Effective interactions, Coulomb displacements, and separation energies for $N = 50$ and $N = 28$ isotones*

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Effective interactions for $N = 50$ and $N = 28$ isotones are obtained by fitting the low-lying excited levels. Coulomb displacements and separation energies are deduced directly from the difference of observed and calculated binding energies.

[NUCLEAR STRUCTURE $N = 50$ and $N = 28$; calculated effective interactions, deduced Coulomb displacements and separation energies.]

It is well known that the Coulomb displacement energy exists only between the binding energies of the ground states for two neighboring mirror nuclei, whereas the J^π assignments and the energy spacings of the excited states remain almost the same. Similar situations exist in the isobaric analog states in medium and heavy nuclei. In fact, the effective interaction adopted in the calculation of energy spectra by the conventional shell model is not presumed to represent the kind of nucleon being studied. The distinction between the p-p, p-n, or n-n interactions exists in the consideration of different isobaric spin among two-body matrix elements of the effective interaction.

Recently, Ball *et al.*[1] and Gloeckner and Serduke[2] calculated the $N = 50$ isotones by treating ^{88}Sr as an inert closed shell. Lips and McEllistrem[3] investigated the $N = 28$ isotones by shell-model calculation with the ^{48}Ca nucleus assumed to be an inert core. All these studies employed the least-squares fit in their calculation of binding energies and treated the two-body matrix elements as adjustable parameters. Since the experimental values of Coulomb displacement energies are not complete for $N = 50$ and $N = 28$ isotones, the observed binding energies, adopted in the above works, still include the effect due to Coulomb repulsion.

The purpose of this paper is to discuss the different aspects which exist in the shell-model calculation of binding energies by the least-squares fit when binding energies of the ground states are included in the fitting (henceforth referred to as model I) or excluded from the fitting (referred to as model II). These may be analyzed from the following three considerations: (i) reliability of the effective interaction obtained from the fitting, (ii) explanation of the Coulomb displacement and separation energy, and (iii) reasonableness of the obtained wave functions. For $N = 50$ isotones, direct comparison between calculated p-p and n-n interactions is not available. However, the reaction matrix elements for the $1f$-$2p$ shell nuclei[4] provide us with the necessary information for comparison. From the above comparisons, the effect of Coulomb repulsion may be investigated. For $N = 28$ isotones, the investigations (i) and (ii) can be reached by direct comparison between the calculated two-body matrix elements for p-p interaction and those for n-n interaction obtained by McGrory *et al.*[5] for Ca isotopes.

Ball *et al.*[1] and Gloeckner and Serduke[2] calculated the $N = 50$ isotones by assuming ^{88}Sr as an inert core with $Z - 38$ protons being distributed in the $2p_{1/2}$ and $1g_{9/2}$ shells. Two single-particle energies for $2p_{1/2}$ and $1g_{9/2}$ orbits and nine two-body matrix elements are treated as adjustable parameters to fit to the binding energies of the ground states and low-lying excited energies for nuclei of $N = 50$, $39 \leq Z \leq 44$. Both of these studies obtained almost the same results.

Therefore, it is only necessary to compare the results obtained in the present study with one of the above studies. In our calculation, ^{88}Sr is assumed to be an inert core and the model space is still assumed to be $2p_{1/2}$ and $1g_{9/2}$ orbits. In the model I calculation, 6 binding energies of the ground states and 49 excitation energies, except the 3^- state in ^{92}Mo and the excited 0^+ state in ^{94}Ru, are included in the least-squares fit. In the model II calculation, we include only the excitation energies in the least-squares fit. The resulting rms deviations are 0.100 MeV for model I and 0.085 Mev for model II. The calculated two-body matrix elements and single-particle energies for

TABLE I. Comparison of the calculated two-body matrix elements (in MeV) for $N = 50$ isotones. Single-particle energies of $2p_{1/2}$ and $1g_{9/2}$ states are listed in the last two rows.

$2j_1$	$2j_2$	$2j_3$	$2j_4$	J	BML	Our	KB
1	1	1	1	0	−0.484	−0.719	−0.249
1	1	9	9	0	0.901	0.907	0.650
1	9	1	9	4	0.690	0.392	•••
				5	0.175	−0.008	•••
9	9	9	9	0	−1.719	−1.937	−1.147
				2	−0.603	−0.896	−0.852
				4	0.164	−0.098	−0.259
				6	0.508	0.128	−0.037
				8	0.570	0.318	0.094
$p_{1/2}$ single-particle energy					−7.094	0.0	
$g_{9/2}$ single-particle energy					−6.255	0.877	

model I are consistent with those obtained by Ball *et al.*[1] Table I lists the calculated two-body matrix elements. Column 2 of Table I shows the two-body matrix elements calculated by Ball *et al.*, and column 3 lists our results with model II. Column 4 gives the results obtained from the reaction matrix elements.[4] The single-particle energies are listed in the last two rows. Since we do not consider the binding energies of the ground states in the least-squares fit for the model II calculation, $\epsilon(2p_{1/2})$ is set equal to zero. Our calculated two-body matrix elements agree reasonably well with those of Kuo and Brown.[4] Comparison between column 2 and column 3 shows the main differences between the two-body matrix elements of Ball *et al.*, and those of the present study are in the diagonal elements. The overall average of the differences for these eight diagonal elements is 0.265 MeV, which can be considered as the Coulomb interaction energy for a pair of protons in the $(2p_{1/2}, 1g_{9/2})$ model space.

The binding energies of the ground states calculated with the parameters in model II are listed in in column 3 of Table II. Column 2 shows the corresponding observed values. The differences between them are given in column 4. This difference will be interpreted as due to the Coulomb interaction energies since these matrix elements are not included in the parameter obtained in model II. If c is the Coulomb interaction of a pair of protons in the $2p_{1/2}$-$1g_{9/2}$ shell, then the total Coulomb interaction energy of n extracore protons can be written as

$$E(n) = \frac{n(n-1)}{2} c \,. \tag{1}$$

The calculated values of c in column 5 are almost constant, varying between 0.222 and 0.277 MeV. The average value of 0.255 MeV is in almost perfect agreement with the mean Coulomb displacement energy, 0.265 MeV, obtained above. The separation energies, which can be calculated from

$$S(n) = S(1) - (n-1)c - [E_B(n) - E_B(n-1)] \tag{2}$$

are listed in column 7, where $S(1)$ is assumed to be the experimental value of ^{89}Y, i.e., 7.067 MeV, and $E_B(n)$ is taken directly from our calculated binding energies. Column 6 shows the corresponding experimental separation energies. The calculated separation energies are found to be in very good agreement with the observed ones.

It is well known that in shell-model calculations, if various effective interactions are employed within the same model space, the most realistic interaction will produce the most configuration mixing of eigenvectors among the components. For $N = 50$ isotones, the eigenvectors obtained by excluding the binding energies of the ground states from the least-squares fit are found to possess more configuration mixing. For instance, the eigenvector for the ground state of ^{92}Mo in model I calculation is

$$|0^+\rangle_I = 0.551\,|1g_{9/2}{}^4, v=0\rangle + 0.014\,|1g_{9/2}{}^4, v=4\rangle + 0.835\,|1g_{9/2}{}^2, 2p_{1/2}{}^2\rangle \,,$$

while that obtained with model II is

TABLE II. Comparison of observed and calculated binding energies, Coulomb displacement energies, and the separation energies (in MeV) for $N = 50$ isotones.

Nucleus	Binding energy Exp.	Binding energy Calc.	Diff.	Coulomb displacement c	Sp Exp.	Sp Calc.
^{90}Zr	−1.289	−1.511	0.222	0.222	8.356	8.323
^{91}Nb	0.619	−0.213	0.832	0.277	5.159	5.259
^{92}Mo	0.219	−1.256	1.475	0.246	7.467	7.345
^{93}Tc	3.182	0.563	2.619	0.262	4.104	4.228
^{94}Ru	4.008	0.092	3.916	0.261	6.241	6.263
^{95}Rh	7.904	2.435	5.469	0.260	3.171	3.194

$$|0^+\rangle_{II} = 0.581\,|1g_{9/2}{}^4, v=0\rangle - 0.016\,|1g_{9/2}{}^4, v=4\rangle + 0.814\,|1g_{9/2}{}^2, 2p_{1/2}{}^2\rangle .$$

Although the difference between $|0^+\rangle_I$ and $|0^+\rangle_{II}$ is not large, it still may produce a considerable effect on the transition rate.

The existence of the states $\frac{3}{2}^-$ at 1.507 MeV and $\frac{5}{2}^-$ at 1.745 MeV for the ^{89}Y nucleus shows that the ^{88}Sr nucleus is actually not a good core for the calculation of $N=50$ isotones. This difficulty may be solved by enlarging the model space to include the $2p_{3/2}$ and $1f_{5/2}$ orbits. However, the calculation becomes more complicated with such consideration because, in addition to the particle-particle interaction, one must take into account the particle-hole and hole-hole interactions in the enlarged model space. However, if the ground-state binding energies are not included in the calculation, one may assume the pseudonucleus ^{100}Sn to be an inert core, and therefore, only the hole-hole interaction has to be considered in this situation.

The effective p-p interaction is the sum of nuclear and Coulomb contributions. It is to be expected that the Coulomb interaction, because of its long range, should have two-body matrix elements which depend rather weakly on J. Since the Coulomb interaction contributes very little to off-diagonal matrix elements, the main effect of the Coulomb interaction is to add a constant to the diagonal elements. For example, in the calculation of $N=50$ isotones, the difference between the off-diagonal elements $\langle p_{1/2}{}^2|V|g_{9/2}{}^2\rangle_{J=0}$ for model I and model II is only a negligible value of 0.006 MeV as shown in Table I. Furthermore, our two-body matrix elements for $N=50$ isotones are fitted to the experimental energy levels. Therefore, the effects of Coulomb interaction on the off-diagonal matrix elements and the J dependence of the diagonal elements are automatically included in our results. The negligible effect of Coulomb interaction on the off-diagonal elements ensures the similarity between the eigenvectors obtained by Ball *et al.* and this study. A slight difference exists between these results because the eigenvectors obtained in our calculation with model II possess more configuration mixing.

In the calculation of $N=28$ isotones, we assume the ^{48}Ca nucleus to be an inert core with $Z-20$ protons being distributed in the $1f_{7/2}$, $2p_{3/2}$, $1f_{5/2}$, and $2p_{1/2}$ orbits. We allow only one proton to jump to a higher orbit from the $1f_{7/2}$ shell. A two-range central-plus-tensor potential, proposed by Schiffer and True,[6] is assumed in the practical calculation. Harmonic oscillator wave functions are employed with the oscillator constant being fixed at $\nu = 0.96 \times A^{-1/3}$ fm^{-2}, where $A=50$. The radial dependence of the effective interaction is assumed to be of the Yukawa type, and the interaction ranges are taken directly from Ref. 6. The interaction strengths of the presumed two-range force and the single-particle energies of $2p_{3/2}$, $1f_{5/2}$, and $2p_{1/2}$ with respect to the $1f_{7/2}$ orbit are treated as free parameters. In the model I calculation, 28 low-lying excited states in addition to 6 binding energies of the ground states for nuclei $N=28$, $Z=22$–28 are included in the least-squares fit and yield an rms deviation of 260 keV. In the calculation with model II, the 6 binding energies are excluded from the least-squares fit, and the rms deviation is 221 keV.

The interaction strengths are listed in Table III. The third column, with the heading I, shows the calculated results with model I while the fourth column, with the heading II, shows those obtained with model II. The interaction strengths obtained by Schiffer and True[6] in their calculation of two-body matrix elements for the nuclei in the vicinity of doubly-closed shells are listed in the last column. The last three rows show the single-particle energies of $2p_{3/2}$, $1f_{5/2}$, and $2p_{1/2}$ referring to the $1f_{7/2}$ orbit. Comparison of the last three columns shows that the results obtained by the calculation with model II give better agreement with the Schiffer and True results than those obtained with model I.

The spectroscopic factor of the low-lying states of ^{49}Sc observed by Henning *et al.*[7] in the ^{48}Ca(^{15}N,^{14}C)^{49}Sc reaction suggests that the centroid of the single-particle strengths of $(2p_{1/2})$ and $(1f_{5/2})$ are 3.32 and 4.25 MeV, respectively. Our calculated single-particle energy is in rather good agreement with the observed values for

TABLE III. Interaction strengths (in MeV) for $N=28$, $22 \leq Z \leq 28$ nuclei. Column I and column II show the calculated results with model I and model II, while column ST represents those obtained by Schiffer and True. The last three rows are the single-particle energies (s.p.e). CSE, CTO, and TTO mean the strengths of central singlet-even, central triplet-odd, and tensor triplet-odd components, respectively.

	Range or s.p.e	I	II	ST
CSE	Short	−102.95	−57.77	−49.32
	Long	33.74	13.53	15.47
CTO	Short	−269.86	−250.92	−155.82
	Long	120.94	105.47	62.06
TTO	Short	4.63	−20.94	−6.10
s.p.e	$\epsilon(2p_{3/2})$	3.09	3.22	
	$\epsilon(2p_{1/2})$	3.94	4.00	
	$\epsilon(1f_{5/2})$	4.38	4.23	

TABLE IV. Two-body matrix elements (in MeV) of $\langle f_{7/2}^2 | V | f_{7/2}^2 \rangle_J$ for $N = 28$ isotones. Column LM lists the results obtained by Lips and McEllistrem. Columns I and II show our calculated results with models I and II, respectively. The last column gives the modified Kuo and Brown two-body matrix elements.

J	LM	I	II	KB′
0	−2.29	−2.31	−2.50	−2.11
2	−0.47	−0.49	−0.81	−1.11
4	0.42	0.30	−0.05	−0.10
6	0.82	0.81	0.37	0.23

$(1f_{5/2})$ and in qualitative agreement for $(2p_{1/2})$.

In this study, the main effect of the Coulomb displacement energy is due to the two-body matrix elements $\langle f_{7/2}^2 | V | f_{7/2}^2 \rangle_J$. Table IV shows the values of $\langle f_{7/2}^2 | V | f_{7/2}^2 \rangle_{J=0,2,4,6}$. Column 2, with the heading LM, lists the two-body matrix elements obtained by Lips and McEllistrem.[3] The columns headed I and II show our calculated results with models I and II, respectively. The last column, KB′, lists the modified Kuo and Brown two-body matrix elements obtained by McGrory *et al.*[5] for the energy spectra of Ca isotopes. Comparison of the second and third columns shows that our calculated results with model I are very similar to those obtained by Lips and McEllistrem,[3] while our calculated results with model II are in good agreement with those listed in the column headed KB′. The overall average of the differences between I and II for $J = 0, 2, 4, 6$ is 0.35 MeV, which is consistent with the value 0.318 MeV obtained by Harchol *et al.*[8] for fitting the Coulomb displacement energies. Since the size of the nucleus increases when the mass number increases, the Coulomb interaction for a larger nucleus is weaker than that for a smaller nucleus. In view of this fact, the Coulomb interaction obtained for $N = 50$ isotones is rather consistent with that obtained for $N = 28$ nuclei.

In conclusion, it is found in the present study that the calculation of $N = 50$ and $N = 28$ isotones with the binding energies of the ground states excluded from the least-squares fit seems to be more practical. Furthermore, more information can be deduced from such a calculation, e.g., Coulomb displacement energy, separation energy, and effective nucleon-nucleon interaction. It is well known that it is difficult to investigate the deformed nuclei within the framework of the shell-model calculation. However, if the ground state and the low-lying excited states possess the same deformation for such nuclei, then one may not consider the ground state. The excitation energies can be calculated with the conventional shell model. After the interaction has been obtained, the binding energy can be reproduced. Information of the deformation for some nuclei can be obtained from the difference between the calculated and the observed binding energies.

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