THE DEPENDENCE OF COULOMB DISPLACEMENT ENERGY ON DEFORMATION OF A NUCLEUS

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The influence of deformation on the Coulomb displacement energy for the nuclei of rare earth elements is considered. The essential contributions which change with deformation were calculated exactly using the shell model. The results were compared with experimental data.

1. *Introduction*

Recently Coulomb displacement energy has been the subject of many theoretical works [1]. However, the majority of them concern spherical nuclei; the influence of deformation was considered to a certain extent through the phenomenological correction terms [2]. In this paper all contributions to the Coulomb displacement energy which could essentially depend on deformation, for example: direct term, exchange term and spin orbit term, are exactly calculated numerically. The Hamiltonian used contains a deformed Woods–Saxon type potential and monopole pairing interaction.

Considerations were limited to the axial deformed nuclei of rare elements for which such a kind of deformation is typical. There is also a remark regarding the influence of the nuclear surface deformation on the Coulomb displacement energy. The obtained results were compared with experimental data.

2. *Method*

The Coulomb displacement energy ΔE_c is defined by the equation:

$$\Delta E_c = E_{AS} - E_{GS}, \tag{1}$$

where E_{GS} is the energy of the parent nucleus $Z_<$ in the ground state, and E_{AS} — the energy of the daughter nucleus $Z_>$ in the excited analog state. Neglecting the isospin mixing, we can describe the states of nuclei with the help of the isospin value and its component M_T on the z-axis in isospin space. Based on the concept of analog isospin [3], the ground state of the analog nucleus $|T_0, T_0-1\rangle_{AS}$ (on the assumption of charge-inde-

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pendence of nuclear forces) can be described by the formula [4]

$$|T_0, T_0-1\rangle_{AS} = (2T_0)^{-1/2}\hat{T}_-|T_0, T_0\rangle_{GS}, \tag{2}$$

where $|T_0, T_0\rangle_{GS}$ is the ground state of the parent nucleus, T_0 — isospin of the parent nucleus. Using (1) and (2), the Coulomb displacement energy can be given in the form [5]

$$\Delta E_c = \frac{1}{2T_0}\langle T_0, T_0|\,[[\hat{T}_+, \hat{V}_{EM}], \hat{T}_-]\,|T_0, T_0\rangle_{GS}. \tag{3}$$

For the ground state $|T_0, T_0\rangle_{GS}$ we have taken the configuration of the axial deformed shell model with the one-particle potential of Woods–Saxon with regard to the short-

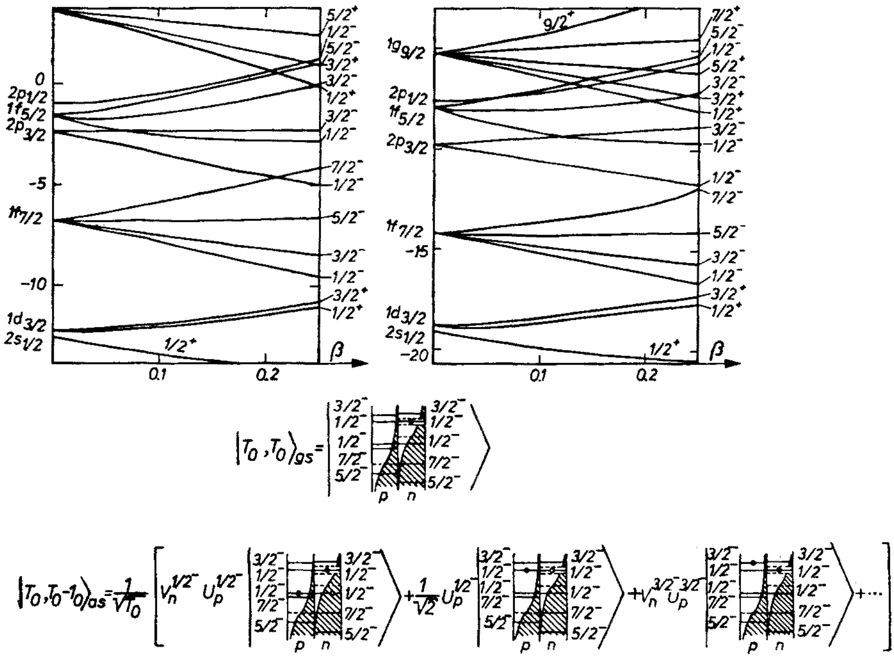

Fig. 1. The structure of the ground state of the parent nucleus $|T_0, T_0\rangle_{GS}$ and analog $|T_0, T_0-1\rangle_{AS}$. The dilution of nucleon occupation through pairing is shown schematically. The odd nucleon is blocked

-range correlation in monopole pairing form. We used an optimalised set of Woods–Saxon parameters for the rare earths [6] and also outside this range [7]. The pairing force was taken from the work [8]. The ground state $|T_0, T_0\rangle_{GS}$ is BCS-state with blocked state of odd nucleon. As an illustration, one-particle states of ^{56}Fe are shown in Fig. 1 and the structure of the states: parent (^{57}Fe) and analog one (^{57}Co). To demonstrate better the dependence of ΔE_c on deformation, we introduce a new value $\delta(\Delta E_c)$, as the difference between the Coulomb displacement of a spherical and deformed nucleus, which essentially depends on the deformation of the nucleus

$$\delta(\Delta E_c)(\beta_2, \beta_4) = \Delta E_c(\beta_2 = 0, \beta_4 = 0) - \Delta E_c(\beta_2, \beta_4). \tag{4}$$

$\delta(\Delta E_c)$ so defined can be indirectly compared with experimental results.

It is true, that if the nucleus in the ground state is deformed, we do not know the experimental value of ΔE_c for its spherical state, but we can profit from a phenomenological formula given in [2] describing the Coulomb displacement energy for spherical nuclei

$$\Delta E_c(\mathrm{SPH}) = \frac{1394.1\,Z}{A^{1/3}} - 416.0 + [1-(-1)^Z]\frac{60}{N-Z} - \frac{86.0\,Z}{A}\,t \;[\mathrm{keV}] \tag{5}$$

The first term in (5) describes a direct Coulomb interaction, the second — exchange forces, the third — Coulomb pairing interaction, the fourth is an approximation of the electromagnetic spin-orbit interaction [9], with the assumption $t = \langle\!\langle \vec{l}\vec{\sigma} \rangle\!\rangle$ [2]. If we extrapolate (5) to the region of deformed nuclei, the experimental equivalent of (4) can be expressed in the form

$$\delta(\Delta E_c)_{\mathrm{EXP}} = \Delta E_c(\mathrm{SPH}) - \Delta E_c(\mathrm{MEASURED}). \tag{6}$$

Since we are interested in $\delta(\Delta E_c)$ (this is the difference), we can neglect such correction terms to the Coulomb displacement energy as the effect of finite nucleon size, vacuum polarization, the short range correlations, the dynamical effect of the neutron-proton mass difference, the charge dependence and charge asymmetry of nuclear forces [1, 10–12], because analysis of these corrections suggests that their dependence on deformation is not significant. If we take (3) and put into this equation $V_{\mathrm{EM}} = \frac{e^2}{|\vec{r}-\vec{r}'|}$, then the main part of the Coulomb displacement energy — direct term — can be expressed in the following form

$$\Delta E_c^{\mathrm{D}} = \frac{1}{2T_0}\iiint \varrho_{\mathrm{EXC}}^{(1\mathrm{p})}(\vec{r})V_c(\vec{r})d^3\vec{r}, \tag{7}$$

where

$$V_c(\vec{r}) = \iiint \varrho_{\mathrm{p}}^{(1\mathrm{p})}(\vec{r}')\frac{e^2}{|\vec{r}-\vec{r}'|}d^3\vec{r}' \tag{8}$$

is the one-particle Coulomb potential. In (7) and (8) $\varrho_{\mathrm{n(p)}}^{(1\mathrm{p})}(\vec{r})$ is one-particle neutron (proton) density matrix, $\varrho_{\mathrm{EXC}}^{(1\mathrm{p})}(\vec{r})$ — density matrix of neutron excess. In addition, one ought to regard the quantum-mechanical exchange term, which can be given in the form

$$\Delta E_c^{\mathrm{EXCH}} = -\frac{1}{2T_0}\int\cdots\int \varrho_{\mathrm{p}}^{(2\mathrm{p})}(\vec{r},\vec{r}')\varrho_{\mathrm{EXC}}^{(2\mathrm{p})}(\vec{r},\vec{r}')\frac{e^2}{|\vec{r}-\vec{r}'|}d^3\vec{r}d^3\vec{r}', \tag{9}$$

where $\varrho^{(2\mathrm{p})}(\vec{r},\vec{r}')$ is two-particle density matrix. Expression (9), in general, is calculated on the basis of a statistical model [13] and nuclear matter [10]. Without difficulty, one can also get $\Delta E_c^{\mathrm{EXCH}}$ in the case of spherical symmetry [9]. In the present work this value was exactly calculated also in the case of deformed nuclei using the method given in the Appendix. In the expression containing the terms of direct and exchange interaction, the electromagnetic sin-orbit interaction gives a small contribution to the Coulomb displacement energy (order of a few keV), hence this term can be estimated without significant error on the basis of [9].

3. *Results and discussion*

The change in nucleon deformation causes a shift of the one-particle states sequence (Fig. 1) as well as the change in the symmetry of the wave functions. These two effects influence in a different way the behavior of the direct and exchange terms.

Let us consider the direct term. The one-particle density matrix can be expressed with the help of multipoles

$$\varrho^{(1p)}(\vec{r}) = \sum_{L=0}^{\infty} \varrho^{[L]}(r) Y_{L0}(\Omega) \tag{10}$$

($M = 0$ because of the assumption of axis symmetry). In Fig. 2 graphs of multipole moments for the proton-density matrix of ^{158}Dy-nucleus for different deformations $\beta_2 (\beta_4 = 0)$

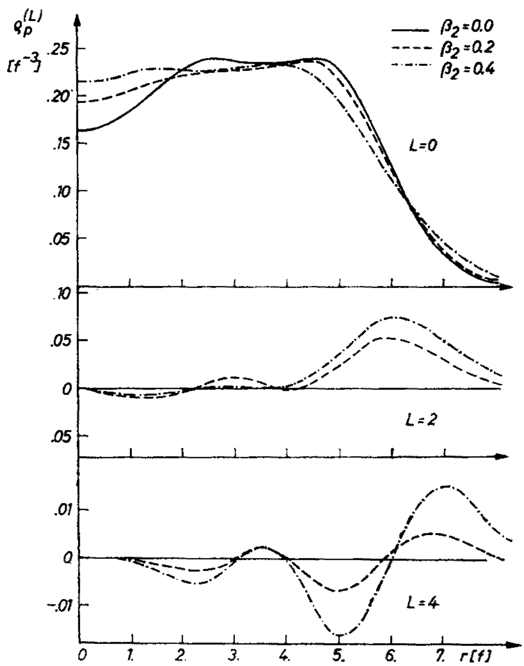

Fig. 2. The graph of the dependence $\varrho_p^{[L]}(r)$ for ^{158}Dy for various values of deformations β_2 ($\beta_4 = 0$)

are given. As expected, the amplitude of the functions decreases very strongly with the higher multipoles. The effect of the proton density matrix deformation influences the one--particle Coulomb potential (8). This potential is given in a form similar to (10)

$$V_c(\vec{r}) = \sum_{L=0}^{\infty} V_c^{[L]}(r) Y_{L0}(\Omega) \tag{11}$$

(see Fig. 3) hence the direct term of the Coulomb displacement energy is

$$\Delta E_c^D = \frac{1}{2T_0} \sum_{L=0}^{\infty} \int_0^{\infty} V_c^{[L]}(r) \varrho_{EXC}^{[L]}(r) r^2 dr. \tag{12}$$

Comparing Fig. 2 and Fig. 3 the averaging effect of integration in expression (8) can be seen.

The contributions from higher multipoles have relative values higher for proton distributions than for a one-particle Coulomb potential generated through these distributions. The direct term depends slightly on the change of sequences of one-particle states and the strength of pairing forces. The exchange term depends more on state sequences.

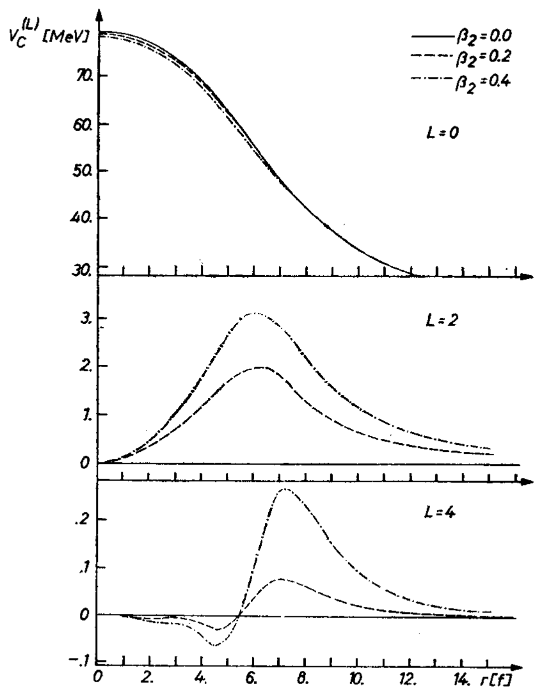

Fig. 3. The graph of dependence $V_c^{[L]}(r)$ for ^{158}Dy for various values of deformations $\beta_2(\beta_4 = 0)$

Contrary to ΔE_c^D, where the proton effect and neutron excess effect are independent, in ΔE_c^{EXCH} the proton states and neutron excess states are combined. The change in deformation causes the change in overlapping of their wave functions and also because of the displacement of one-particle states, causes removing of some states by adding and including of others. The pairing interaction weakens this effect due to the dilution of the occupation of one-particle states. This effect becomes visible when superfluid correlations disappear.

The exchange term depends stronger on nucleon deformation than the main term. This is illustrated in Fig. 4 for the nucleus ^{151}Nd, where $\delta(\Delta E_c^D)$ and $\delta(\Delta E_c^{EXCH})$ depending on deformation $\beta_2(\beta_4 = 0)$ are given. As we see, the consideration of the deformation effect through the correlation correction in the direct term [2] seems to be insufficient. In Table I numerical values of $\delta(\Delta E_c)_{TH}$ are given for a few nuclei from the rare earth region

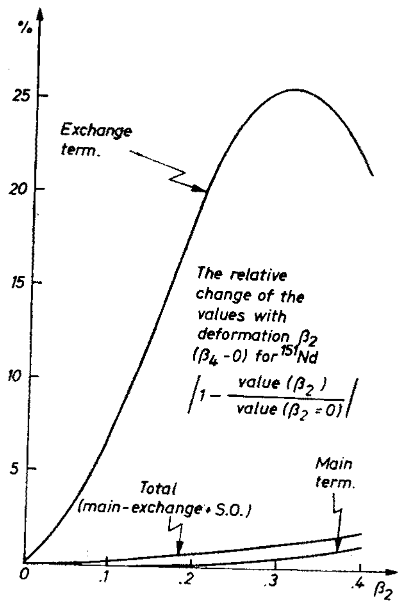

Fig. 4. The dependence of ΔE_c^D, ΔE_c^{EXCH} and ΔE_c on deformation β_2 ($\beta_4 = 0$) for ^{151}Nd

which are calculated in the minimum of Strutinski's deformation. One can see, that in all examples the value of $\delta(\Delta E_c)_{TH}$ is higher than $\Delta(\delta E_c)_{EXP}$, and the divergence is growing with deformation. It seems, that the reason for this effect is the inadequacy of fitting (5) for nuclei far from the magic ones. In general, the difference does not exceed 80 keV. Summarising this, we can conclude with the following suggestions:

TABLE I

Analog pair	β_2	β_4	$\delta(\Delta E_c)_{TH}$ [MeV]	$\delta(\Delta E_c)_{EXP}$ [MeV]	$\Delta\delta$ [keV]
^{149}Nd–^{149}Pm	0.197	0.063	0.099	0.127	28 ±20
^{151}Nd–^{151}Pm	0.237	0.080	0.1385	0.121	17.5±25
^{169}Er–^{169}Tm	0.300	0.0	0.164	0.123	41 ±22
^{169}Yb–^{169}Lu	0.300	0.0	0.174	0.136	38 ±23
^{171}Yb–^{171}Lu	0.300	−0.012	0.207	0.121	86 ±20

Table I contains the results of theoretical calculations for a few analog pairs from the region of the rare earths. Columns 2 and 3 represent theoretically calculated deformations β_2 and β_4 (on the basis of Strutinski's shell correction). Columns 4 and 5 represent the values $\delta(\Delta E_c)_{TH}$ calculated from the fit (5). The value $\Delta\delta$ in column 6 is a difference between $\Delta(\Delta E_c)_{TH}$ and $\delta(\Delta E_c)_{EXP}$ with experimental error. Experimental values are taken from publication [2].

1. One cannot neglect the deformation effect in the exchange term; it is comparable with this effect in the direct term.

2. The value of Coulomb displacement energy depends rather strongly on the deformation of the nuclei, therefore one must take it into consideration in theoretical and experimental research concerning the analysis of Coulomb displacement energies.

APPENDIX

The calculation of the direct and exchange term

The Schrödinger equation with the deformed Woods–Saxon potential was solved with the help of the diagonalisation method (see [14]) on the basis of a spherical harmonic oscillator. It is shown that the use of 11 oscillator shells sufficiently reproduces the results of a 9-shell calculation performed on the basis of a deformed oscillator for the considered range of nuclei and deformation. Wave function of the Woods–Saxon potential indicated by projecting the angular momentum Ω on the axis "z" and by parity, has the following form

$$\psi_\alpha^{(\Omega,\pi)}(\vec{r},\vec{\sigma}) = \sum_{\substack{nlm\Sigma \\ \left(m+\frac{\Sigma}{2}=\Omega\right)}} a^\alpha_{nlm\Sigma}\frac{R_{nl}(r)}{r}\,Y_{lm}(\Omega)\chi_\Sigma(\vec{\sigma}), \tag{A1}$$

where $a^\alpha_{nlm\Sigma}$ are the decomposition coefficients of the function $\psi_\alpha^{(\Omega,\pi)}$ on the deformed oscillator basis.

In the Woods–Saxon basis, the one-particle density matrix is given by the expression

$$\varrho^{(1p)} = \sum_\alpha 2v_\alpha^2|\psi_\alpha^{(\Omega,\pi)}|^2, \tag{A2}$$

where v_α^2 denotes the coefficient of the occupation of the state α taken from the BCS--method. Using the theorem of addition of spherical harmonics we can decompose the density matrix (A2) on the multipoles

$$\varrho^{(1p)}(\vec{r}) = \sum_{L=0}^{\infty}\varrho^{[L]}(r)Y_{L0}(\Omega), \tag{10}$$

where

$$\varrho^{[L]}(r) = \frac{1}{\sqrt{4\pi(2L+1)}}\sum_\alpha 2v_\alpha^2\left\{\sum_{\substack{nl,n'l'\\ m,\Sigma}} a^{\alpha *}_{nlm\Sigma}a^\alpha_{n'l'm\Sigma}\right.$$

$$\left.\frac{R_{nl}(r)R_{n'l'}(r)}{r^2}(-1)^m\sqrt{(2l+1)(2l'+1)}\,\langle l0l'0|L0\rangle\,\langle l-ml'm|L0\rangle\right\}. \tag{A3}$$

Using now the well known decomposition

$$\frac{1}{|\vec{r}-\vec{r}'|} = \sum_{k=0}^{\infty}\frac{4\pi}{2k+1}\frac{r_<^k}{r_>^{k+1}}\sum_{\lambda=-k}^{+k}Y^*_{k\lambda}(\Omega)Y_{k\lambda}(\Omega') \tag{A4}$$

TABLE II

L	0	1	2	3	4
$\Delta E_c^D[L](\beta_2 = 0)$	14.788	0.0	0.0	0.0	0.0
$\Delta E_c^D[L](\beta_2 = 0.3)$	14.607	0.0	0.097	0.0	0.0
$\Delta E_c^{EXCH}[L](\beta_2 = 0)$	−0.290	−0.081	−0.031	−0.018	−0.008
$\Delta E_c^{EXCH}[L](\beta_2 = 0.3)$	−0.361	−0.100	−0.046	−0.020	−0.012

In Table II the components of the decomposition of the direct and exchange term are given (see (A 6) and (A 7)) towards the L-value for the analog pair ^{151}Nd–^{151}Pm at two deformations $\beta_2 = 0$ $\beta_2 = 0.3$ ($\beta_4 = 0$). All the values are given in MeV. As can be seen, when considering differences between deformed and spherical shape, calculations should be limited to $L \leqslant 4$. The contribution coming from $L = 5$ would be of order of magnitude ca 1 keV.

it is easy to perform the integration (8). As a result we get

$$V_c^{[L]}(r) = \frac{4\pi}{2L+1} \int_0^\infty \varrho_p^{[L]}(r') \frac{r_<^L}{r_>^{L+1}} r'^2 dr'. \tag{A5}$$

The integration in (A5) can be expressed through the elementary sum containing polynomials, exponential functions and an error function (ERF).

Now carrying out the decomposition of (10) for $\varrho_{EXC}^{(1p)}$ and going back to (11), we get after simple calculations

$$\Delta E_c^D = \frac{1}{2T_0} \sum_{L=0}^{\infty} \int_0^\infty V_c^{[L]}(r) \varrho_{EXC}^{[L]}(r) r^2 dr \tag{12}$$

$$= \sum_{L=0}^{\infty} \Delta E_c[L]. \tag{A6}$$

If a similar procedure is applied to the exchange term, this term can be expressed in a form analogous to (A6)

$$\Delta E_c^{EXCH} = \sum_{L=0}^{\infty} \Delta E_c^{EXCH}[L], \tag{A7}$$

where ΔE_c^{EXCH} [L] is a single integral depending on r. As an example the values of the sum components (A6) and (A7) for ^{151}Nd for different values of deformations $\beta_2(\beta_4 = 0)$ are shown in Table II. It can be seen that, the components decrease fast to zero if the L-value increases. Practically one can limit the calculations to $L_{max} = 4$.

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