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Effective interactions and energy spectra for $N = 28, 29$ and 30 nuclei†

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Abstract. A two-range central-plus-tensor potential is assumed for the effective nucleon-nucleon interactions in the shell-model calculation of $N = 28, 29$ and 30 isotones. A model space of $[[f_{7/2}^{-1}, (p_{3/2}, p_{1/2}, f_{5/2})]]$ is assumed for the proton configuration of $N = 28$ nuclei. The correct isospin wavefunctions proposed by Osnes are considered. For $N = 29$ and 30 nuclei, the protons are restricted to the $1f_{7/2}$ orbit, and the valence neutrons are allowed to distribute in the $2p_{3/2}, 2p_{1/2}$ and $1f_{5/2}$ shells. Energy level spectra for $N = 28, 29$ and 30 nuclei are calculated in a Talmi-type calculation. The calculated results are in good agreement with the experimental observations.

1. Introduction

In recent years, numerous shell-model calculations have been performed with considerable success on the $N = 28, 29$ and 30 isotones. Different effective interactions were obtained for each of these regions. Osnes (1970) studied the $N = 28$ nuclei with the consideration of correct isospin states. In his calculation, the two-nucleon matrix elements entering the description of the $N = 28$ nuclei also describe uniquely the $N = 29$ nuclei in their lowest configuration. It should be interesting to extend the work of Osnes to investigate the possibility that the energy spectra of $N = 28, 29$ and 30 isotones can be described by a single effective interaction.

A few years ago the energy spectra of the $N = 28$ isotones were calculated by Auerbach (1967) and Lips and McEllistrem (1970) within the proton $f_{7/2}^n$ and $f_{7/2}^{n-1}, p_{3/2}$ configurations outside a ^{48}Ca core. The latter authors also included the $(f_{7/2}^{n-1}, f_{5/2})$ configuration. Considerable improvement over the pure configuration of previous works (Edmonds and Flowers 1952, Lawson and Uretsky 1957, Talmi and Unna 1960, McCullen *et al* 1964) was obtained. Despite the success of the above works, the calculated states do not have definite isospin. Osnes and Warke (1970) constructed good isospin states in the $(f_{7/2})^n$ and $(f_{7/2}^{n-1}, p_{3/2})$ configuration. The inclusion of correct isospin states would introduce several new parameters, namely proton-neutron and neutron-neutron matrix elements. These additional interaction matrix elements can be expanded in terms of the proton-proton matrix elements and the proton-neutron matrix elements $\langle \pi f_{7/2} \nu p_{3/2} | V | \pi f_{7/2} \nu p_{3/2} \rangle_J$, which describe completely the $N = 29$ isotones in their lowest configuration.

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It was shown in previous calculations (Ohnuma 1966, Horie and Ogawa 1971) that the configuration intensities of the wavefunctions for the low-lying states of $N = 29$ nuclei are concentrated in the $|\pi f_{7/2}^n, \nu j\rangle$ configuration, where $j = p_{3/2}, p_{1/2}$ and $f_{5/2}$. With this model space, good agreement with the experimental results can be obtained for a large number of energy levels and spectroscopic factors. Therefore, for $N = 29$ isotones, we restrict the protons to the $f_{7/2}$ shell and allow the extra core neutron to occupy the $p_{3/2}, p_{1/2}$ and $f_{5/2}$ shells. For $N = 30$ isotones, previous calculations also assumed ^{48}Ca as an inert core. The protons are also restricted to the $f_{7/2}$ shell, and the two extra core neutrons are distributed in the $p_{3/2}, p_{1/2}$ and $f_{5/2}$ shells. In the work of McGrory (1967) for $N = 30$ nuclei the proton-proton interaction is taken from spectroscopic data and the neutron-neutron interaction is taken from the shell-model calculation of the Ni isotopes by Cohen *et al* (1967). The proton-neutron interaction is assumed to be the delta function introduced by Vervier (1966). Later, Horie and Ogawa (1973) performed a similar calculation on $N = 30$ isotones, but they used the best-fit matrix elements of $N = 29$ nuclei for the proton-neutron interaction. As indicated above, the effective proton-proton, proton-neutron and neutron-neutron interactions in $N = 30$ nuclei are adopted from different sources and the physical implications of the interactions are somewhat ambiguous. This is mainly because the number of reliable experimental energy levels for $N = 30$ isotones is not very great, thus making a Talmi-type calculation for the $N = 30$ isotones rather difficult.

In a rather extensive analysis of the data over the entire nuclear chart, Schiffer and True (1976) have found a similarity exists in the 'angular distributions' and the multipole coefficients of the effective two-body interactions of different multiplets. This remarkable discovery suggests the possibility that the energy spectra of the nuclei in different regions might be explained by a single effective interaction. Therefore, it is our purpose to investigate the possibility that the energy spectra of $N = 28, 29$ and 30 isotones can be explained simultaneously by a single effective interaction. In the meanwhile, we also wish to extend the work of Osnes (1970) to include the proton excitation to the $p_{1/2}$ and $f_{5/2}$ orbits for the $N = 28$ isotones.

2. Assumption

In the present work, we analyse the effective interaction by investigating the low-lying states of nuclei with $N = 28, 22 \leq Z \leq 26, N = 29$ and 30 with $21 \leq Z \leq 27$. As indicated above, a ^{48}Ca inert core is assumed. For $N = 28$ isotones, the protons are restricted to the $[f_{7/2}^{-1}(p_{3/2}, p_{1/2}, f_{5/2})]$ configuration with good isospin correction. In $N = 29$ and 30 nuclei the protons are restricted to the $f_{7/2}$ shell only, while the extra core neutrons are allowed to occupy the $p_{3/2}, p_{1/2}$ and $f_{5/2}$ orbits. Under these assumptions, the wavefunctions of states for $N = 28, 29$ and 30 nuclei can be written as linear combinations of basic states of the form

$$\Psi_1^J = |\pi f_{7/2}^n \rangle_J \quad \text{or} \quad |\pi f_{7/2}^{n-1}, j \rangle_J$$

where $j = p_{3/2}, p_{1/2}$ or $f_{5/2}$ for $N = 28$,

$$\Psi_2^J = |(\pi f_{7/2}^{Z-20}) J_\pi, \nu j_1 \rangle_J$$

where $j_1 = p_{3/2}, p_{1/2}$ or $f_{5/2}$ for $N = 29$ and

$$\Psi_3^J = |(\pi f_{7/2}^{Z-20}) J_\pi, (\nu j_1 \times \nu j_2) J_\nu \rangle_J$$

where $j_1, j_2 = p_{3/2}, p_{1/2}$ of $f_{5/2}$ for $N = 30$. The Hamiltonian in this space then has the form

$$H = H_0 + H_{pp} + H_{pn} + H_{nn}$$

where H_0 is the single-particle Hamiltonian which includes

$$\epsilon_n(2p_{3/2}) = 3.32 \text{ MeV} \quad \epsilon_n(2p_{1/2}) = 5.35 \text{ MeV} \quad \epsilon_n(1f_{5/2}) = 7.31 \text{ MeV}$$

for the neutron states (these values are taken from the neutron separation energies of ^{49}Ca) and

$$\epsilon_p(1f_{7/2}) = 0.0 \text{ MeV}$$

for the protons. For $N = 28$ proton single-particle energies we use $\epsilon_n(j)$ values but with corrections for the symmetry energy between neutrons and protons and the Coulomb displacement energy. H_{pp}, H_{pn} and H_{nn} represent the interactions between the $1f_{7/2}$ protons, the protons and the neutrons outside the ^{48}Ca core and the neutrons in the $2p_{3/2}, 2p_{1/2}$ and $1f_{5/2}$ shells respectively. In practical calculations, the effective interactions between the identical nucleons (i.e. proton-proton and neutron-neutron interactions) and those between the non-identical nucleons (i.e. proton-neutron interactions) are assumed to be the same for all nuclei and the single-particle energies are kept constant throughout the calculation. For the residual interaction a two-range central-plus-tensor potential proposed by Schiffer and True is used. The radial part of the potential is taken to be of Yukawa type with the interaction ranges $r_0 = 1.415 \text{ fm}$ and $r_1 = 2.0 \text{ fm}$. These values for the interaction ranges are also used in the recent work of Schiffer and True (1976). Harmonic oscillator wavefunctions with oscillator constant $\nu = 0.96A^{-1/3} \text{ fm}^{-2}$ are used and an average value of $A = 50$ is assumed. In this way, the effective interaction between the nucleons has the same form for all $N = 28, 29$ and 30 nuclei. With this prescription, the interaction strengths of the central $T = 0$, singlet-odd (CSO), triplet-even (CTE), and $T = 1$, singlet-even (CSE), triplet-odd (CTO) components and the tensor-even (TTE), tensor-odd (TTO) components of both ranges are considered as free parameters. Since the results of the least-squares fit are not sensitive to the long-range tensor-even and tensor-odd components, we therefore set these two components to be zero and leave only ten parameters in the least-squares-fit calculation for 92 observed energy levels of the low-lying states of $N = 28, 29$ and 30 nuclei. In order to avoid the core-polarisation effect, we select only the excitation energies of those levels which can be accounted for by our model spaces. $N = 28$ nuclei with proton number up to 6 and $N = 29$ and 30 nuclei with proton number up to 7 are considered in the calculation. With these criteria, 23, 35 and 34 low-lying levels are selected respectively for $N = 28, 29$ and 30 nuclei. The total RMS deviation for the least-squares fit is 0.216 MeV .

3. Results

3.1. Effective interaction

The best-fit interaction strengths obtained from the least-squares fit are listed in table 1. The strengths obtained by Schiffer and True (1976) are also displayed in the last column. The third, sixth, ninth and twelfth rows give the ratios of the short-range to long-range components of CSO, CTE, CSE and CTO respectively. The strengths

Table 1. Strengths (in MeV) and relative ratios of the best-fit potential parameters compared with those of Schiffer and True (ST).

		This work	ST
CSO	short	59.96	37.62
	long	-73.97	-36.37
	ratio	1.23	0.97
CTE	short	-44.97	-35.39
	long	37.99	22.25
	ratio	0.85	0.63
CSE	short	-22.45	-14.78
	long	21.76	12.68
	ratio	0.97	0.86
CTO	short	-98.41	-46.69
	long	112.06	50.87
	ratio	1.14	1.09
TTE	short	-3.89	-12.74
TTO	short	-6.09	-1.83

of CSE, CTE, TTE and TTO components for both ranges are similar to those of Schiffer and True. The strengths of the long-range component of CSO and the short-range component of CSE are found to be more attractive, and the strengths of the short-range component of CSO and the long-range component of CTO are found to be more repulsive, than those of Schiffer and True. The reason for this may be that we restrict the protons to the $f_{7/2}$ shell only and neglect the effect of excitation to $2p_{3/2}$, $2p_{1/2}$ and $1f_{5/2}$ proton orbits for $N = 29$ and 30 isotones. In the calculations of the E2 properties of ^{48}Ti , Lesser *et al* (1972) found that the inclusion of the configuration of excitation of one proton from $(f_{7/2})^n$ to upper orbits produced better results than if this excitation effect was omitted. In fact, we have performed a calculation which includes one- and two-proton excitations to the $2p_{1/2}$ and $1f_{5/2}$ shells for $N = 28$ isotones and found that the strengths of the effective interactions get closer to the values obtained by Schiffer and True when two-proton excitations are taken into account (Chuu *et al* 1978). If we consider the ratios only, then table 1 shows that our results give quite similar values to those obtained by Schiffer and True.

Table 2. Proton-proton two-body matrix elements in the $1f_{7/2}$ or $2p_{3/2}$ orbit.

$2j_1$	$2j_2$	$2j_3$	$2j_4$	J	This work	KB'	KB
7	7	7	7	0	-2.448	-2.11	-1.81
				2	-0.884	-1.11	-0.78
				4	-0.047	-0.10	-0.09
				6	0.380	0.23	0.23
7	3	7	3	2	-0.766	-0.56	-0.86
				3	0.096	0.25	-0.03
				4	0.371	0.28	-0.05
				5	0.373	0.49	0.15
7	7	7	3	2	-0.337	-0.50	-0.50
				4	-0.254	-0.31	-0.31

Table 3. Two-body matrix elements of the proton in the $1f_{7/2}$ and the neutron in the $2p_{3/2}, 2p_{1/2}$ or $1f_{5/2}$ orbits.

$2j_1$	$2j_2$	$2j_3$	$2j_4$	J	This work	HO
7	1	7	1	3	-0.841	-0.760
				4	-0.638	-0.695
7	1	7	3	3	-0.694	-0.536
				4	0.510	0.202
7	1	7	5	3	-0.444	-0.866
				4	-0.503	-0.602
7	3	7	3	2	-1.096	-0.787
				3	-0.788	-0.444
				4	-0.028	-0.141
				5	-1.076	-1.026
				2	0.532	0.294
7	3	7	5	3	-0.238	0.306
				4	0.164	0.034
				5	-0.309	-0.074
				1	-3.146	-2.544
7	5	7	5	2	-1.640	-1.430
				3	-0.674	-0.592
				4	-0.844	-1.336
				5	-0.209	-0.005
				6	-1.725	-1.345

Tables 2 and 3 display the most important two-body matrix elements of the proton-proton interaction and the proton-neutron interaction respectively. The column entitled KB' lists the modified Kuo-Brown two-body matrix elements obtained by McGrory *et al* (1970) for the energy spectra of calcium isotopes. Column KB represents the two-body matrix elements calculated by Kuo and Brown (1968) using the Hamada-Johnston potential. Column HO shows the proton-neutron interaction matrix elements calculated by Horie and Ogawa (1971) for the $N = 29$ nuclei. As indicated in the tables, all studies give almost the same results. This fact exhibits the reasonable results of our effective interactions.

3.2. Energy levels

As indicated above, we include for each nucleus in this calculation all the available low-lying excited states with reliable J^π assignments which may be accounted for in our model space in the least-squares fit. Those levels that could not be reproduced in previous shell-model calculations with the same model space are also excluded here. The calculated energy spectra for $N = 28$ nuclei, $22 \leq Z \leq 26$, are presented in figure 1. The experimental values are also shown for comparison. The gross features of the predicted energy spectra are in satisfactory agreement with the observed values. For ^{51}V , no conclusive J^π assignment has been made for the state at 2.7 MeV. However, studies on the γ -ray angular distribution (Poletti *et al* 1974a) strongly suggest the assignment $J^\pi = \frac{1}{2}^{\pm}$ for this state and our calculated level of $J^\pi = \frac{1}{2}^{\pm}$ at 2.66 MeV gives favourable support to this observation. For ^{52}Cr , two states of $J^\pi = 2^+$ and 4^+ are produced. The first 2^+ state is mainly seniority 2 with an intensity of 96% and the second 2^+ state is mainly seniority 4 with an intensity of 97%. This is consistent with the conclusions of previous results (Talmi 1962, Komoda 1964). For the lower 4^+ state, there is a large seniority mixing for $v = 2$ and 4

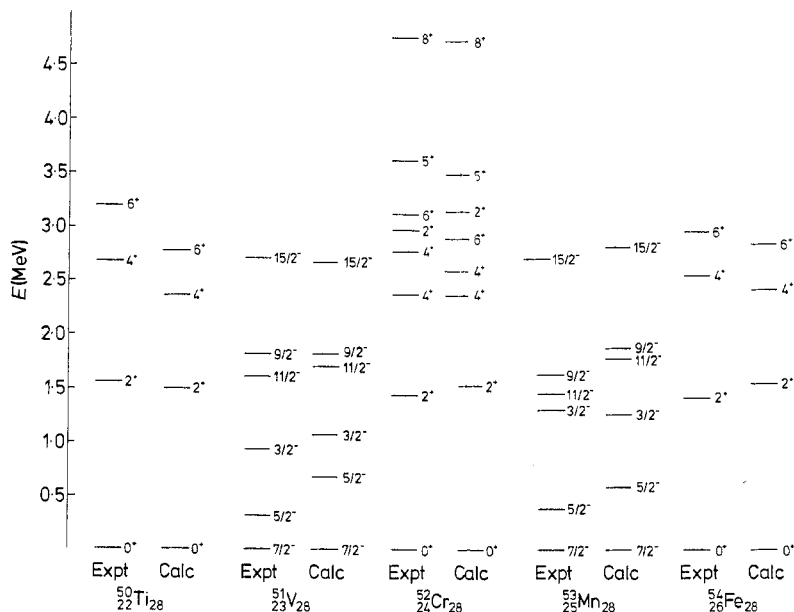


Figure 1. Calculated and experimental energy spectra for $N = 28$ isotones.

of the $f_{7/2}^4$ configuration with intensities of 50% and 45% respectively. For the upper 4^+ state, $v = 2$ and $v = 4$ components have intensities of 47% and 51% respectively. It can be shown that the seniority mixing cannot be accounted for when a pure $(f_{7/2})^n$ model space is considered provided that a same-type interaction is considered. The seniority mixings increase as the model space is enlarged from $(f_{7/2})^n$ to $(f_{7/2}^{-1}, p_{3/2})$. However, large seniority mixings can be obtained only for the cases when isospin is taken into account correctly. Federman and Talmi (1965) have shown that seniority mixing exists in the 4^+ states, and the main component is $v = 4$ for the

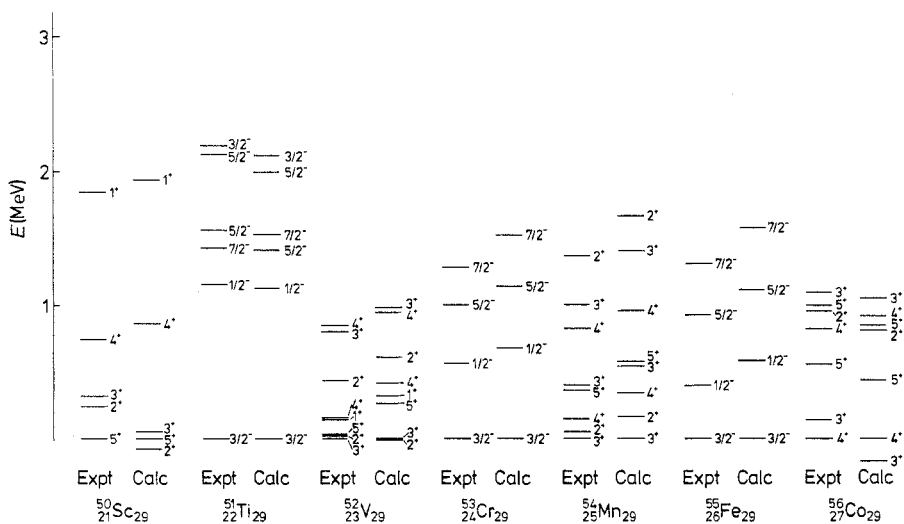


Figure 2. Calculated and experimental energy spectra for $N = 29$ isotones.

lower state and $v = 2$ for the higher state. It has been shown (Chuu *et al* 1978) that this seniority inversion can be produced if the model space is enlarged to include two-proton excitations. The 4.75 MeV level of ^{52}Cr can be reproduced quite well. In fact, Poletti *et al* (1974b) have identified a spin assignment of $J^\pi = 8^+$ for this level from the investigation of the γ transition in the reaction $^{51}\text{V}(^7\text{Li}, \alpha 2n)^{52}\text{Cr}$. Our calculated 8^+ level at 4.72 MeV agrees strikingly well with the observed value and suggests that this level is a pure $(1f_{7/2})^4$ state (99%).

In figure 2, the calculated energy levels of $N = 29$ isotones are compared with the experimental ones. For odd-mass isotones, the agreement between the observed and calculated levels is satisfactory. For these nuclei, the ground states are $J^\pi = \frac{3}{2}^-$, and excitation states of $J^\pi = \frac{1}{2}^-$, $\frac{5}{2}^-$ and $\frac{7}{2}^-$ lie just above these ground states. The results of our calculation show that the lowest $J^\pi = \frac{3}{2}^-$ and $\frac{7}{2}^-$ levels are of almost single-particle nature, i.e. the wavefunctions have predominant components of $|J_p = 0; \nu p_{3/2}\rangle_{J=3/2}$ and $|v = 2, J_p = 2; \nu p_{3/2}\rangle_{J=7/2}$. For the lowest $\frac{1}{2}^-$ levels, the wavefunctions are composed mainly of the admixture of $|J_p = 0; \nu p_{1/2}\rangle_{J=1/2}$ and $|v = 2; J_p = 2; \nu p_{3/2}\rangle_{J=1/2}$. In the lowest $\frac{5}{2}^-$ states, the wavefunction contains a predominant component of $|J_p = 2; \nu p_{3/2}\rangle_{J=5/2}$ in ^{51}Ti , but shifts to the $|J_p = 0; \nu f_{5/2}\rangle_{J=5/2}$ component in ^{55}Fe . The low-lying levels of even-mass isotones do not possess this similarity. The lowest $J = 5^+, 2^+, 3^+$ and 4^+ states in ^{50}Sc are almost pure $|\pi f_{7/2}, \nu p_{3/2}\rangle$. For ^{52}V and ^{54}Mn , the wavefunctions are in general admixtures of different components except for the lowest $J = 5^+$ state and the ground state of both nuclei and the lowest 4^+ state of ^{54}Mn . The intensities of the $|J_p = \frac{7}{2}, \nu p_{3/2}\rangle_{J=5}$ components for the lowest $J = 5^+$ states of ^{52}V and ^{54}Mn are more than 87% and 79% respectively and the $|J_p = \frac{7}{2}, \nu p_{3/2}\rangle_{J=3}$ components for the ground state of ^{52}V and ^{54}Mn are more than 68% and 63% respectively. The component $|J_p = \frac{7}{2}, \nu p_{3/2}\rangle_{J=4}$ for the state $J = 4^+$ of ^{54}Mn has an intensity of 69%. For ^{56}Co , the dominant component in the lowest $J = 2^+, 3^+, 4^+$ states is $|\pi(f_{7/2}^-); \nu p_{3/2}\rangle_J$ with an intensity of more than 90%, except the lowest 2^+ state which has an intensity of 61%.

For $N = 30$ isotones, the general features of level ordering and the agreement between calculated and observed energy levels are satisfactory. The results are presented in figure 3. Levels marked with an asterisk are excluded from the least-squares fit. For ^{51}Sc , the level ordering is in good agreement with the observed one. The ground-state $\frac{7}{2}^-$ is found to be almost a single $f_{7/2}$ proton state, i.e. the wavefunction has the predominant component $|J_p = \frac{7}{2}, J_n = 0\rangle_{J=7/2}$. The lowest $\frac{3}{2}^-$ and $\frac{1}{2}^-$ levels are found to possess the predominant component $|J_p = \frac{7}{2}, J_n = 2\rangle_J$. These two levels are in satisfactory agreement with the corresponding experimental ones. A larger discrepancy occurs in the lowest $\frac{1}{2}^-$ state. It is found that the $\frac{1}{2}^-$ state has the predominant component $|J_p = \frac{7}{2}, \nu(p_{3/2}, f_{5/2})J_n = 4\rangle_{J=1/2}$. This larger discrepancy may be due to the following reason. Since there is only one proton state with $J_p = \frac{7}{2}^-$ in the nucleus of ^{51}Sc , in order to form a $J = \frac{1}{2}^-$ state, one must couple a $f_{5/2}$ neutron and a $p_{3/2}$ neutron to either $J_p = 3$ or 4 . Such states are much too high in energy in this calculation to account for the level at 2.33 MeV. The second $\frac{3}{2}^-$ state, which is not well reproduced, also possesses the predominant component $|J_p = \frac{7}{2}, \nu(p_{3/2}, f_{5/2})J_n = 4\rangle_{J=3/2}$. Therefore the discrepancy may be due to a similar reason as that for the $J = \frac{1}{2}^-$ state. These large discrepancies would be reduced if we took the proton excitation from the $f_{7/2}$ orbit to the upper orbits into account. The strong excitations to the lower two levels in the $^{48}\text{Ca}(d, p)^{51}\text{Sc}$ reaction also seem to suggest the necessity of including the $(p_{3/2}, p_{1/2}, f_{5/2})^3$ configuration for higher

One of the interesting features known experimentally is that among nuclei lying in the f - p shell region, ^{56}Fe has the largest prolate deformation in its ground state, and the first 2^+ (0.857 MeV) and 4^+ (2.095 MeV) states can be understood as members of the ground-state quasirotational band (Lesser *et al* 1972). In order to compare our results with the prediction given by the rotational model, we plot the calculated energies of the lowest levels for each even- J state as a function of $J(J+1)$ for ^{52}Ti , ^{54}Cr and ^{56}Fe . Our calculated values for these states presented in figure 4 agree satisfactorily with the results of Horie and Ogawa (1973) and Bendjaballah *et al* (1977). It is found that the curve for ^{52}Ti is not linear, but those for ^{54}Cr and ^{56}Fe become almost linear. Therefore, the calculated spectra in ^{54}Cr and ^{56}Fe resemble the ground-state band spectra of deformed nuclei (Sakai 1967). The appearance of a rotation-like spectrum in ^{56}Fe (two proton hole-two neutron system) but not in ^{52}Ti (two proton-two neutron system) is because a rotational spectrum is apt to appear when proton and neutron systems have the same kind of deformation (Tanaka *et al* 1971).

4. Summary and conclusion

The $N = 28, 29$ and 30 nuclei are described by the shell model based upon the assumption that the ^{48}Ca nucleus is an inert core. One-proton excitation from the $f_{7/2}$ orbit to $(p_{3/2}, p_{1/2}, f_{5/2})$ is allowed for the $N = 28$ isotones. The correct isospin consideration proposed by Osnes is considered for these nuclei. For $N = 29$ and 30 isotones, the extra core protons are restricted in the $f_{7/2}$ orbit, and the extra core neutrons are allowed to distribute between the $p_{3/2}, p_{1/2}$ and $f_{5/2}$ orbits. The effective two-body n - n , p - p and p - n interactions are assumed to be the two-range

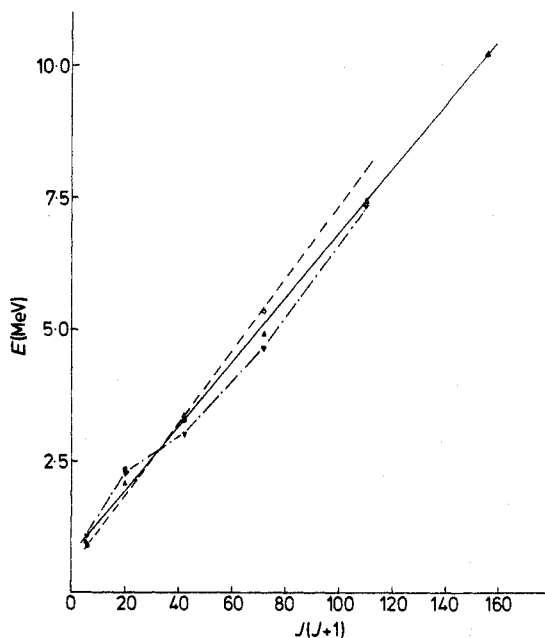


Figure 4. Calculated energies of the yrast even- J states as a function of $J(J+1)$. \blacktriangledown , chain curve, $^{52}\text{Ti}_{30}$; \triangle , full curve, $^{54}\text{Cr}_{30}$; \circ , broken curve, $^{56}\text{Fe}_{30}$.

central-plus-tensor potential proposed by Schiffer and True. Ninety-two reliable energy levels are selected in a Talmi-type calculation to determine the ten residual interaction strengths. The general features of the calculated level spectra agree satisfactorily with the experimental results. The overall RMS deviation is 0.216 MeV. The effective interactions obtained are used to calculate the two-body matrix elements for identical and non-identical nucleons. The results are in satisfactory agreement with those of previous works.

The large seniority mixture displayed in the calculated 4^+ states in ^{52}Cr shows the importance of the consideration of good isospin. The inversion of the seniority order of 4^+ states in ^{52}Cr cannot be obtained in this work. However, it was shown in another work that this may be reached if two protons are allowed to excite to the $(p_{3/2}, p_{1/2}, f_{5/2})$ orbits, i.e. if the model space for $N = 28$ is enlarged from $(f_{7/2})^{n-1}(p_{3/2}, p_{1/2}, f_{5/2})$ to $(f_{7/2})^{n-2}(p_{3/2}, p_{1/2}, f_{5/2})^2$ (Chuu *et al* 1978). The rotation-like spectrum appears in ^{54}Cr and ^{56}Fe , but does not appear in ^{52}Ti . This may be explained by the difference in deformation of the proton wavefunctions between these three nuclei. The failure in describing most of the low-lying levels of ^{51}Sc and ^{57}Co is probably due to the neglect of the proton excitation from $f_{7/2}$ to other higher orbits.

In conclusion, our calculation shows that a single effective interaction of a two-range central-plus-tensor potential can be used to explain simultaneously the energy spectra of the $N = 28, 29$ and 30 isotones provided that enough model spaces are taken into account.

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