69×69 , 56×56 , 42×42 , 28×28 , 19×19 , and 12×12 for $J^{\pi} = \frac{1}{2}$, $\frac{3}{2}$, $\frac{5}{2}$, $\frac{7}{2}$, $\frac{9}{2}$, $\frac{11}{2}$, $\frac{13}{2}$, $\frac{15}{2}$, $\frac{17}{2}$, and $\frac{19}{2}$, respectively. In the following, these two cases will be referred to as approximations A and B, respectively.

Figure 1 shows a comparison of the experimen-

 sc^{43}

FIG. 1. Level spectrum of Sc^{43} in approximations A and B. The observed spectrum is taken from Ref. 7.

tal and calculated level spectra for Sc^{43} . It is clear that the effect of configuration mixing is to lower the low-spin states $\frac{1}{2}$, $\frac{3}{2}$, and $\frac{5}{2}$. These states did not make their appearance in the calculation of McCullen et al. below an excitation of 3 MeV. On the whole, the results of approximation A agree better with the experimental values. This is contrary to expectation but can be easily understood if one notices the large value of the reaction matrix element $\langle (0f_{7/2})^2_{0} | G | (0g_{9/2})^2_{0} \rangle_{T=1} = 2.602$ MeV. In approximation A, the lowest eigenvalue for J^{π} $=\frac{7}{2}$ is -5.98 MeV, but on the inclusion of $0g_{9/2}$ orbital, this state is pushed down to -6.66 MeV. Most of this depression is caused by the matrix element $\langle (0f_{7/2})^2 \circ |G| (0g_{9/2})^2 \circ \rangle_{T=1}$, without which the state is depressed only to -6.23 MeV. All the other states are pushed down by 0.5 MeV or less when $0g_{9/2}$ orbital is included, thus making the agreement with the experimental data worse. The large value of the matrix element $\langle (0f_{7/2})^2_{0} |G|$ $(0g_{\omega/2})^2$ ₀ γ _{r=1} arises because of the large correction $\langle (0f_{7/2})^2 \cdot (G_{8p1h})(0g_{9/2})^2 \cdot (g_{7-1})^2 = 1.984$ MeV. The reason for this large correction is not clear, except that it involves negative-parity excitations of the core.

The theoretically calculated levels can be perhaps identified with the experimental levels at: 1.18 MeV $(\frac{3}{2})$, 1.81 MeV $(\frac{1}{2}^{-}, \frac{3}{2}^{-})$, 1.83 MeV $(\frac{11}{2}^{-})$, 2.29 MeV $(\frac{5}{2}, \frac{7}{2})$, and 2.62 MeV $(\frac{9}{2}, \frac{11}{2})$. The predicted $J^{\pi} = \frac{15}{2}$, $\frac{19}{2}$ states have not been observed experimentally. The model does not reproduce the low-lying $\frac{3}{2}$ (0.47-MeV), $\frac{5}{2}$ (0.85-MeV), and $\frac{7}{2}$ (1.41-MeV) low-lying states, and it is necessary to postulate that they mainly arise from core excitations. Data from the $Ca^{42}(He^3, d)Sc^{43}$ reaction tend to support these conclusions. Johnstone and Payne^{20,21} have shown that the mixing of $(f p)^3$ states with a low-lying $K = \frac{3}{2}$ rotational band can account for the observed low-lying levels. In the present calculation, the lowest positive-parity state occurs at 9.07 MeV with $J^{\pi} = \frac{9}{5} +$.

As a test of the wave functions obtained in the calculation, the spectroscopic factors for the reaction $Ca^{42}(He^3, d)Sc^{43}$ are also calculated and are listed in Table I. The results for the Ca⁴² spectrum were checked against those given in Ref. 3. It is found that the calculated spectroscopic factors are smaller than the experimental values. This may be partly due to the various uncertainties associated with the application of the distorted-wave Born-approximation analysis as employed by Schwartz and Parker Alford,¹² and partly due to the unreliability of the wave functions, as the agreement for the level spectrum is not complete. The ground-state magnetic moment is found to be 4.42 μ_N in quite good agreement with the experimental value $(4.61 \pm 0.4)\mu_N^{10}$

The theoretical values correspond to approximation A. For the blank cases there are no corresponding theoret-
ical levels.

TABLE I. Spectroscopic factors S for Ca^{42} (He³,d)Sc⁴³.

^aSee Ref. 12. The experimental values for 1.81 and 2.²⁹ MeV are calculated from those quoted in this paper by multiplying by factors of 2 and $\frac{4}{3}$, respectively, and ignoring the j dependence of the single-particle wave functions. In their analysis, Schwartz and Alford had assumed spins of $\frac{3}{2}$ and $\frac{7}{2}$ for these levels. For Ca⁴², Kuo and Brown wave functions have been used.

3. SHELL-MODEL CALCULATION OF Ca⁴³

As for Sc^{43} , here also the calculations are carried out in two approximations, A' and B'. In approximation A', the three identical nucleons $(T=$ $\frac{3}{2}$ are distributed in all possible ways amongst the $0f_{7/2}$, $0f_{5/2}$, $1p_{3/2}$, and $1p_{1/2}$ levels, and in approximation B' , the level $0g_{9/2}$ is also included. For (i) B' , the level $0g_{9/2}$ is also included. For $\frac{1}{2}$, $\frac{3}{2}$, $\frac{5}{2}$, $\frac{7}{2}$, $\frac{9}{2}$, $\frac{11}{2}$, $\frac{13}{2}$, $\frac{15}{2}$, and $\frac{17}{2}$, the dimensions of the matrices to be diagonalized are 12×12 , 25×25 , 28×28 , 27×27 , 23×23 , 16×16 , 8 \times 8, 5 \times 5, and 1 \times 1. They increase to 16 \times 16, 32 \times 32, 37 \times 37, 37 \times 37, 33 \times 33, 26 \times 26, 17 \times 17, 13 \times 13, and 7×7 when the orbital $g_{9/2}$ is included. It is clear from Fig. ² that the effective matrix elements of Kuo and Brown reproduce the observed energy-level spectrum²³ reasonably well, though, in general, these calculated energy levels are slightly higher than the experimentally observed ones up to 1.0 MeV and slightly lower above that energy. As for Sc^{43} , here also the agreement is better in approximation A' and deteriorates contrary to expectation when $g_{9/2}$ orbital is included. This can also be understood in terms of the large value of the reaction matrix element $\langle (0f_{7/2})^2_{0} | G |$ $(0g_{9/2})^2$ ₀)_{T=1}. The inclusion of $g_{9/2}$ orbital has the effect of depressing the ground state from -2.279 to -3.005 MeV, while all other states are depressed by 0.55 MeV or less. The matrix element $\langle (0f_{7/2})^2 \rangle$ $|G| (0g_{9/2})^2_{0}$ _{r=1} alone causes a depression of 0.5 MeV in the ground state. There are observed levels corresponding to the calculated ones at 2.48 $(\frac{15}{2})$ and 2.87 $(\frac{1}{2})$ MeV, though their spins are as yet undetermined. The ground state $(\frac{7}{2})$ mainly consists of the $[(f_{7/2})^3]_{7/2}$ $\nu = 1$ configuration with nonnegligible contributions from $(f_{5/2}^20f_{7/2})$ and

FIG. 2. Level spectrum of Ca^{43} in approximations A' and B'. The observed spectrum is taken from Ref. 23.

 $(p_{3/2}^{20}q_{7/2}^{2})$ configurations. Similarly, the lowest $\frac{5}{2}$ and $\frac{3}{2}$ have large $[(f_{7/2})^3$ _{5/2,3/2} $\nu=3]$ components. The second excited $\frac{3}{2}$ level has a large $(f_{7/2}^{20} \rho_{3/2})$ component. The $\frac{1}{2}$ state has components mainly distributed amongst the $(f_{7/2}^2 p_{3/2})$ and $(f_{7/2}^2 p_{1/2})$ configurations. In their fit to calcium isotopes, Federman and Talmi⁴ use a model space consisting of $(f_{7/2}^n)$, $(f_{7/2}^n{}^{-1}p_{3/2})$ and $(f_{7/2}^n{}^{-2}p_{3/2}^n)$ configurations, whereas Engeland and Osnes²⁴ omit the latter. However, the Hamada- Johnston potential couples the $0f_{5/2}$, $1p_{1/2}$, and $0g_{9/2}$ orbits rather strongly with the $0f_{7/2}$ and $1p_{3/2}$ orbits. Thus the configuration space of $0f_{7/2}$ and $1p_{3/2}$ alone, as chosen by Federman and Talmi, would not be adequate for describing the Ca isotopes, at least when the Hamada- Johnston potential is used. In other words, the effective interactions of Talmi and Federman determined in the $0f_{7/2}$ -1 $p_{3/2}$ -model space should already have contained strong renormalization effects due to the neglect of the $0f_{5/2}$, $1p_{1/2}$, and $0g_{9/2}$ orbits. The Kuo and Brown matrix elements do not contain these renormalizations, since they include these three orbits as active orbits as well.

Table II lists the spectroscopic factors for the reaction $Ca^{42}(d,p)Ca^{43}$. Except for the ground state, the calculated spectroscopic factors are not in good agreement with the experimental values, perhaps because the calculated levels are not in perfect agreement with the experimental

6.04 0.023 3.76

approximation A' . $(2 J_f + 1)S$ $(2J_f+1)S$ J^{π} expt^a theor.

5.5 0.21 3.00

TABLE II. Spectroscopic factors for $Ca^{42}(d,p)Ca^{43}$ in

^aSee Ref. 23. For Ca⁴², Kuo and Brown wave functions have been used.

ones. The first $\frac{3}{2}$ level is too high by 0.29 MeV, and the second $\frac{3}{2}$ level is too low by 0.52 MeV. Their wave functions are, therefore, perhaps unreliable. The ground-state magnetic moment is found to be $-1.15\mu_N$, compared to the experimental value $-1.315\mu_N$.

4. OUASIPARTICLE SPECTRUM OF Ca^{43} , Ca^{45} , AND Ca^{47}

In this section we report the results of the spectra of Ca⁴³, Ca⁴⁵, and Ca⁴⁷, as obtained by applying the MTDA method. In a very restricted configuration space, shell-model calculations for these nuclei have been performed by Engeland and Osnes, and Federman and Talmi, but in the configuration space considered here such calculations become very involved for Ca⁴⁵ and Ca⁴⁷, though they can be easily carried out by the quasiparticle method. In order to predict the detailed spectrum of an odd nucleus, one has to mix one- and threequasiparticle states. The detailed method and all working formulas are given in Ref. 22. Only some of the relevant formulas are given below.

The chemical potential λ and the energy-gap parameter Δ_{a} are obtained by solving the BCS equations

$$
\Delta_a = \frac{1}{4} \sum_{b} \left(\frac{2b+1}{2a+1} \right)^{1/2} \left[G \left(aabb0 \right) / E_b \right] \Delta_b, \tag{1}
$$

and

$$
N = \frac{1}{2} \sum_{a} \left(2a + 1\right) \left(1 - \frac{\hat{\epsilon}_a - \lambda}{E_a}\right) + \frac{(\hat{\epsilon}_j - \lambda)}{E_j} \,. \tag{2}
$$

Here, N is the actual number of nucleons (neutrons in our case) present in the unfilled major shell, $\hat{\epsilon}_a$ is the single-particle energy corrected for self-energy, and $G(abcdJ)$ is the antisymmetric two-body matrix element for total angular momentum J. The quasiparticle energy E_a is given by

$$
E_a = [(\hat{\epsilon}_a - \lambda)^2 + \Delta_a^2]^{1/2}
$$

The probability of occupancy $V_a^{\;\;2}$ and nonoccu The probability of occupancy v_a and honoccupancy U_a^2 of a given state a are determined from

$$
U_a^2 = \frac{1}{2} \left[1 + (\hat{\epsilon}_a - \lambda) / E_a \right], \tag{3}
$$

and

$$
V_a{}^2 = 1 - U_a{}^2. \tag{4}
$$

The energy matrix to be diagonalized may be written as

$$
\binom{E\quad S}{S\quad L+E'}
$$

where E and E' are the unperturbed energies of one- and three-quasiparticle states, L is the matrix connecting the three-quasiparticle subspaces, while S connects one- and three-quasiparticle subspaces. The explicit expression for the matrices S and L are contained in Ref. 22.

The effect of including the correlations in the

TABLE III. Experimental and calculated energies (in MeV) of Ca^{43} . The entries under KB and TP give the results obtained by the quasiparticle method using the two-body reaction matrix elements of Kuo and Brown, and of the Tabakin potential, respectively, and the numbers in the parentheses denote the percentage admixture of the one-quasiparticle state. The column SM gives the energies calculated by the shell-model method employing the KB two-body matrix elements.

		TP						
J^{π}	Expt	SM	ΚB	Without G_{2h}	With G_{2h}	a	b	
$7/2^-$	0.00	0.00	0.00(97,82)	0.00(96.15)	0.00(96.44)	0.00	0.00	
$5/2^{-}$	0.37	0.46	0.76(0.23)	0.49(0.71)	0.71(0.70)	0.30	0.410	
$3/2^{-}$	0.59	0.88	1,26(1,20)	1,02(0.09)	1.23(4.10)	0.60	0.645	
3/2,7	2.05	1.53	1.54(92.69)	1.49(89.62)	1.45(87.97)	2.10	2.094	
$11/2^-$	1.68	1.59	1.83	1.69	1.98	1.93	1.743	
$9/2^-$	2.10	1.79	2.00	1.97	2.27	2.08	2.049	
$15/2^{-}$			2.78	2.74	3.11			
$1/2^{-}$			2.90(43.42)	2,81(32,81)	2,95(45,69)			

^aResults of Ref. 4.

^bResults of Ref. 24.

 $7/27$ $3/27$ $3/2₂$

 $\overline{1}$

ground state changes the spectrum only slightly and has not been considered here. The numerical calculations are carried out using the reaction matrix elements of Hamada-Johnston as mell as Tabakin nucleon-nucleon potentials. In addition to the contribution of the 3-particle-1-hole term (G_{sub}) , the Tabakin matrix elements also include the G_{2h} term. The results indicated in Table III show that there is reasonably good agreement between the shell-model results and the MTDA results for Ca for the different sets of matrix elements. The number of particles in the unfilled levels considered in this case is only three, and the quasiparticle method is not expected to yield very good quantitative results for this nucleus; therefore, such an agreement should be taken as an indication about the reliability of the approximations involved in the quasiparticle method. A similar agreement should be expected in Ca^{45} and Ca^{47} . However, in the quasiparticle spectrum for $Ca⁴⁵$ (see Table IV), the energy of the first excited state is relatively high, and the ordering of the levels is not tively high, and the ordering of the levels is not reproduced. In Ca^{47} (see Table V), the energy of the first excited state $J^{\pi} = \frac{3}{2}$ is relatively too low.

In all the cases, the ground state is predominantly of the one-quasiparticle type. In Ca⁴³ the first $\frac{5}{2}$ and $\frac{3}{2}$ states are practically of the three-quasiparticle type. This is purely the effect of configuration mixing, because of which these three-quasiparticle states are pushed much lower than their predominantly one-quasiparticle states. In $Ca⁴⁵$, the first excited $\frac{5}{2}$ state is of the three-quasiparticle type but the first $\frac{3}{2}$ state is of the one-quasiparticle type out the n_{B} is state is of the one-quase. lowest excited $\frac{3}{2}$ and $\frac{1}{2}$ states are predominantly of the one-quasiparticle type. Experimentally, very few levels are known in $Ca⁴⁵$ and $Ca⁴⁷$, and therefore no comments are made about the other levels.

In general, the calculated excitation energies of the few low-lying states by the MTDA method are high compared to the observed ones except in Ca⁴⁷. The observed energies of the first excited states in Ca⁴³ and Ca⁴⁵ are quite low $(0.37 \text{ MeV} \text{ in Ca})$ and 0.18 MeV in Ca^{45} , but comparatively too high in Ca⁴⁷ (\simeq 2.01 MeV). The quasiparticle theory is unlikely to explain such a change, since it describes only the average property of the neighbor-

TABLE IV. Experimental and calculated energies (in MeV) of Ca⁴⁵. For other details see caption of Table III.

				TP		
J^{π}	Expt	KВ	Without G_{2h}	With G_{2h}	а	$\mathbf b$
$7/2^{-}$	0.00	0.00(95.80)	0.00(93.59)	0.00(93.77)	0.00	0.00
$5/2^-$	0.18	1.06(0.11)	0.85(0.36)	1.07(0.35)	0.20	0.195
$3/2^-$	(1, 43)	0.90(88.99)	0.83(80.41)	0.72(85.00)	1.41	
$3/2^{2}$	(1.90)	1,59(4,06)	$1,48$ ($9,02$)	1.65(6.48)	1.93	
$11/2^-$		2.11	2.01	2.32		
$9/2^-$		2.26	2.21	2.51		
$1/2^{-}$		2.40 (57.37)	2,40(49,56)	2,42(63,07)		
$3/2_{3}^{-}$		2,84(3,16)	$2,88$ ($3,83$)	3.15(2.41)		
$7/2^{2}$		2,96(1,57)	2.78(3.49)	2,93(3,36)		

^aResults of Ref. 4.

 b Results of Ref. 24.

TABLE V. Experimental and calculated energies (in MeV) of Ca^{47} . For other details see caption of Table III.

	TP						
J^{π}	Expt	KВ	Without G_{2h}	With G_{2h}	a	b	
$7/2^{-}$	0.00	0.00(94.05)	0.00(91.40)	0.09(91.35)	0.00	0.00	
$3/2^-$	2.01	0.10(92.71)	0.07(87.76)	0.00(88.66)	2.06	1.943	
$1/2^{-}$		1.80(85.36)	1.92(78.73)	1,85(83,98)			
$5/2^-$		1.82(0.00)	1.62(0.01)	1.85(0.04)			
$3/2^{2}$		2.05(2.65)	1.91(4.71)	2.01(4.19)			
$7/2$ ₂		2.77(2.45)	2.68(4.28)	2.81(4.50)			
$5/2$ ₂		2.79(0.01)	2.71(0.05)	2,80(0,40)			
$11/2^-$		2.85	2.76	3.07			
$9/2^-$		2.88	2.73	2.96			
$3/2_{3}^{-}$		2,93(0,12)	3.00(0.01)	3.27(0.09)			

^aResults from Ref. 4.

^bResults from Ref. 24.

ing nuclei. This is further borne out by the fact that for even Ni isotopes, where such large fluctuations in the energies of the first excited states are not observed, the quasiparticle method gives a good description of the first few excited states.⁵

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