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COULOMB DISPLACEMENT ENERGIES
OF THE $T = 1$, $J = 0$ STATES OF $A = 42$ NUCLEI[†]

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Abstract: Coulomb displacement energies of the $T = 1$, $J = 0^+$ and 6_1^+ states of $A = 42$ nuclei are analyzed with previously known charge dependent forces and effects, and with the available Hartree-Fock single-particle wave functions. From the study of the Coulomb displacement energies of the 6_1^+ states, it is found that the present knowledge on the charge dependence, including a phenomenological charge symmetry breaking force previously introduced so as to help explain the Nolen-Schiffer anomaly, gives a sufficient and consistent explanation for both single-particle and two-particle systems. From the study of the 0^+ states, we found that the Coulomb displacement energies of the second 0_2^+ states can be explained with a compensation between the smaller Coulomb energies of the second lowest two-particle state and larger ones of the deformed 4p-2h state.

1. Introduction

In a previous paper [1]), we investigated the Nolen-Schiffer anomaly [2]) of the $T = \frac{1}{2}$ mirror nuclei with the best available Hartree-Fock (HF) wave functions [the density matrix expansion [3]) (DME) and the Skyrme II (SKII) interaction [4])]. In the course of the study, we found several important facts. These are: The raw experimental Coulomb displacement energy is not the experimental value of the single-particle (s.p.) Coulomb displacement energy, because of the existence of the core excitation. The sum rule is a quite powerful method to extract the experimental s.p. Coulomb displacement energy. The core-excitation correction in the s.p. system is always negative, while it is always positive in the single-hole (s.h.) system. Consequently, the core-excitation correction (or correction due to many-body effects), alone, cannot resolve the Nolen-Schiffer anomaly, because, if this kind of correction resolves the anomaly in a s.p. system, it gives trouble in the s.h. system with the same core. Therefore, besides the charge dependent forces and effects of electromagnetic (e.m.) origin, the introduction of some kind of the charge symmetry breaking (CSB) force is necessary to explain the Nolen-Schiffer anomaly. We then found that a

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simple phenomenological CSB force can account for a wide range of the observed anomalies with few exceptions.

In this paper, we extend our investigation to the Coulomb displacement energies of the $T = 1$ two-particle system. The Coulomb displacement energies of two-particle systems have been studied by many people, extensively by Bertsch [5]) and his co-workers [6-8]). Those studies can be classified into two types of analysis. In the first type of analysis the s.p. and the two-body Coulomb energies are parameterized with the employment of the generalized seniority scheme, and the best parameters are searched [8-10]). The second one is the investigation of the relative shifts in the spectra of the Coulomb displacement energies of the two-particle system [5-7,11]). Unfortunately, those two analyses are subject to a definite shortcoming in that there is no consistent analysis of the relationship between the s.p. Coulomb displacement energy and the two-body charge dependent spectra. For now, however, we have an appropriate calculational method for the s.p. Coulomb displacement energy, and we investigate the consistency between the s.p. Coulomb displacement energy and the spectra of the Coulomb displacement energies of the two-particle system, choosing the $T = 1, 0^+$ and 6_1^+ states of $A = 42$ nuclei. This system is a particularly interesting subject for study. It has been shown that a naive 4p-2h picture of the second 0_2^+ state, which has been studied by Gerace and Green [12]) and Flowers and Skouras [13]), shows a $\approx$ 7–800 keV overestimation for ^{42}Ti-^{42}Ca, in spite of the great success of this model in other fields [14]). Therefore, in this paper, employing reliable two-particle configurations and the deformed 4p-2h states, we carefully re-examine the Coulomb displacement energies of the $T = 1, 0^+$ states, and seek the possible resolution of the overestimation. In sect. 2, employing the HF s.p. wave function generated with the SKII interaction [15]), we calculate the Coulomb displacement energies of the $T = 1, 0^+$ and 6_1^+ states of $A = 42$ nuclei with the known charge dependent forces and effects of e.m. origin and the possible CSB force, which is fitted so as to help explain the Nolen-Schiffer anomaly in the previous paper. We then show what the problem is in the calculation of the Coulomb displacement energies of this system by using the generalized sum rule for the Coulomb displacement energy. In sect. 3 we investigate the origin of this problem, and discuss the possible resolutions.

2. Wave functions and Coulomb displacement energies

2.1. GENERAL TREATMENT

The wave functions of the $T = 1$ states of a particular spin and parity α can be expressed in terms of the two-particle configuration and the particle-hole excitation as follows:

$$|\alpha^i\rangle = \sum_t A_t^i |\alpha_t : 2p\rangle + \sum_s B_s^i |\alpha : n_s p - (n_s - 2)h\rangle, \tag{1}$$

where the subscripts t specify the eigenstates in the two-particle configuration space, and the subscripts s stand for the core-excited states. The superscripts i are the identification numbers of the states, starting with $i = 1$ for the lowest state. In general, the state with $i = 1$ has a predominant lowest two-particle state $|\alpha_{t=1} : 2\mathrm{p}\rangle$. For the truncated space with M two-particle states and N p-h excitations, the amplitudes A_t^i and B_s^i satisfy the relationships

$$\sum_{t=1}^{t_M} |A_t^i|^2 + \sum_{s=1}^{s_N} |B_s^i|^2 = 1, \qquad \sum_{i=1}^{M+N} |A_t^i|^2 = 1, \qquad \sum_{i=1}^{M+N} |B_s^i|^2 = 1, \qquad (2)$$

where $M = \sum_{t=1}^{t_M} 1$ and $N = \sum_{s=1}^{s_N} 1$. The summation of t is undertaken over all the possible two-particle states up to t_M, while that of s is over all the possible p-h core excitations up to s_N.

The charge dependent energy $\mathscr{E}^{T_x}(\alpha^i)$ of the state $|\alpha^i\rangle$, which corresponds to the raw experimental value, is defined in terms of the binding energy difference,

$$\mathscr{E}^{.T_x}(\alpha^i) = \mathrm{B.E.}^{T_x=1}(\alpha^i) - \mathrm{B.E.}^{T_x}(\alpha^i). \qquad (3)$$

Employing the wave function (1), the $\mathscr{E}^{T_x}(\alpha^i)$ is given by

$$\mathscr{E}^{T_x}(\alpha^i) = \sum_t |A_t^i|^2 \varepsilon^{T_x}(\alpha_t : 2\mathrm{p}) + \sum_s |B_s^i|^2 \varepsilon^{T_x}(\alpha : n_s\mathrm{p} - (n_s - 2)\mathrm{h}), \qquad (4)$$

$$+ \text{off-diagonal terms,}$$

where the $\varepsilon^{T_x}(\alpha_t : 2\mathrm{p})$ is the Coulomb displacement energy of the two-particle state and the $\varepsilon^{T_x}(\alpha : n_s\mathrm{p} - (n_s - 2)\mathrm{h})$ is that of the s-type core excited state. Here the quantities ε^{T_x} are defined by

$$\varepsilon^{T_x}(\alpha_t : 2\mathrm{p}) = \langle \alpha_t : 2\mathrm{p}|\mathscr{H} + \mathrm{V}|\alpha_t : 2\mathrm{p}\rangle^{T_x} - \langle \alpha_t : 2\mathrm{p}|\mathscr{H} + V|\alpha_t : 2\mathrm{p}\rangle^{T_x=1}, \qquad (5)$$

$$\varepsilon^{T_x}(\alpha : n_s\mathrm{p} - (n_s - 2)\mathrm{h}) = \langle \alpha : n_s\mathrm{p} - (n_s - 2)\mathrm{h}|\mathscr{H} + V|\alpha : n_s\mathrm{p} - (n_s - 2)\mathrm{h}\rangle^{T_x}$$

$$- \langle \alpha : n_s\mathrm{p} - (n_s - 2)\mathrm{h}|\mathscr{H} + V|\alpha : n_s\mathrm{p} - (n_s - 2)\mathrm{h}\rangle^{T_x=1}, \qquad (6)$$

where the $\mathscr{H}$ is a sum of the s.p. Hamiltonian and the V is the residual interaction Summing up both sides of the eq. (4) for all possible i states within the truncated space, we can obtain the following relationship between the sum of the calculated Coulomb displacement energies and that of the experimental values from relationship (2)

$$\sum_{i=1}^{M+N} \mathscr{E}^{T_x}(\alpha^i) = \sum_{t=1}^{t_M} \varepsilon^{T_x}(\alpha_t : 2\mathrm{p}) + \sum_{s=1}^{s_N} \varepsilon^{T_x}(\alpha : n_s\mathrm{p} - (n_s - 2)\mathrm{h}), \qquad (7)$$

where the off-diagonal terms are cancelled out in this relationship. The sum rule relationship (7) puts a quite important and strong condition on both the wave function employed and the charge dependent forces and effects to be calculated: If we have reliable wave functions for the system, eq. (7) can be utilized to obtain the information about the charge dependent forces and effects, or vice versa.

2.2. WAVE FUNCTIONS

For the two-particle states, we employ two different configurations. The first one consists of a simple $1f_{\frac{7}{2}}^2$ configuration (SC). The second is obtained with the Kuo-Brown realistic two-body matrix elements [16]) within fp configurations (KB). While Bertsch pointed out the importance of the $1g_{\frac{9}{2}}^2$ configuration in the calculation of the Coulomb energy shift of the ^{42}Ti-^{42}Ca ground states, we found that the $1g_{\frac{9}{2}}^2$ configuration can be neglected in a much more realistic Coulomb energy calculation. The calculation undertaken by Bertsch is based upon a quite low $1g_{\frac{9}{2}}$ s.p. level [i.e. $\Delta\varepsilon(1g_{\frac{9}{2}}\text{-}1f_{\frac{7}{2}}) = 5.9$ MeV compared to $\Delta\varepsilon(1f_{\frac{5}{2}}\text{-}1f_{\frac{7}{2}}) = 6.5$ MeV] in the calculation of the Kuo-Brown wave function and also based upon harmonic oscillator s.p. wave functions which drop quickly in the tail region. However, there is so far no reason to expect that the $1g_{\frac{9}{2}}$ level is so low. For instance, the DME gives the $1g_{\frac{9}{2}}$ neutron level at 11.25 MeV above the $1f_{\frac{7}{2}}$ level, and the SKII interaction gives it at 13.05 MeV above the $1f_{\frac{7}{2}}$ level. These energies are almost 2–2.5 times higher than those used in the original Kuo-Brown wave function. Moreover, these $1g_{\frac{9}{2}}$ states are unbound, so that the contribution from overlaps in the tail region is not negligible. Two effects, which are the higher $1g_{\frac{9}{2}}$ level in the calculation of the two-particle wave function and the broader distribution of the $1g_{\frac{9}{2}}$ level especially in the tail region, reduce the contribution from $1g_{\frac{9}{2}}^2$ configuration. Fig. 1 shows the Coulomb energy contribution from the $1g_{\frac{9}{2}}^2$ configuration. The solid lines are the Coulomb energies calculated with the Kuo-Brown wave function whose s.p. $1g_{\frac{9}{2}}$ level changes from 4.9 MeV to 12.9 MeV above the $1f_{\frac{7}{2}}$ level. The Coulomb energy $\Delta\varepsilon_{\text{C}}$ is defined by $\Delta\varepsilon_{\text{C}} = \varepsilon_{\text{C}}^{T_z=-1}(\alpha_1: 2p) - 2\varepsilon_{\text{C}}(1f_{\frac{7}{2}})$ where the $\varepsilon_{\text{C}}(1f_{\frac{7}{2}})$ is the s.p. Coulomb energy of the $1f_{\frac{7}{2}}$ state. In this paper HO stands for the case of the harmonic oscillator s.p. wave functions, while the SKII is for the case of the SKII interaction. Only the Coulomb force is employed as a charge dependent force. From fig. 1, we find that the Coulomb energy calculated with the SKII interaction is quite sensitive to the choice of the $1g_{\frac{9}{2}}$ level, while that of the HO case is insensitive. This stems from the fact that the SKII interaction (or realistic calculation) gives large s.p. Coulomb energy differences among fp and $1g_{\frac{9}{2}}$ levels. For comparison, the Coulomb energies calculated with the Kuo-Brown wave function having only fp configurations are also shown in fig. 1 by dashed lines. Thus we conclude that the contribution from the $1g_{\frac{9}{2}}^2$ configuration is quite small in the realistic calculation of the Coulomb energy with the higher $1g_{\frac{9}{2}}$ level generated with the HF potential. We cannot find any difference between the Coulomb energies calculated with and without the $1g_{\frac{9}{2}}^2$ configuration. The wave functions of the 0^+ states derived with the Kuo-Brown two-body matrix elements within fp configurations are shown in table 1 together with that of 6_1^+ state.

We employ the deformed 4p-2h core-excited state having a particle isospin $T_{\text{p}} = 0$ and a hole isospin $T_{\text{h}} = 1$ by following Gerace and Green [12]), and Flowers and Skouras [13]). The four particles fill Nilsson orbit no. 14 with a deformation $\delta = 0.2$
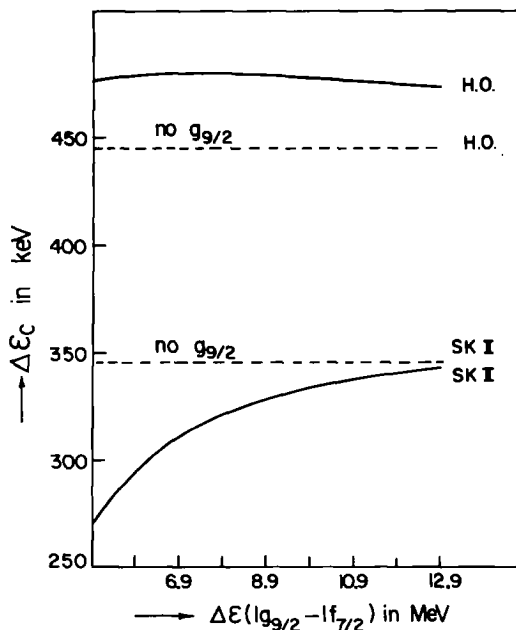
Fig. 1. The Coulomb energy contribution from the $1g_{9/2}^2$ configuration. The solid lines show the Coulomb energy calculated with the Kuo-Brown wave function whose s.p. $1g_{9/2}$ level changes its energy from 4.9 to 12.9 MeV above the $1f_{7/2}$ level. The Coulomb energy $\Delta\varepsilon_C$ is defined by $\Delta E_C = \varepsilon_C^{T_z=-1}(\alpha_1:2p) - 2\varepsilon_C(1f_{7/2})$ where $\varepsilon_C(1f_{7/2})$ is the s.p. Coulomb energy of the $1f_{7/2}$ state. The HO stands for the case obtained with the HO s.p. wave functions (HO constant $\nu = 0.2451$ fm^{-2}). The SKI is for the case obtained with the SKII interaction. The dashed lines correspond to $\Delta\varepsilon_C$ calculated with the Kuo-Brown realistic two-body matrix elements within fp configurations.

TABLE 1

Two-particle wave functions of the $T = 1, 0^+$ and 6_1^+ states derived with the Kuo-Brown matrix elements within fp configurations

State	$1f_{7/2}^2$	$2p_{3/2}^2$	$2p_{1/2}^2$	$1f_{5/2}^2$	$1f_{7/2}1f_{5/2}$
0_1^+	0.958	0.188	0.102	0.194	
0_2^+	−0.217	0.941	0.257	0.024	
6_1^+	0.992				0.130

and the two holes are given simply by the $1d_{\frac{5}{2}}^{-2}$ configuration. This 4p-2h state is equivalent to that employed in method A by Flowers and Skouras [13]. The radial part of the s.p. wave functions are assumed to be given by a simple HF s.p. wave function.

2.3. CHARGE DEPENDENT FORCES AND EFFECTS

It has been shown in the previous paper [1]) that, besides s.p. charge dependent energies of e.m. origin and other known charge dependent corrections of s.p. nature, some kind of a CSB force is necessary to explain the Nolen-Schiffer anomaly. However, so far we do not know whether presently known charge dependent forces and other known corrections, including the phenomenological CSB force obtained previously, are sufficient or not to explain the Coulomb displacement energies of the two-particle system. To answer this question, we examine the Coulomb displacement energies of the $T = 1$, 6_1^+ states with the presently known charge dependent forces and corrections. Since so far no extra 6^+ state has been found experimentally [17]), the $T = 1$, 6_1^+ states of $A = 42$ nuclei are considered to have a pure lowest two-particle configuration. Hence the Coulomb displacement energies to be calculated must exactly coincide with experimental data because of relationship (7). Table 2

TABLE 2

The Coulomb displacement energies of the $T = 1, 6_1^+$ states of $A = 42$ calculated with the SKII interaction, and the experimental data

States	$\varepsilon_{s.p.}$ [a])		V_{tot}	(V^C	$V_{f.s.p.}$	$V_{s.r.c.}$	V_C^{per}	V^{CSB})	AKWI	AKWII	V^{CIB}	Total	Exp [b])
^{42}Sc-^{42}Ca	SC	7232							31	−3	−24±6	7236±6	7250
	KB	7229							32	2	−28±7	7235±7	
^{42}Ti-^{42}Ca	SC	14464	310	(304	−2	2	−6	12)	63	−5		14832	14837
	KB	14459	318	(310	−3	4	−6	13)	64	3		14844	

For notation see text. All quantities are in keV.
[a]) Estimated with the s.p. Coulomb displacement energies calculated in ref. [1]).
[b]) Refs. [24,25]).

shows the Coulomb displacement energies of the $T = 1$, 6_1^+ states calculated with the SKII interaction. Here SC stands for a simple $1f_{\frac{7}{2}}^2$ configuration, and KB is for the Kuo-Brown configuration mixing. To estimate the s.p. contribution $\varepsilon_{s.p.}$, we employ the s.p. Coulomb displacement energies calculated in the previous paper. These are 7412 keV for $1d_{\frac{3}{2}}^{-1}$, 7232 keV for $1f_{\frac{7}{2}}$, 6578 keV for $2p_{\frac{3}{2}}$, 6318 keV for $2p_{\frac{1}{2}}$, and 6943 keV for $1f_{\frac{5}{2}}$. These are including the charge dependent forces of e.m. origin, other known charge dependent corrections of s.p. nature and the phenomenological CSB force denoted by V_2 in table 7 in the previous paper

$$V^{CSB} = \left[\tfrac{1}{12}(3 + \tau_1 \cdot \tau_2) - \tfrac{1}{4}[\tau_1 + \tau_2]_0^1 + \tfrac{1}{2}\sqrt{\tfrac{1}{6}}[\tau_1 \times \tau_2]_0^2\right] \times \left[a_2 f(\mu_2) + b_1 \sigma_1 \cdot \sigma_2 f(\mu_1)\right], \quad (8)$$

$$f(\mu_n) = -\tfrac{1}{100} v_n \exp(-\mu_n r_{12})/\mu_n r_{12}, \qquad v_n = 135\,\mu_n^3 \text{ MeV}, \quad (9)$$

where $\mu_n = n m_\pi c/\hbar = 0.7071n$ fm^{-1}. The coefficients a_2 and b_1 are taken to be -1.26 and -0.43, respectively. The correction to the Auerbach-Kahana-Weneser effect (AKWI) [18]) is the additional core-polarization correction due to a different isospin

assignment ($T = 1$) of the system from that ($T = \frac{1}{2}$) of the s.p. system. According to Auerbach [19]), this correction is given by

$$AKWI = (1 - T_z)(\sqrt{\tfrac{3}{2}} - 1)\varepsilon_{c.p.}, \tag{10}$$

where the core-polarization correction $\varepsilon_{c.p.}$ is taken from the previous paper [1]). The Auerbach-Kahana-Scott-Weneser effect [20]) in the two-body interaction energy (AKWII) is obtained by employing the nuclear residual interaction of a Yukawa radial shape, having a one-pion exchange range, and the Ferrel-Vischer type mixture (i.e. Rosenfeld mixture for the $T = 1$ state and Serber mixture for $T = 0$), because this force can well reproduce the $1f_{\frac{7}{2}}^2$ particle-particle matrix elements [21]). The AKWII is given by

$$AKWII = \tfrac{1}{2}(1 - T_z)[\langle\alpha:2p|V_N^{\text{res}}|\alpha:2p\rangle_{\pi\pi} - \langle\alpha:2p|V_N^{\text{res}}|\alpha:2p\rangle_{\nu\nu}]. \tag{11}$$

The energies of two-body nature, shown in table 2, are the Coulomb interaction, V_C, the correction due to the finite proton size, $V_{\text{f.s.p.}}$, the short range correlation correction, $V_{\text{s.r.c.}}$, the second-order Coulomb perturbation, V_C^{per}, and the CSB force, V^{CSB}. Since the corrections due to two-body e.m. interactions are small [22]), we neglect these corrections. The second-order Coulomb perturbation, V_C^{per}, is estimated by

$$V_C^{\text{per}} = \tfrac{1}{2}(1 - T_z)\left[\langle\alpha:2p\,|\frac{e^2}{r_{12}}\,|\alpha:2p\rangle_{\pi\pi} - \langle\alpha:2p|\frac{e^2}{r_{12}}|\alpha:2p\rangle_{\mu\mu}\right], \tag{12}$$

which is similar to eq. (11). It is well known that the nucleon-nucleon (NN) interaction has a $(2.0\pm0.8)\,\%$ charge independence breaking (CIB) component [23]). To estimate the contribution from this CIB component of the NN interaction, we employ a phenomenological CIB force given by

$$V^{\text{CIB}} = \tfrac{1}{2}(1 - \tau_{1z}\tau_{2z})\delta_{\text{CIB}}f(\mu_1), \tag{13}$$

where the force $f(\mu_1)$ is defined by eq. (9) and δ_{CIB} is 2.0 ± 0.8.

The results obtained are compared with experimental data in table 2. We obtain an excellent agreement between the calculated and experimental values. Although this agreement cannot give additional evidence for the need of a CSB force because of its small amount of two-body interaction energy (≈ 15 keV), this agreement indicates that the present knowledge on the charge dependent forces and corrections can give a sufficient and consistent explanation for both Coulomb displacement energies of the s.p. system and of the two-particle system.

2.4. COULOMB DISPLACEMENT ENERGIES OF THE $T = 1, 0^+$ STATES

Thus far we have obtained the wave functions and the charge dependent forces and corrections. Here we calculate the Coulomb displacement energies of the $T = 1, 0^+$ states, and compare these with the experimental data through relationship (7). One of the advantages of this relationship is that we can neglect the off-diagonal

TABLE 3

The Coulomb displacement energies of the $T = 1, 0^+$ states of $A = 42$ calculated with the SKII interaction, and the experimental data

States		$\varepsilon_{s.p.}$ [a]	V_{tot}	AKWI	AKWII	V^{CIB}	Total	Exp [b]
^{42}Sc-^{42}Ca								
	0_1^+ SC	7232		31	28	-85 ± 21	7206 ± 21	7204
	KB	7188		36	93	-106 ± 26	7211 ± 26	
	0_2^+ 4p-2h	7412	253	-35	65	-59 ± 14	7636 ± 14	7240
	0_3^+ SC	6578		109	175	-39 ± 10	6823 ± 10	7164 [c]
	KB	6592		104	210	-41 ± 10	6865 ± 10	
^{42}Ti-^{42}Ca								
	0_1^+ SC	14464	437	63	57		15021	14985
	KB	14377	469	72	186		15104	
	0_2^+ 4p-2h	14825	915	-70	129		15799	15001
	0_3^+ SC	13155	263	218	351		13987	
	KB	13184	272	208	418		14083	

For notation see text. All quantities are in keV.
[a]) Estimated with the s.p. Coulomb displacement energies calculated in ref. [1]).
[b]) Refs. [24,25]).   [c]) Refs. [24,26]).

TABLE

Contributions from charge dependent forces and effects in the Coulomb

States		E_C	$E_{f.s.p.}$	$\varepsilon_{s.o.}^{c.m.}$	$\varepsilon_{v.p.}$
^{42}Sc-^{42}Ca					
	0_1^+ SC	6780	-73	-106	41
	KB	6738	-72	-93	40
	0_2^+ 4p-2h	7259	-93	114	42
	0_3^+ SC	6268	-60	-28	38
	KB	6264	-59	-26	38
^{42}Ti-^{42}Ca					
	0_1^+ SC	13962	-168	-213	81
	KB	13905	-175	-186	81
	0_2^+ 4p-2h	14902	-196	228	84
	0_3^+ SC	12843	-127	-56	75
	KB	12837	-127	-53	75

E stands for a sum of the s.p. energy ε and the two-body energy V.
For all subscripts and superscripts see text in ref. [1]). All quantities are in keV.
[a]) A sum of the s.p. core-polarization correction $\varepsilon_{c.p.}$ and the additional corrections AKWI and AKWII

terms between the states. Therefore we simply define the states as

$$|\alpha'\rangle = |\alpha_1 : 2p\rangle, \qquad |\alpha^2\rangle = |\alpha : 4p\text{-}2h\rangle, \qquad |\alpha^3\rangle = |\alpha_2 : 2p\rangle.$$

The Coulomb displacement energies of these states are calculated and compared with the experimental data in table 3. Also, contributions from each charge dependent

force and effect are shown in table 4. All the subscripts and superscripts in table 4 are consistent with those in the previous paper [1]).

The Coulomb displacement energies of the SC 0_1^+ states show nice agreement with the experimental values of the 0_1^+ states. The KB of the 0_1^+ state shows nice agreement with the experimental value for ^{42}Sc-^{42}Ca, and it differs by 120 keV from the experimental value for ^{42}Ti-^{42}Ca. The third 0_3^+ state, which is the second lowest two-particle state, is about 300 keV lower than the experimental value for ^{42}Sc-^{42}Ca. The Coulomb displacement energy of the 4p-2h state is about 400 keV larger than the experimental 0_2^+ value for ^{42}Sc-^{42}Ca, and it is about 800 keV larger than the value for ^{42}Ti-^{42}Ca. These disagreements in the 0_2^+ states cause serious trouble for the so-called coexistence model [12,13]), in spite of the great success of this model in other fields. Since the coexistence model, which has been studied by Gerace and Green, and Flowers and Skouras [13]), includes only the lowest two-particle states and the 4p-2h state, relationship (7) must be satisfied for the Coulomb displacement energies of the 0_1^+ and 0_2^+ states. However, the calculated values show an overestimation by 400 keV for ^{42}Sc-^{42}Ca and by 900 keV for ^{42}Ti-^{42}Ca. Following the discussion undertaken in subsect. 2.1, we can have two possible explanations for these over-estimations. The first is the introduction of an unknown extra charge dependent

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displacement energies of the $T = 1, 0^+$ states of $A = 42$

$E_{\text{s.r.c.}}$	$\varepsilon_{\text{k.e.c.}}$	E_C^{per}	AKW [a])	E^{CSB}	E^{CIB}	Total
121	34	-60	200	354	-85 ± 21	7206 ± 21
119	33	-88	290	350	-106 ± 26	7211 ± 26
133	26	-70	-128	412	-59 ± 14	7636 ± 14
124	24	-594	771	319	-39 ± 10	6823 ± 10
123	24	-550	775	317	-41 ± 10	6865 ± 10
253	68	-128	403	763		15021
262	67	-193	579	764		15104
273	52	-145	-256	857		15799
258	47	-1248	1542	653		13987
258	48	-1154	1553	646		14083

given by eqs. (10) and (11).

effect within the Gerace-Green and Flowers-Skouras type of the truncated space. The second is the expansion of the truncated space. Since the Coulomb displacement energies of the three 0_1^+, 0_2^+ and 0_3^+ states of the ^{42}Sc-^{42}Ca satisfy well the sum rule relationship (7), the second explanation seems to be more plausible than the first. In the next section we examine these explanations and discuss the possible resolution.

3. Discussion

3.1. CHARGE DEPENDENT EFFECTS INDUCED BY THE DEFORMATION

Since it has been shown that the previously known charge dependent forces and effects are sufficient to account for the Coulomb displacement energies of the 6_1^+ state of the spherical two-particle configuration, the extra charge dependent effect, in terms of the first kind of the explanation, is expected to be present in the Coulomb displacement energies of the deformed 4p-2h state. Since the only difference in the theoretical treatment between the spherical two-particle and the deformed 4p-2h states is the nuclear deformation of the 4p-2h state, we study the charge dependent phenomena induced by the nuclear deformation.

3.1.1. Isotope shifts of the charge radii. Here we show the importance of the core deformation in the study of the isotope shifts of the charge radii. Since the main part of the ground-state wave function of an even Ca isotope (Ca+2n neutrons) is given by

$$|2n: {}^{40}\text{Ca}\rangle = \sqrt{1-B^2}|2n: {}^{40}\text{Ca}_{\text{s.s.m.}}\rangle + B|2(n+1)\text{p}-2\text{h}: {}^{40}\text{Ca}_{\text{d.s.m.}}\rangle, \quad (14)$$

the experimental mean square (m.s.) radius $\langle r^2 \rangle_{\text{exp}}^{(2n)}$ can be expressed by

$$\langle r^2 \rangle_{\text{exp}}^{(2n)} = \langle r^2 \rangle_{\text{s.s.m.}}^{(2n)} + B^2[\tfrac{1}{20}(2\langle r^2 \rangle_{\text{d.p.}}^{(2n)} - 2\langle r^2 \rangle_{\text{d.h.}}^{(2n)})] + B^2[\langle r^2 \rangle_{\text{d.s.m.}}^{(2n)} - \langle r^2 \rangle_{\text{s.s.m.}}^{(2n)}], \quad (15)$$

where the isospins of the deformed core excited states are assumed to be $T_{\text{p}} = n-1$ and $T_{\text{h}} = 1$. Here the subscripts s.s.m. and d.s.m. stand for the spherical and the deformed shell-model states of the ${}^{40}\text{Ca}$ core, respectively, while d.p. and d.h. stand for the deformed particle and the deformed hole states, respectively. The superscripts $2n$ specify that all the basis is defined in the $40+2n$ system. The second term of the right-hand side of eq. (15) stems from the deformed 2p-2h proton state, while the third term is from the deformation of the core states. For the cylindrically symmetric deformed harmonic oscillator wave functions with a quadrupole deformation δ [ref. [27]], the second and the third terms of the right-hand side of eq. (15) are given by

$$B^2[\tfrac{1}{20}(2\langle r^2 \rangle_{\text{d.p.}}^{(2n)} - 2\langle r^2 \rangle_{\text{d.h.}}^{(2n)})] = \tfrac{1}{10}B^2 \left[\frac{1}{\gamma^2} - \frac{2}{3}\gamma \right] \langle r^2 \rangle_{\text{s.s.m.}}^{(2n)}, \quad (16)$$

$$B^2[\langle r^2 \rangle_{\text{d.s.m.}}^{(2n)} - \langle r^2 \rangle_{\text{s.s.m.}}^{(2n)}] = B^2 \left[\frac{1}{3\gamma^2} + \frac{2}{3}\gamma - 1 \right] \langle r^2 \rangle_{\text{s.s.m.}}^{(2n)}, \quad (17)$$

where $\gamma = [(3-4\delta)/(3+2\delta)]^{\frac{1}{2}}$. Here we employ the particle and hole states which are denoted by the asymptotic quantum numbers (330) and (202) [ref. [27]]. Hence for a given deformation δ and a mixing B^2, we can deduce the charge radius of the spherical core state from the experimental one as

$$\langle r^2 \rangle_{\text{s.s.m.}}^{(2n)} = \langle r^2 \rangle_{\text{exp.}}^{(n)} \bigg/ \left[1 + \tfrac{1}{10}B^2 \left[\frac{1}{\gamma^2} - \frac{2}{3}\gamma \right] + B^2 \left[\frac{1}{3\gamma^2} + \frac{2}{3}\gamma - 1 \right] \right]. \quad (18)$$

The important implication with relationship (18) is that the isotope shifts of the charge radii of the spherical core states are not those of the experimental charge radii because of the existence of the deformed core excitation in the ground state.

Although eq. (17) is also a good approximation for the realistic HF core states, eq. (16) is not a good approximation for the realistic HF particle state, which has a much larger m.s. radius than the HO particle state. Therefore, to deduce the $\langle r^2 \rangle^{(2n)}_{\text{s.s.m.}}$ from the experimental data for the realistic HF states, we evaluate the second term of eq. (15) with the employment of the HF s.p. wave functions and the Nilsson amplitudes generated by the deformed Woods-Saxon potential [28], whose spherical potential depth and spin-orbit coupling are adjusted to fit the HF s.p. energies of the neutron $1d_{\frac{3}{2}}$ and $1f_{\frac{7}{2}}$ levels with fixed shape parameters $a = 0.6$ fm and $r_0 = 1.24$ fm. Employing the second term of eq. (15) calculated with this method, we can deduce the charge radius of the spherical core state from the experimental one as

$$\langle r^2 \rangle^{(2n)}_{\text{s.s.m.}} = [\langle r^2 \rangle^{(2n)}_{\text{exp}} - \tfrac{1}{10}B^2[\langle r^2 \rangle_{\text{d.p.}} - \langle r^2 \rangle_{\text{d.h.}}]] \Big/ \left[1 + B^2 \left[\frac{1}{3\gamma^2} + \frac{2}{3}\gamma - 1\right]\right]. \quad (19)$$

The root mean square (r.m.s.) charge radii of the spherical core states of the Ca isotopes are deduced from the experimental data with eq. (18) for the HO case and with eq. (19) for the DME and the SKII interaction, and are shown in table 5 and fig. 2. Here we employ the deformation $\delta = 0.3$ and the mixing $B^2 = 0.2$, which are not inconsistent with Gerace and Green. The nucleus ^{48}Ca is assumed not to have such a core excitation. The numerals in parentheses are calculated with the ^{40}Ca Gerace-Green wave function. The results obtained show a much smaller deviation

TABLE 5

The r.m.s. charge radii of the spherical core states of the Ca isotopes deduced from the experimental ones with the inclusion of the corrections due to the deformed core excitation

Nucleus	A [a]	B [a]	C [a]	Exp [c]
^{40}Ca	(3.470) [b]	(3.473) [b]	(3.476) [b]	3.487
^{42}Ca	3.476	3.482	3.489	3.517
^{44}Ca	3.475	3.480	3.487	3.515
^{46}Ca	3.471	3.477	3.483	3.511 [d]
^{48}Ca [e]	3.476	3.476	3.476	3.476

All quantities are in fm. Charge radii of spherical core states are obtained with eq. (19) with a deformation $\delta = 0.3$ and a mixing $B^2 = 0.2$.

[a] A, B and C stand for the type of s.p. wave functions employed to evaluate the correction from the deformed 2p-2h proton state. The Nilsson amplitudes [28] are used to evaluate the correction for A (SKII) and B (DME) cases. For the C (HO) case, eq. (16) is used.

[b] Corrections from the deformed p-h state are evaluated with the Gerace-Green wave function [12].

[c] Ref. [29].

[d] Derived from refs. [29, 30].

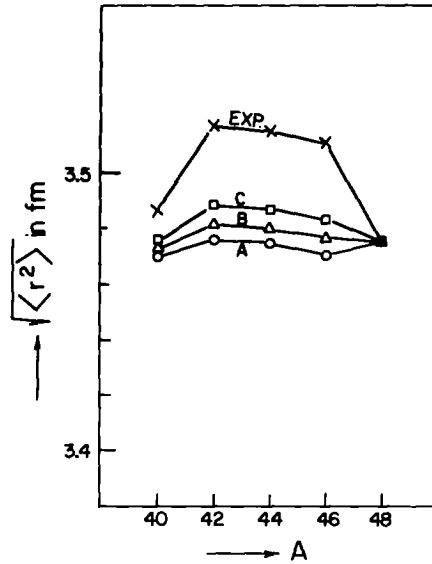[e] ^{48}Ca is assumed not to have a deformed core excitation.

Fig. 2. Isotope shifts of r.m.s. charge radii of the spherical core states of Ca deduced from the experimental ones with the inclusion of the corrections due to the deformed core excitation. Charge radii are obtained using eq. (19) with a deformation $\delta = 0.3$ and a mixing $B^2 = 0.2$ for the various types of s.p. wave functions employed to evaluate the correction from the deformed 2p-2h proton state. The Nilsson amplitudes [28]) are used to evaluate the correction for the cases A (SKII) and the B (DME). For the case C (HO), eq. (19) is used. Experimental data are taken from refs. [29, 30]).

through the isotopes than that of the raw experimental data. Therefore we can conclude that the charge radii of the core states are almost constant through the even Ca isotopes.

It is very interesting to compare this conclusion with the recent shell-model analysis undertaken by Sherr [10]). Assuming a simple functional form for the A-dependence of the charge dependent matrix elements, Sherr analyzed the relationship between charge independence breaking and A-dependent effects in isotope shifts of Coulomb displacement energies using the least square method. Although Sherr could not obtain a definite answer for the A-dependence, he found that the magnitudes of the CIB matrix elements depend strongly upon the functional form of the A-dependence. In this $1f_{\frac{7}{2}}$ shell analysis, our conclusion about the isotope shifts of the charge radii corresponds to the case of the least r.m.s. deviation ($\sigma = 7.4$), and gives a CIB matrix element $V^{CIB}(SC: 0_1^+)$ of -74 keV, which is comparable to our value of -85 ± 21 keV in table 3.

3.1.2. Deformation effects on the Coulomb energy. The deformation effects on the Coulomb displacement energy of the 4p-2h state are classified into two parts. The first effect is caused by a mixing of configurations due to a deformation. However, the configuration mixing only affects the energy of the p-h interaction in our case, and this effect is already accounted in the previous section with the employment of

Nilsson orbit no. 14 with $\delta = 0.2$. Therefore we only note that a change of the deformation $\Delta\delta = +0.2$ (-0.2) from $\delta = 0.2$ gives -5 keV $(+5$ keV$)$ shift for ^{42}Sc-^{42}Ca and -6 keV $(+16$ keV$)$ shift for ^{42}Ti-^{42}Ca. The second effect stems from the core renormalization due to volume conservation. To see this effect, we calculate the direct term of the total Coloumb energy of the ^{40}Ca core and those of the s.p. Coulomb energies of the 1f state having a zero z-component of the angular momentum, $|1f0\rangle$, and the states having asymptotic quantum numbers (330) and (202), using the deformed harmonic oscillator s.p. wave functions with a deformation δ. The results are shown in fig. 3 as a function of δ. Here the harmonic oscillator constant v at $\delta = 0$ is taken to be 0.2451 fm^{-2}, and results are normalized to 1 for $\delta = 0$. The values obtained with the SKII interaction at $\delta = 0$ are 80672 keV for ^{40}Ca, 7038 keV for the $|1f0\rangle$ state, 6677 keV for (330), and 7682 keV for (202).

Since the s.p. Coulomb energies of the $1d_{\frac{3}{2}}$ and $1d_{\frac{5}{2}}$ states are almost equal, the deformation effect upon the s.p. Coulomb energy of the (202) state stems mainly from the core renormalization. For $\delta = 0.2$ this effect is 35 keV. Since this effect is not included in the previous calculation, we add the extra Coulomb displacement energies of 35 keV for ^{42}Sc-^{42}Ca and 70 keV for ^{42}Ti-^{42}Ca. If the deformation does not change its value from ^{42}Ca to ^{42}Ti, these extra energies are the only correction due to the deformation. On the other hand, if the deformation changes from $\delta = 0.2$ to $\delta = 0.35$ as from ^{42}Ca to ^{42}Sc, a 400 keV difference between the theoretical and the experimental values can be explainable. Also the same change (0.2 to 0.35) of the
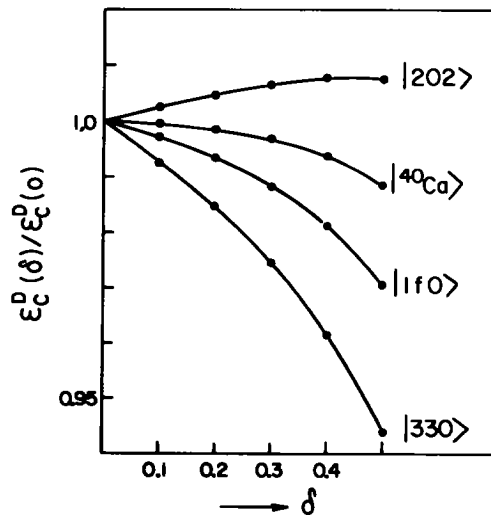

Fig. 3. The direct term of the total Coulomb energy of the ^{40}Ca core and those of the s.p. Coulomb energies of the 1f state, having zero z-component of the orbital angular momentum $|1f0\rangle$, and the states, having asymptotic quantum numbers (330) and (202), calculated using the deformed HO s.p. wave functions with a deformation δ [ref. [27]]. The HO constant v at $\delta = 0$ is taken to be 0.2451 fm^{-2}, and the results are normalized to 1 for $\delta = 0$.

deformation can explain a 800–900 keV difference in the Coulomb displacement energies of ^{42}Ti-^{42}Ca. However, these changes are unrealistic, because, if the deformation changes its value from 0.2 to 0.35 as from ^{42}Ca to ^{42}Sc, it may also change the value from ^{42}Sc to ^{42}Ti by approximately the same amount. Moreover, the underestimation of the theoretical Coulomb displacement energies of the third 0_3^+ state is not explainable within this coexistence model of the two states. Therefore, we must expand the truncated space.

3.2. THE EXPANSION OF THE TRUNCATED SPACE

3.2.1. Coexistence model of the three states. It is very interesting to note that, from table 3, the Coulomb displacement energies of the three 0_1^+, 0_2^+ and 0_3^+ states of ^{42}Sc-^{42}Ca satisfy the sum rule relationship (7). For instance, the differences between the sum of the three theoretical values and that of the experimental data are 92 keV for the SC case and 139 keV for the KB case, respectively. These differences correspond to 0.43 % of the sum of the experimental data for the SC case and 0.64 % for the KB case. On the other hand, the difference ($\approx$ 435 keV) between the sum of the theoretical values and that of the experimental data, within the coexistence model of the two states, corresponds to 3 % of the sum of the experimental data for both the SC and KB cases. Therefore, the better agreement between the sum of the theoretical Coulomb displacement energies and that of the experimental data for the three 0^+ states suggests that the lower three 0^+ states of the $T = 1$, $A = 42$ nuclei can be described with the admixture of the three states (the two lower two-particle states and the 4p-2h state).

According to this model, we can explain the 400 and 800 keV excess of the calculated Coulomb displacement energies of the second 0_2^+ states in table 3 as a compensation between the smaller Coulomb energies of the second lowest two-particle state and larger ones of the deformed 4p-2h state. Note that this model is also consistent with recent experimental data on the small branching ratio for the isospin symmetry hindered positron decay of ^{42}Sc to ^{42}Ca (1.837 MeV) [31]).

The main difficulties of this assignment are: (i) there are no experimental data on the third 0_3^+ state of ^{42}Ti and (ii) there still exists a small difference between the theoretical and the experimental sums for ^{42}Sc-^{42}Ca. However, the second difficulty is expected to be resolved when the first one is resolved. For instance, if we explain the difference in the Coulomb displacement energies of ^{42}Sc-^{42}Ca with a change of the deformation (0.2 to 0.25), the third 0_3^+ state of ^{42}Ti is expected to be 5.34 MeV above the ground state of the ^{42}Ti with the deformation $\delta = 0.3$ of the 4p-2h state. Thus the reliability of this model depends strongly upon the experimental determination of the third 0_3^+ state of ^{42}Ti.

3.2.2. Other resolution. As another resolution, one may assign the second 0_2^+ state as the 6p-4h state having $T_p = 1$ and $T_h = 0$. In fact, this 6p-4h state carries almost the same Coulomb displacement energies as the lowest two-particle state does.

However, since this 6p-4h state cannot explain the underestimation in the theoretical Coulomb displacement energy of the third 0_3^+ state, we need at least one extra 0^+ state, which may be assigned as the 4p-2h state, to explain this underestimation. Therefore, to assign the 0_2^+ state as the 6p-4h state, we must treat the $T = 1$, 0^+ states of $A = 42$ nuclei as the admixture of four or more states. However, we cannot solve this problem from the study of the Coulomb displacement energy because of the lack of experimental information.

4. Conclusion

The main difficulty with the theoretical investigation of the Coulomb displacement energy stems from the simultaneous uncertainty of the nature of the nucleon-nucleon interaction and of the many-body structure in the nuclear wave function. Therefore the study of the sum rule relationship (7) between the theoretical Coulomb displacement energies and the experimental data is essential to get rid of this difficulty. Also the use of the realistic s.p. wave functions is quite important step to deduce reliable information from the experimental data. With the employment of the best HF s.p. wave functions and the sum rule relationship (7), we first analyzed the Coulomb displacement energies of the $T = 1$ 6_1^+ state of $A = 42$ nuclei. Then we found that the present knowledge on the charge dependent forces and corrections, including a phenomenological CSB force previously introduced so as to help explain the Nolen-Schiffer anomaly, can give a sufficient and consistent explanation for Coulomb displacement energies both of the single-particle and the two-particle systems. Next we analyzed the Coulomb displacement energies of the $T = 1, 0^+$ states, employing realistic two-particle wave functions and the well known deformed 4p-2h state. Although the simplified coexistence model, which is given by the admixture of the lowest two-particle states and the deformed 4p-2h state, could not account for the sum of the corresponding experimental data, the extended coexistence model, which is given by the admixture of two lower two-particle states and the deformed 4p-2h state, is found to be able to account for the sum of the experimental data. Thus we can conclude that the study of the Coulomb displacement energies gives strong criteria on the determination of the spectroscopic amplitude, although we cannot determine the amplitude solely from this study.

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