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РОЛЬ ВЗАИМОДЕЙСТВИЯ В КОНЕЧНОМ СОСТОЯНИИ В ИОНИЗАЦИИ К-ОБОЛОЧЕК ПРИ β-РАСПАДЕ ЯДЕР

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Аннотация

Вычислен вклад взаимодействия в конечном состоянии в ионизацию К-оболочки в β^-- и β^+- распадах ядер. Найден вклад в спектр β-частиц и в полную вероятность ионизации К-оболочки. Для последней величины расхождение экспериментальных и теоретических данных значительно уменьшилось. Вычислено также влияние на распределение вторичных электронов.

Abstract

We have calculated the contribution of the final state interaction to the ionization of the K-shell during the β^- and β^+ decays. The contributions to the spectra of the β particles and to the total probability of the K-shell ionization are obtained. The disagreement between the calculated values and the experimental data for the latter is shown to diminish strongly. The influence of the secondary electrons on the distribution is also determined.

It is well known that the ionization of the internal electrons during the nuclear β-decay takes place mainly due to the sudden change of the nuclear charge - the shake-off (SO) - see papers /1-6/ and the references therein. The β-electron can also interact with the bound electrons - the final state interaction (f.s.i.) or the direct collisions. The role of the f.s.i. was discussed in a number of papers /3,4/ (and some more references therein) partially in connection with the discrepancy between the experimental data and the theoretical predictions.

The f.s.i. can be treated as perturbation if it's parameter is small enough:

$$\xi^2 = \frac{\alpha^2 E^2}{p^2} = \frac{\alpha^2}{v^2} \ll 1 \qquad (1)$$

with E(p,v) - the energy (momentum, velocity) of the β-electron In the previous studies the first order f.s.i. contribution to the amplitude was calculated.

But that is not enough for the calculation of the lowest order f.s.i. contribution to the probability of the process. As it was shown in /7/ the lowest order f.s.i. correction is included by the equation

$$|F_n|^2 = |F_n^{(0)}|^2 + 2ReF_n^{(1)}F_n^{(0)} + |ImF_n^{(1)}|^2 + 2ReF_n^{(2)}F_n^{(0)}, \qquad (2)$$

where $F_n^{(i)}$ denotes the amplitude of the i-th order of the f.s.i. which causes the transition of the atomic electrons to the state $|\chi_n\rangle$. The first term in the right side of eq.(2) is the SO contribution. The other terms give the f.s.i. correction $\sim \xi^2$. The last term of eq. (2) was overlooked in the previous works.

For the SO amplitude

$$F_n^{(0)} = \varphi(E) \cdot f_n^{(0)} \qquad (3)$$

with φ (E) - the Fermi function of the β-electron,

$$f_n^{(0)} = \langle \chi_n | \psi \rangle \qquad (4)$$

while $|\Psi\rangle$ stands for the initial state of the atom. It was shown in /7/ that the factorization of the interactions of the β -electrons with the nucleus and the bound electrons takes place for the amplitudes $F_n^{(1,2)}$ also takes place if the kinetic energy of the β -electron is large enough

$$T = E - m \gg B_k \tag{5}$$

with $B_k > 0$ - the binding energy of the K-electron.

Thus,

$$F_n^{(1,2)} = \varphi(E)\, f_n^{(1,2)} \tag{6}$$

while $f_n^{(1,2)}$ describe the interaction of the free β-electron with the bound electrons (fig. 1).

The explicit expression for the amplitudes $f_n^{(1,2)}$ was obtained for the nonrelativistic case in the papers /7,8/ and for the relativistic case in the paper /9/. We use them to calculate the lowest order f.s.i. contribution to the probability of creating the vacancy in the K-shell at any point of the β -spectrum (sec. II). The process is referred to as ionization though it includes the small contribution of the excitation of the K-electron. In sec. III we calculate the f.s.i. correction to the total probability. The results are presented in Tables 1, 2. In sec. IV we study the f.s.i. influence on the distribution of the secondary electrons.

II. THE SPECTRUM OF THE β -ELECTRONS

We use eq. (2) for the calculation of the probability of the K-shell ionization at any point of the β -electron spectrum

$$dW = |\mathcal{M}|^2 \cdot |\varphi(E)| \cdot \sum_{n'} (E_0^{n'} - E)\, p E\, |f_n|^2 dE \tag{7}$$

Here $\mathcal{M}$ is the nuclear matrix element of the β-decay, E_0 is the limit energy of the β -electron

$$|f_n|^2 = |f_{Tn}^{(0)}|^2 + \theta_n \tag{8}$$

and the sum over n is taken over all the states but the one with the two electrons on the K-shell. The term θ_n describes the f.s.i. contribution.

In the nonrelativistic case

$$\theta_n = \xi^2 \cdot \Lambda_n \tag{9}$$

with

$$\Lambda_n = \langle\psi|\chi_n\rangle\langle\chi_n|\sum_i \frac{\partial}{\partial z_i}|\psi\rangle \cdot z_0 + \tag{10}$$

$$|\langle\chi_n|\sum_i \ln(z_i - z_{i_2})\lambda|\psi\rangle|^2 - \langle\psi|\chi_n\rangle\langle\chi_n|\sum_{ij} \ln(z_i - z_{i_2})\lambda \ln(z_j - z_{j_2})\lambda|\psi\rangle$$

In eq. (10) the sums are taken over the atomic electrons, z is the direction of the momentum of the β-electron, λ is the infrared cutoff. The terms which contain ln λ are just the Coulomb phase terms of the elastic scattering of the β-electrons on the bound electrons. One can see that they do cancel out. The three terms in the right side of eq.(10) correspond to those of eq. (8). If $T = E - m \gg B_K$ the transitions of the bound electrons do not change strongly the other quantities in eq. (7) and we can obtain

$$\sum_{n'} |f_n|^2 = \sum_n |f_n|^2 - |f_0|^2 \tag{11}$$

with f_0 describing the process in which the state of the atomic electrons does not change. The sum over all the states n can be calculated with the closure condition. Thus

$$\sum_{n'} |f_n|^2 = \tau + \theta \tag{12}$$

Here

$$\tau = 1 - |\langle\chi_0|\psi\rangle|^2 \tag{13}$$

is the SO expression which was often used for the calculation of the probability of the K-shell ionization. $|\chi_0\rangle$ is the final state with two electrons in the K-shell. The f.s.i. contribution is

$$\Theta = \xi^2 \cdot \Lambda \tag{14}$$

with

$$\begin{aligned}\Lambda = & -\langle\psi|\sum_i \tau_i^{-1}|\psi\rangle\cdot\tau_0 - \langle\psi|\chi_0\rangle\langle\chi_0|\sum_i \frac{\partial}{\partial\tau_i}|\psi\rangle\cdot\tau_0 - \\ & -|\langle\chi_0|\sum_i \ln(\tau_i - \tau_{iz})\lambda|\psi\rangle|^2 + \\ & + \langle\psi|\chi_0\rangle\langle\chi_0|\sum_{i,j} \ln(\tau_i - \tau_{iz})\lambda\cdot\ln(\tau_j - \tau_{jz})\lambda|\psi\rangle; \quad \tau_0 = 1/m\alpha\end{aligned} \tag{15}$$

Now we can estimate the relative contribution of the f.s.i. ionization of the K-shell. Eq. (4) leads to the known estimation $f^2 \;\; z^{-2}$ with z - the charge of the decaying nucleus. Since $\langle\chi_{n'}|\psi\rangle \sim z^{-1}$ while $\tau_0\langle\chi_{n'}|\frac{\partial}{\partial\tau}|\psi\rangle \sim Z$ the first term of eq. (9) gives the contribution of the order of unity. The same referes to the two last terms of eqs. (9) and (15). Thus the relative contribution of the f.s.i. is

$$\frac{\Theta}{\tau} \sim \xi_Z^2 = \xi^2 \cdot Z^2 \tag{16}$$

Since for the single-particle wave functions of the electrons of the parent atom ψ_i and the daughter atom χ_j we have

$$(\chi_j, \psi_i) \ll 1 \tag{17}$$

if $i \neq j$. Thus we can neglect the exchange terms in eq. (15) for Λ and express the latter through the single-particle functions ψ_s, χ_s of the K-electrons. We present eq. (15) as

$$\Lambda = d + l \tag{18}$$

while

$$l = l_1 + l_2; \tag{19}$$

$$l_1 = 2[|\langle\psi_s|\ln(1-t)|\psi_s\rangle|^2 - \langle\psi_s|\chi_s\rangle\langle\chi_s|\ln^2(1-t)|\psi_s\rangle] \tag{19a}$$

$t = \tau_z/\tau$

$$l_2 = 2[|\langle\psi_s|\ln\tau|\psi_s\rangle|^2 - \langle\psi_s|\chi_s\rangle\langle\chi_s|\ln^2\tau|\psi_s\rangle] \tag{19b}$$

$$d = -2\tau_0[\langle\psi_s|\tau^{-1}|\psi_s\rangle + \langle\psi_s|\chi_s\rangle\langle\chi_s|\frac{d}{d\tau}|\psi_s\rangle] \tag{20}$$

We can obtain the approximate explicit equation for using the nonrelativistic Coulomb functions for ψ_s and χ_s. In this case

$$d = -2\bar{z}\,\left(1 - \frac{(1+1/\bar{z})^{3/2}}{(1+1/2\bar{z})^3}\right) \sim -3/4\bar{z}. \qquad (21)$$

Thus using also the expansion in powers of $\bar{z}^{-1}$ we can replace χ_s by ψ_s in eqs. (19),(20) and obtain

$$d = 0; \quad \theta = 1 > 0. \qquad (22)$$

The explicit calculation gives

$$\Lambda = 2(1+\psi'(3)) \qquad (23)$$

The two terms in the right side of eq. (23) are l_1 and l_2.

In the relativistic case the contribution of the second and third terms of eq. (7) to θ is still $\xi^2 \cdot \ell$ /9/ while the first term has a more complicated structure. At $E \gg m$ the latter obtains the small factor $\sim m/E$ and

$$\theta = \xi^2 \cdot \ell \qquad (24)$$

In the cases considered in the paper $\bar{z}$ is large enough and eq. (24) is a good approximation (with the accuracy better than 10%) - the fact prompted by the Coulomb calculation mentioned above.

III. THE CONTRIBUTION TO THE TOTAL PROBABILITY

Now we calculate the probability of the ionization of the K-shell

$$P = W_i/W_0 \qquad (25)$$

with

$$W_0 = |\mathcal{M}|^2 \cdot \int_0^{T_0} (E_0 - E)\, pE\, |\varphi(E)|^2 dE \qquad (26)$$

while w_i is obtained by integration of eq. (4)

$$W_i = |\mathcal{M}|^2 \sum_{n'} \int_0^{T_0^{n'}} (E_0^{n'} - E)\, pE\, |\varphi(E)|^2 |f_{n'}|^2 dE \qquad (27)$$

we present

$$P = P_s + P_f \qquad (23)$$

with ρ_s and ρ_ℓ corresponding to the shake-off term τ and the f.s.i. term θ. The value of ρ_s was calculated for many transitions in a number of works. Our aim is to obtain ρ_ℓ.

We carry out the calculations using the Fermi function of the point nucleus

$$|\varphi(E, Z+1)|^2 = \frac{2\pi \cdot \xi_{Z+1}}{1-\exp(-2\pi\xi_{Z+1})} \tag{29}$$

$$\xi_{Z+1}(E) = \frac{\alpha(Z+1)E}{p}$$

There are the approximate equations for the limit cases.

If the limit energy E_0 is so large that

$$\pi^2 \xi^2_{Z+1}(E_0) \ll 1 \tag{30}$$

the integrals (26),(27) are dominated by the regions where $\pi\xi_{Z+1}(E) \ll 1$. Under this condition $|\varphi|^2 \simeq 1$ and one can calculate the integrals explicitly. We obtain the simple equations for the limit cases:

$$\rho_\ell = 4 \cdot \xi^2_{Z+1}(E_0) \cdot \Lambda \tag{31}$$

for the nonrelativistic case $E_0 - m \ll m$ and

$$\rho_\ell = \alpha^2 \cdot \Lambda \tag{32}$$

for the ultrarelativistic case $E_0 \gg m$. Since $B_K \doteq m(\alpha Z)^2/2$ we can replace the condition (30) by

$$B_K \ll \pi^2 \cdot T_0 \tag{33}$$

in the nonrelativistic case.

If

$$\pi \xi_{Z+1}(E_0) \gtrsim 1 \tag{34}$$

one can obtain $|\varphi|^2 \sim 2\pi\xi_{Z+1}(E)$ and the integral (27) is $\int dT/T$ at $T \ll T_0 . m$. Thus there is a large contribution coming from the region $T \sim B_K$ where our model is not valid. This can be illustrated by the nonrelativistic equation in the case (34)

$$P_f = 3 \xi^2_{Z+1} (E_0) \Lambda \cdot \left(\ln \frac{T_0}{B_K} - \frac{3}{2} \right) \qquad (35)$$

while the region $T \sim B_k$ adds to the expression in brackets the values of the order of unity. Thus in the case (34) our model gives only a rough estimation but not the quantitative result.

In the case of β^+ decay the model is free from the latter shortcoming. Indeed, for the positron

$$\varphi(E, Z-1) = \frac{2\pi \xi_{Z-1}}{\exp(2\pi \xi_{Z-1}) - 1} \qquad (36)$$

and the region of small $T \sim B_k$ is suppressed.

In the Table I we present the experimental data on the K-shell ionization in the β^- decay for the cases when eq. (5) is true while eq. (34) is not /10-20/. We calculate the term P_f. The Dirac-Fock wave functions /21/ were used to obtain Λ - eqs. (16)-(20) and the numerical calculations of the integrals which enter eqs. (25)-(27) was carried out. Note that the discrepancy between the values of Λ calculated with the functions /21/ and those given by a simple calculation (eq. (23)) do not exceed 10%. There ar several sets of the calculated values of the SO contribution p_B. One can see that being composed with those obtained in /1/ the f.s.i contributions either remove or strongly diminish the discrepancy between the theoretical and the experimental data.

In the Table II we present the data on the β^+ decay. The two sets of the SO calculations are given. One can see the effect of the f.s.i. to be rather large. It also draws nearer the experimental and theoretical data.

IV. THE DISTRIBUTION OF THE SECONDARY ELECTRONS

The equations obtained in sec. II enable us to calculate the distribution of the secondary electrons:

$$\frac{1}{W_0} \cdot \frac{dW_i}{dT\,d\mathcal{E}\,dt_p} = |f_\mathcal{E}|^2 \tag{37}$$

with $f_\mathcal{E}$ describing the transition of the K-electron to the final state with the energy $\mathcal{E}$; $t_p = (p_1 p)/p_1 p$, $p(p_2)$ is the momentum of the β (secondary) electron.

The partial-wave expansion of the secondary electron wave function gives

$$|f_\mathcal{E}|^2 = \tau_{\mathcal{E}0} + \sum_{\ell=0} \theta_{\mathcal{E}\ell} \tag{38}$$

with the shake-off contribution

$$\tau_{\mathcal{E}0} = (\chi^{\tau}_{\mathcal{E}0}, \psi^{\tau}_{1s})^2 \tag{39}$$

Here the indices denote the radial wave function, the normalization of the functions $\chi^{\tau}_{\mathcal{E}}$ being $(\chi^{\tau}_{\mathcal{E}\ell}, \chi^{\tau}_{\mathcal{E}'\ell}) = 2\pi\delta(\mathcal{E}-\mathcal{E}')$
The f.s.i. contribution of the s wave is

$$\theta_{\mathcal{E}0} = 2\xi^2(\mathcal{E})\Big[\langle\chi^{\tau}_{\mathcal{E}0}|\psi^{\tau}_{1s}\rangle\langle\chi^{\tau}_{\mathcal{E}0}|\frac{d}{d\tau}|\psi^{\tau}_{1s}\rangle + |\langle\chi^{\tau}_{\mathcal{E}0}|\ln\tau|\psi^{\tau}_{1s}\rangle|^2 - \langle\chi^{\tau}_{\mathcal{E}0}|\psi^{\tau}_{1s}\rangle\langle\chi^{\tau}_{\mathcal{E}0}|\ln^2\tau|\psi^{\tau}_{1s}\rangle\Big] \tag{40}$$

with the last term vanishing in the ξ^1 powers expansion. Eq. (40) is presented for the nonrelativistic energies T. For $l \geqslant 1$ only the angular parts of the logarithmic terms of eq. (10) contribute and

$$\theta_{\mathcal{E}\ell} = K\langle\chi^{\tau}_{\mathcal{E}\ell}|\psi^{\tau}_{1s}\rangle\Big|^2\frac{(2\ell+1)^2}{\ell^2(\ell+1)^2}\mathcal{P}^2_\ell(t_p)\cdot\xi^2(\mathcal{E}) \tag{41}$$

The integration over t_p gives the energy distribution of the secondary electrons

$$\frac{1}{W_0}\cdot\frac{dW_i}{dTd\mathcal{E}} = 2\Big[\ \tau_{\varepsilon 0} + \xi^2(E)\cdot\Big(\theta_{\varepsilon 0} + \sum_{\ell=1}\frac{2\ell+1}{\ell^2(\ell+1)^2}\big|\langle\chi^2_{\varepsilon\ell}|\psi^2_{1s}\rangle\big|^2\Big]\quad(42)$$

We illustrate the results obtained in this section by the calculation of the spectrum of the secondary electrons in the β-decay of $^{45}_{20}Ca$ integrated over the energies of β-electrons. The Hartree-Fock-Slater wave functions /21/ were used for the description of the electrons. The separate integration of the terms which compose the right side of eq. (42) gives the distribution of the partial waves in $\Lambda = \sum_\ell \Lambda_\ell$

$$\Lambda_0 = 0.71;\quad \Lambda_1 = 1.2;\quad \Lambda_2 = 0.27.\qquad(43)$$

All the integrals over $\mathcal{E}$ are saturated by $\mathcal{E}\sim B_K$. At large $\mathcal{E} \gg B_K$ the distribution (37) can be obtained from the general equations of the paper /8/. The process is dominated by the f.s.i. and the distribution (37) is determined by the region near $t_\rho = 0$ corresponding the small virtuality of the intermediate electron of fig. 1b. The spectrum is /10/

$$\frac{1}{W_0}\,\frac{dW_i}{dTd\mathcal{E}} = \frac{\langle\psi|r^{-2}|\psi\rangle}{2\pi}\cdot\frac{dW_0}{dT}\cdot\frac{d\sigma(T)}{d\mathcal{E}_2}\cdot\frac{1}{W_0}\qquad(44)$$

with $\sigma(T)$ - the cross section of the scattering of the free electrons.

V. THE SUMMARY

We have calculated the final state interaction contribution to the ionization of the K-shell following the β-decay. Our calculations were based on the consistent study of the f.s.i. in the β-decay /7/ taking into account all the terms contributing to the lowest order f.s.i. correction.

We have shown (Tables I, II) the f.s.i. terms to be rather large. The should be taken into account in any attempt to improve the theory of the phenomena. For the β^--decay the f.s.i. contributions being added to the SO results /1/ either remove or strongly diminish the discrepancy between the theoretical and experimental data (Table I). The same referes to the β^+ decay (Table II).

Table I

The probability of the K-shell ionization in the β -decay.

Atom	B_k/T_0	$P_s \cdot 10^{-4}$ /1/	$P_f \cdot 10^{-4}$	$P \cdot 10^{-4}$	Experiment
$^{32}_{15}P$	1.4·(-3)	24.9	2.4	27	47 /10/ 99 /11/ 72 /12/
$^{35}_{16}S$	1.7 (-2)	17.6	16.8	34	23 ± 7 /13/ 20 /14/
$^{36}_{17}Cl$	4.5 (-3)	18.8	4.7	23.5	22 ± 4 /15/
$^{45}_{20}Ca$	1.8 (-2)	12	11.3	23	24.3±3.9 /16/
$^{89}_{38}Sr$	1.2 (-2)	4.11	2.5	6.6	8.6±0.7/16, 17/
$^{90}_{39}Y$	8 (-3)	4.12	2.0	6.1	7 ± 1 /18/ 7.4±1.4 /16/ 5.0±1.1 /19/
$^{114}_{43}In$	1.5 (-2)	2.62	2.1	4.7	5.4±0.4 /20/

Table II

The probability of the K-shell ionization in the β decays. The upper and the lower lines for P_s and P correspond to the calculations of the SO contribution in the models /5/ and /6/.

Atom	$P_s \cdot 10^{-4}$	$P_f \cdot 10^{-4}$	$P \cdot 10^{-4}$	Experiment
$^{58}_{27}Co$	6.7-9.2 13.1	3.3	10-12.5 16.4	13.8±2.4 /22/ 16.6±2.1 /28/
$^{64}_{29}Cu$	5.8-8.25 11.5	4.1	9.9-12.35 15.6	13.2-0.8 /24/ 13.3-1.1 /25/
$^{65}_{30}Zn$	4.8±6.6 10.8	2.8	7.6±9.4 13.6	16.1±3.0 /26/
$^{68}_{31}Ga$	5.54-6.53 9.7	1.8	7.3-8.3 11.5	10.3±1.0 /27/

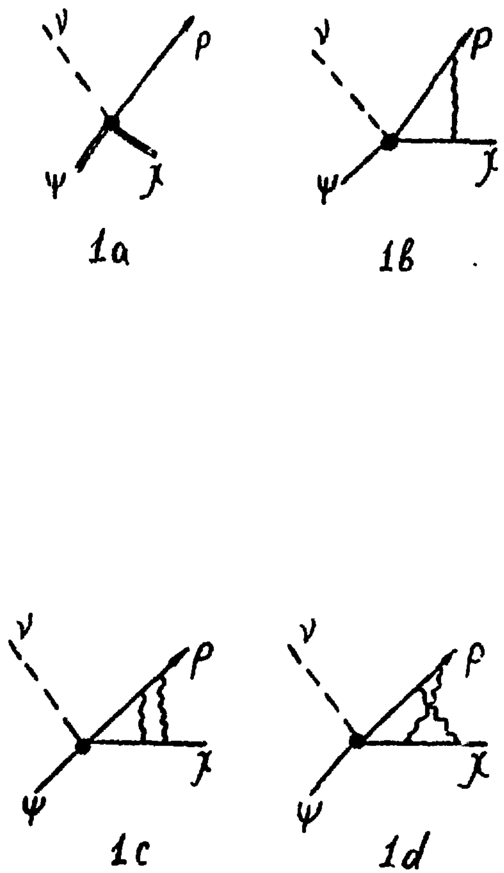

Fig.1. The Feynman diagrams contributing to the final state interaction.

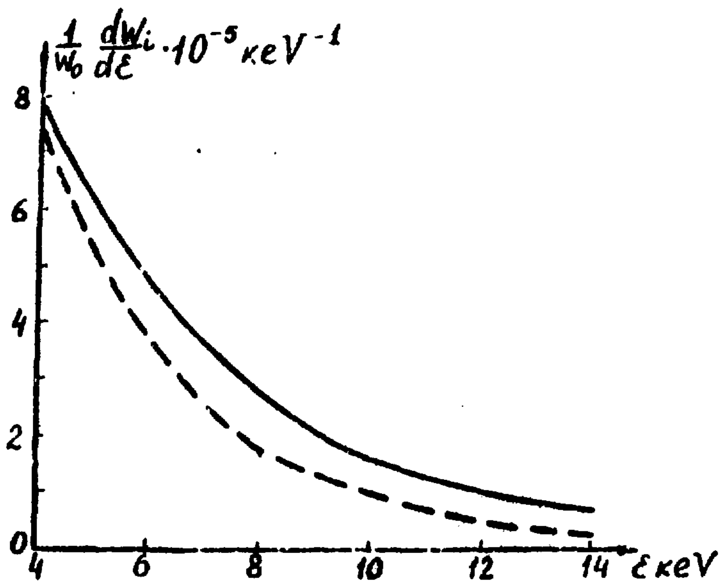

Fig.2. The spectrum of the secondary electrons emitted in the β-decay of $^{45}_{20}Ca$ integrated over the energies of the β-electrons. The dotted line - the f.s.i. are neglected; the solid line - the f.s.i. terms are included.

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