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EFFECT OF THE SURFACE LAYER AND THE DEFORMATION OF THE NUCLEUS ON THE REDUCED E0 CONVERSION PROBABILITY

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The dependence of the reduced E0 electron conversion probability on the parameters α , β , and γ^0 defining the thickness of the surface layer and the deformation of the nucleus is investigated.

L T has been shown in a number of papers [1-4] that agreement between theory and experiment in calculations of the isotope shift of spectral lines can only be achieved if improved electron wave functions are used, which take into account the nonuniformity of the nuclear charge distribution at the nuclear surface as well as the deformation and compressibility of the nucleus. It is natural to ask to what extent these improvements affect other processes depending in one way or another on the electron wave functions, in particular, the E0 conversion probability. The present paper is devoted to this question.

The expression for the reduced E0 electron conversion probability, assuming $\alpha ZR \ll 1$ and $k \ll 50$ (α is the fine-structure constant, Z the charge, k the transition energy, and R the nuclear radius¹), can be written in the form ^[5]

$$\Omega_{\mp \varkappa} = A_{\mp \varkappa, n}(Z, k, \varepsilon) B_{\mp \varkappa}, \qquad (1)$$

where the first factor is equal to

$$A_{\pm^{\varkappa, n}}(Z, k, \varepsilon) = \frac{4\alpha\gamma^{4}\Gamma(2\gamma + n')(\varkappa + \gamma)(\varepsilon\varkappa \pm \gamma)(E\varkappa \pm \gamma)p}{Z\varkappa(2\varkappa + 1)n'!\Gamma^{2}(2\gamma + 1)} \times \left(\frac{2\alpha Z\varepsilon}{n' + \gamma}\right)^{2\gamma+2} \frac{F(Z, p)}{R^{2\gamma-2}},$$
(2)

and is independent of the finite dimensions of the nucleus, whereas the second factor, \overline{B} , does depend on them. Here

$$F(\mathbf{Z} \ p) = \frac{2(\varkappa + \gamma) (2pR)^{2\gamma-2} e^{\pi\alpha ZE/p}}{\Gamma^2 (2\gamma + 1)} \left| \Gamma \left(\gamma + \frac{i\alpha ZE}{p} \right) \right|^2, (3)$$

$$\overline{B}_{-\varkappa} = R^{4\gamma} \left[(\varkappa + \gamma) g'_{-\varkappa, \varepsilon}(R) + \alpha Zf'_{-\varkappa, \varepsilon}(R) \right]^{-2}$$

$$\times \left[(\varkappa + \gamma) g'_{-\varkappa, E}(R) + \alpha Zf_{-\varkappa, E}(R) \right]^{-2}, (4)$$

$$f_{\mp\varkappa'} = \sum_{\nu=0} c_{\nu} r^{\nu} \qquad g_{\mp\varkappa'} = \sum_{\nu=0}^{\infty} d_{\nu} r^{\nu}, \qquad (5)$$
$$= 2 |\lambda| \left(j + \frac{1}{2} \right), \quad \lambda = \mp \frac{1}{2}, \quad l = j + \lambda,$$

l and j are the orbital and total angular momenta of the electron, $\mathbf{n'} = \mathbf{n} - \kappa$, **n** is the principal quantum number, $\gamma = (\kappa^2 - \alpha^2 \mathbf{Z}^2)^{1/2}$, ϵ and **E** $= \epsilon + \mathbf{k}$ are the total energies of the conversion electron in the bound and free states, $\mathbf{p} = (\mathbf{E}^2 - 1)^{1/2}$, and the coefficients \mathbf{c}_{ν} and \mathbf{d}_{ν} satisfy recurrence formulas obtained from the system of Dirac differential equations for the radial functions for a given form of the potential energy V(r) of the electron inside the nucleus.^[6] $\overline{\mathbf{B}}_{+\kappa}$ is obtained from $\overline{\mathbf{B}}_{-\kappa}$ by the replacement

$$g'_{-\varkappa} \to f'_{+\varkappa}, \qquad f'_{-\varkappa} \to g'_{+\varkappa}.$$

To obtain the numerical values of the factors $\overline{B}_{\mp \kappa}$ one has usually used an equivalent²⁾ uniform charge distribution over the volume of a spherical nucleus whose radius is equal to ³⁾

$$R = 1.20 A^{1/3} \cdot 10^{-13} \text{ cm}. \tag{6}$$

²⁾By equivalent we mean here a distribution of the nuclear charge for which the mean square radius is equal to the mean square radius of the nucleus obtained on the basis of experimental data [⁷] (mainly on the scattering of electrons by nuclei).

³⁾Such an equivalent uniform distribution was used in more exact calculations of Ω based on a numerical integration of the system of Dirac differential equations for the radial functions with account of screening by the TFD method. [*, *] It should be noted that the results of the calculation of Ω for the K electrons differ only by 1 to 3% from the results calculated by formula (1) with account of screening by introducing the Slater parameters. For example, for Z = 62, A = 152 we obtain in the first case $\Omega = 2.42 \times 10^{10} \text{ sec}^{-1}$ and in the second case $\Omega = 2.38 \times 10^{10} \text{ sec}^{-1}$. We shall find about the same result for Ω , if we use the electron functions obtained by Babushkin.[¹]

¹⁾All quantities are taken in relativistic units.

σ

Later it turned out [7] that for spherical nuclei with A > 16 better agreement with experiment could be attained with an equivalent radius with a more complicated dependence on A:

$$R = \{1.123 A^{1/3} + 2.352 A^{-1/3} - 2.070 A^{-1} + O(A^{-5/3})\} \cdot 10^{-13} \text{ cm.}$$
(7)

This formula was obtained by Elton^[7] with the help of the Fermi distribution. In the present paper we shall also base the calculation of $B_{\mp K}$ on this distribution.

The two parameter distribution function will be written in the form

$$\rho(\mathbf{r},\vartheta,\varphi) = \rho(0) \frac{1 + \exp[-R_0(\vartheta,\varphi)/a]}{1 + \exp[(\mathbf{r} - R_0(\vartheta,\varphi))/a]}, \qquad (8)$$

where

$$R_{0}(\vartheta,\varphi) = R_{0} \left(1 + \sum_{\mu=-2}^{+2} \alpha_{\mu} Y_{2\mu}(\vartheta,\varphi) - \frac{1}{4\pi} \beta^{2} - \frac{1}{84\pi} \sqrt{\frac{5}{\pi}} \beta^{3} \cos 3\gamma^{0}\right), \qquad (9)$$

 R_0 is the radius at half-density, a is a parameter connected with the surface thickness by the relation [7] s = 4a ln 3, β and γ^0 are the parameters of the quadrupole deformation of the nucleus (parameters of nonsphericity and nonaxiality). In a system referred to the principal axes of the nuclear ellipsoid

$$\boldsymbol{\alpha}_{0} = \boldsymbol{\beta} \cos \boldsymbol{\gamma}^{0}, \qquad \boldsymbol{\alpha}_{\mp 1} = 0, \qquad \boldsymbol{c}_{\mp 2} = 2^{-1/2} \boldsymbol{\beta} \sin \boldsymbol{\gamma}^{0}. \tag{10}$$

The two last terms in (9) are added to conserve the volume (incompressible nucleus), and $\rho(0)$ is the charge density at the center of inertia of the nucleus.

After normalizing $\rho(\mathbf{r}, \vartheta, \varphi)$ to unity,

$$\rho(0) = 3/4\pi R_0^3 \left[1 + \frac{\pi^2 a^2}{R_0^2} \left(1 - \frac{\beta^2}{4\pi} - \frac{1}{84\pi} \sqrt{\frac{5}{\pi}} \beta^3 \cos 3\gamma^0 \right) \right].$$
(11)

Introducing the quantity $l = [4\pi A\rho (0)/3]^{-1/3}$, i.e., the radius of the spherical region taken up by one nucleon in infinite nuclear matter,^[7] we obtain for R_0 and for the radius of the equivalent uniform distribution R the following expressions:

$$R_{0} = lA^{\frac{1}{3}} \left[1 - \sigma + \frac{1}{3} \sigma^{3} - \dots + \left(\frac{1}{4\pi} \beta^{2} + \frac{1}{84\pi} \right) \sqrt{\frac{5}{\pi}} \beta^{3} \cos 3\gamma^{0} \right) (\sigma - \sigma^{3} + \dots) \right], (12)$$

$$R = lA^{\frac{1}{3}} \left[1 + \frac{5}{2} \sigma - \frac{21}{8} \sigma^{2} + \dots + \frac{5}{8\pi} \beta^{2} \left(1 - \frac{13}{2} \sigma + \frac{173}{10} \sigma^{2} - \dots \right) \right]$$

$$+\frac{25}{168\pi}\sqrt[]{\frac{5}{\pi}}\beta^{3}\cos 3\gamma^{0}\left(1-\frac{73}{10}\sigma+\frac{1053}{50}\sigma^{2}-\ldots\right)\right],$$

= $\frac{1}{3}(\pi a/lA^{\frac{1}{3}})^{2}.$ (13)

The best agreement of (13) with the data on the scattering of electrons on spherical nuclei ($\beta = 0$) is obtained, according to Elton,^[7] for $l = 1.123 \times 10^{-13}$ cm and s = 2.49 × 10⁻¹³ cm [substituting these values in (12) and setting $\beta = 0$, we get (7)].

We shall regard (12) as a generalization of (7) to the case of nonspherical nuclei. As seen from (12), the deformation of the nucleus leads to an increase of the equivalent nuclear radius, which is tantamount to a certain increase of the nuclear surface thickness. The effective thickness of the surface layer of a nonspherical nucleus can be defined with the help of the relation⁴⁾

$$s' = 4a' \ln 3,$$
 (14)

where a' is connected with the quantity σ' by

$$\sigma' = \frac{1}{3} (\pi a' / lA^{1/3})^2, \tag{15}$$

and σ' is given approximately by the formula

$$\sigma' \approx \sigma + \frac{1}{4\pi} \beta^2 \left(1 - \frac{22}{5} \sigma \right) + \frac{5}{84\pi} \sqrt[7]{\frac{5}{\pi}} \beta^3 \cos 3\gamma^0 \left(1 - \frac{26}{5} \sigma \right).$$
(16)

Let us first consider the changes coming from calculating Ω with the help of (12) for an equivalent uniform nuclear charge distribution. These changes will be described by the relation

$$\omega = \Omega' / \Omega = \overline{B}_{\mp \varkappa}(R') / \overline{B}_{\mp \varkappa}(R), \qquad (17)$$

where R and R' are given by (6) and (12), respectively.

The calculation of ω performed with different Z, k, and A for the K shell with account of screening according to Slater (Z \rightarrow Z - 0.3) shows that ω depends very weakly on k. As k increases from 0.1 to 3 the quantity ω decreases by less than 1% (thus, e.g., with Z = 92, A = 234 we find ω = 0.960 for k = 0.1 and ω = 0.956 for k = 3). ω depends much more strongly on A and Z. In the case of spherical nuclei, ω may differ from unity by 5% for A > 60 (see Table I). Only for A < 60 does ω differ from unity significantly (thus, e.g., ω = 1.48 for Ca⁴⁰).

The inclusion of the deformation parameters

⁴⁾The numerical value of s' may be found on the basis of an analysis of the experimental data on electron scattering by non-spherical nuclei. Such an analysis (an approximate one) has so far only been done for Ta¹⁸¹. The value found was [⁷] s'= 2.8×10^{-13} cm.

Table I

Table II

| Z | A | ω | | | Sm | | Gd | | | |
|----------------------------|-------------------------------|----------------------|------------------|-----------------------|-----------------------|-----------------------|---------------------|----------------------|----------------------|----------------------|
| 20 40 62 80 92 | 40 90 152 200 234 | 1,481,121,010,970,96 | A βaxial ω | 150 0.179 1.036 | 152 0,280 1,091 | 154 0,315 1,114 | 154 0.3 1.106 | 156 0.41 1.111 | 158 0,46 1.146 | 160 0.47 1.149 |

 β and γ^0 may change ω at most by 15 and 0.5%, respectively (in the following we shall neglect the nonaxiality parameter). In tables II and III we give the values of ω as a function of β and γ^0 for various isotopes of Sm and Gd. The values of the parameter β for Sm were found from the experimental values of the nuclear electric quadrupole moments ^[3] according to the formula

$$Q_{0} = 3(5\pi)^{-1/2} Z \left[lA^{1/2} \left(1 + \frac{5}{2} \sigma - \frac{21}{8} \sigma^{2} \right) \right]^{2} \\ \times \beta \left[\cos \gamma^{0} + 0.36\beta (1 - 2 \sin^{2} \gamma^{*}) \right]$$
(18)

with values of γ^0 taken from ^[10,11]. For Gd we used the values of β given in ^[12].

If we calculate $\partial \Omega' / \partial N$ for Gd^{154, 156, 158} from the data of table II, where N is the neutron number, then this quantity will be about proportional to $\partial \beta^2 / \partial N$.

Let us now consider an equivalent distribution somewhat different from the uniform one. Its shape will be established on the basis of relation (8). Starting from (8) with account of (11) and averaging the density $\rho(\mathbf{r}, \vartheta, \varphi)$ over the angles, we can find the potential energy $V(\mathbf{r})$ of the electron according to the formula

$$V(r) = -4\pi \alpha Z \left\{ \frac{1}{r} \int_{0}^{r} r'^{2} dr' \,\overline{\rho(r', \vartheta, \varphi)} + \int_{r}^{\infty} r' \, dr' \,\overline{\rho(r, \vartheta, \varphi)} \right\}$$
(19)

[the bar over $\rho(\mathbf{r}', \vartheta, \varphi)$ indicates the averaging mentioned above]. A study of V(r) as a function of r shows that near $\mathbf{r} = \mathbf{R}_0$ the function V(r) is to a high approximation (quantities smaller than $3\beta^2/8\pi$ by two orders of magnitude are neglected) equal to

$$V(r) = \frac{-aZ}{R_0 [1 + (\pi a / R_0)^2]} \times \left[-\frac{1}{2} \left(\frac{r}{R_0} \right)^2 + \frac{3}{2} + \frac{1}{2} \left(\frac{\pi a}{R_0} \right)^2 - \frac{3}{8\pi} \beta^2 \right], \quad (20)$$

i.e., it differs little from V(r) for the uniform charge distribution. If, in calculating ω , we use an equivalent charge distribution which corresponds to V(r) as given by (20), we obtain values

 Table III

 Sm

 A
 152
 150

 βnonaxial
 0.289
 0.201

 γ⁰,degrees
 13.2
 26

for ω which differ only by 1 to 2% from those given in Table II (for example, for Sm¹⁵² the value of ω will be 1.100 instead of 1.091, for Gd¹⁶⁰, $\omega = 1.149$ instead of 1.132).

1.088

The magnitude of the reduced E0 conversion probability may change considerably if we calculate it with the help of an equivalent nonuniform charge distribution using (12) instead of (6). As an example, let us take the nonuniform equivalent charge distribution given by the function [13] 5)

$$\rho(r) = \frac{21}{16\pi R''^3} \left[1 - \left(\frac{r}{R''}\right)^4 \right]$$
(21)

with the radius

$$R'' = 3R' / \sqrt{7}, \tag{21'}$$

1.036

where R' is given by (12).

| Та | ble | IV |
|----|------------|----|
| | ~ <u> </u> | |

| Ζ | 20 | 40 | 62 | 64 | 80 | 92 |
|----|-------|-------|-------|-------|-------|-------|
| Α | 40 | 90 | 152 | 158 | 200 | 234 |
| ω' | 2.316 | 1.806 | 1.773 | 2.057 | 1.462 | 1.397 |

In Table IV we give the values of ω' , defined as the ratio of Ω' as computed with the help of (21) over Ω calculated with a uniform equivalent charge distribution with a radius given by (6). It is seen from this table that Ω' may in some cases be twice larger than Ω . The values of ω for Sm and Gd were obtained assuming $\beta = 0.289$ and $\beta = 0.46$, respectively (in all other cases $\beta = 0$).⁶

All results shown in Tables I to IV are for the K shell. The calculations of ω for the subshells $L_{I,II}$ show that the effect of the surface layer and the deformation of the nucleus on $\Omega_{LI,LII}$ is

⁶⁾For $\beta = 0$, $\omega(\text{Sm}^{152}) = 1.581$ and $\omega(\text{Gd}^{158}) = 1.566$.

⁵⁾According to [¹³], this distribution better approximates the experimental curves than the uniform distribution.

somewhat weaker than in the K shell (an effect of 1 to 2% for large and 2 to 3% for small Z). The effect on the relative probabilities L_I/L_{II} , K/L_I is even smaller (they change only by 1 to 2% in comparison with their standard values).

If the nonspherical nuclei are regarded as compressible and ω is calculated taking into account the parameter of deformation compressibility $\xi = -5\beta^2/8\pi$ (according to Fradkin^[3]), the effect of the deformation on Ω will become weaker by a factor of about one half.

The theoretical values of the reduced E0 conversion probability Ω are used for the determination of the reduced nuclear electric monopole matrix element ρ from experiment (cf. the review ^[14]) according to the formula

$$\rho = 1 / \sqrt[\gamma]{\tau \Omega_{\gamma}} \tag{22}$$

where τ is the lifetime of the excited nucleus against E0 transitions with emission of a conversion electron as measured by experiment. The change of the numerical values of Ω as discussed in this paper leads thus to a change of the experimental values of ρ . Although these changes are often small, it may be useful to take them into account in a more precise comparison of the theoretical and experimental values of ρ . ³É. E. Fradkin, JETP 42, 787 (1962), Soviet Phys. JETP 15, 550 (1962).

⁴ M. J. Ionesco-Pallas, Ann. Physik 8, 9 (1961).
⁵ L. A. Borisoglebskiĭ, Vestnik MGU, seriya fiz, astr. 5, 74 (1963).

⁶ L. A. Sliv and B. A. Volchok, Tablitsy kulonovskikh faz i amplitud s uchetom konechnykh razmerov yadra (Tables of Coulomb Phases and Amplitudes with Account of the Finite Dimensions of the Nucleus), Izd. AN SSSR, 1956.

⁷ L. R. B. Elton, Nuclear Sizes, Oxford, 1961 (Russ. Transl. IIL, 1962).

⁸ E. L. Church and J. Weneser, Phys. Rev. 103, 1035 (1956).

⁹ M. A. Listengarten and I. M. Band, Izv. AN SSSR, seriya fiz. **23**, 235 (1959), Columbia Tech. Transl. p. 225.

¹⁰ E. P. Grigoriev and M. P. Avotina, Nucl. Phys. **19**, 248 (1960).

¹¹ J. Hiura and S. Suekane, Progr. Theor. Phys. 24, 462 (1960).

¹² B. V. Thosar, Current Sci. **31**, 368 (1962).

 13 E. L. Church and J. Weneser, Ann. Rev. Nucl. Sci. 10, 193 (1960).

¹⁴ L. A. Borisoglebskiĭ, UFN 81, 271 (1963), Soviet Phys. Uspekhi 6, 715 (1964).

Translated by R. Lipperheide 217

¹ F. A. Babushkin, JETP 44, 1661 (1963), Soviet Phys. JETP 17, 1118 (1963).

² F. A. Babushkin, JETP 45, 1479 (1963), Soviet Phys. JETP 18, 1022 (1964).