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ATOMIC CHEMICAL COMPOSITION EFFECT ON THE BETA DECAY PROBABILITIES

Within a new theoretical scheme for sensing the atomic chemical environment effect on the beta decay characteristics there are presented numerical results for chemical environment effect on the beta decay in the fluorine, sulphur and nickel. Despite on the relative smallness of the atomic chemical environment effect on the b

1. Introduction

Though in a modern nuclear physics there is a number of principally new problems, connected with an unprecedented progress in the physical experiment, nevertheless the classical problems, including the beta decay or low energy nucleus-nucleus collision etc. are remained under intensive theoretical and experimental interest (c.f.[1-11]). This paper goes on our investigations on estimating the beta decay characteristics and sensing an influence of the chemical environment on the b decay parameters with using an optimal theoretical schemes (c.f.[11-16]). In last years a calculating the b decay processes and sensing an influence of the chemical environment on the beta b characteristics attracts a great interest especially due to the new experimental studies of the b decay for a number of nuclei [1-10]. A number of experimental and theoretical papers appeared where the different aspects of the b decay theory and accounting for different factors are considered. One of the important topics is problem to get the data about the neutrino mass from the beta decay spectra shape. An exact value of the half-decay period for the whole number of heavy radioactive nuclei is important for standardisation of data about their properties. Disagreement between different experimental data regarding the b-decay in heavy radioactive nuclei is provided by different chemical environment radioactive nucleus. For

example, such disagreement in data on the half-decay period for the ^{241}Pu (see, for example, ref. [1,5,8,9]) is explained in some papers by special beta decay channel. The beta particle in this channel does not transit into free state, but it occupies the external free atomic level. According to ref. [1-5], differences in population of these levels are to be a reason of an influence of the chemical environment on the beta decay. So, a sensing the chemical environment effect on the beta decay is very important to be studied as within a consistent, high accurate theoretical calculation scheme as experimental high precise measurement. Under theoretical consideration of the problem, one has to consider the following effects:

- i.). A changing electron wave functions because of the changing atomic electric field due to the difference in the valence shells occupation numbers in different chemical substances;
- ii). A changing up limit of integration under calculating the Fermi integral function in different chemical substances [1,6].

As a rule, the beta particle and neutrino bring away the difference between energies of the mother and daughter atoms. This difference energy is equal to sum of values, provided by atomic nucleus reconstruction and atomic electron shell reconstruction. The entire energy of electron shell of an atom in the different chemical compounds is different. Due to the changing the nuclear charge Z on unite during the beta decay, this entire en-

ergy of electron shell of an atom changes in different chemical compounds by different way; iii). Together with beta decay and ejection of the beta particle out atom it is possible additional channel when the beta electron occupies non-occupied place on the bonded external orbitals of atom. As a rule, special tables [9] for the Fermi function and integral Fermi function is used for calculating the beta spectrum shape. In ref. [9] calculation scheme is based on the non-relativistic Hartree-Fock-Slater approach, but the finite size of nucleus is taken into account. In paper [4] the relativistic Dirac-Fock (DF) method was used. Note that the DF approach is the most wide spread method of calculation, but, as a rule, the corresponding orbitals basis's are not optimized. Some problems are connected with correct definition of the nuclear size effects, QED corrections etc. We are applying below the gauge invariant DF (GIDF) type approach [11-17] for estimating the atomic chemical environment effect on the b decay characteristics for fluorine, , sulphur and nickel.

2. Method

As it is well known a distribution of the b particles on energy in the permitted transitions is as follows [9]:

$$dW_{\beta}(E)/dE = \frac{1}{2\pi^3} G^2 \cdot F(E, Z) \cdot E \cdot p \cdot (E_0 - E)^2 \cdot |M|^2. \quad (1)$$

Here G is the weak interaction constant; E and $p = (E^2 - 1)^{1/2}$ are an entire energy and pulse of beta particle; $E_0 = 1 + (E_{bn} / m_e c^2)$, E_{bn} is the boundary energy of β -spectrum; $|M|$ is a matrix element, which is not dependent upon an energy in a case of the permitted β - transitions.

As usually for calculation of the b decay shape and decay half period one should use the tables of the Fermi function and integral Fermi function. The Fermi function F and integral Fermi function f are defined as follows:

$$F(E, Z) = \frac{1}{2p^2} (g_{-1}^2 + f_{+1}^2), \quad (2a)$$

$$f(E_0, Z) = \int_1^{E_0} F(E, Z) \cdot E \cdot p \cdot (E_0 - E)^2 dE. \quad (2b)$$

Here f_{+1} and g_{-1} are the relativistic electron radial functions; the indexes $\pm l = c$, where $c = (l-j)/(2j+1)$. Two schemes of calculation are usually used: i). the relativistic electron radial wave functions are calculated on the boundary of the spherical nucleus with radius R_0 (it has done in ref. [4]); ii). the values of these functions in the zero are used (see ref.[9]).

The normalisation of electron radial functions f_i and g_i provides the behaviour of these functions for large values of radial valuable as follows:

$$g_i(r) \rightarrow r^{-1} [(E+1)/E]^{1/2} \sin(pr + d), \quad (3a)$$

$$f_i(r) \rightarrow r^{-1} (i/|i|) [(E-1)/E]^{1/2} \cos(pr + d) \quad (3b)$$

An effect of interaction in the final state between beta electron and atomic electrons with an accuracy to $(\alpha Z/v)^2$ is manifested and further accounted for in the first non-vanishing approximation [8]. This contribution changes the energy distribution of the beta electron on value:

$$\frac{dW_{\beta}(E)/dE}{dW_{\beta}^{(0)}(E)/dE} = 1 - (\alpha E/p)^2$$

$$\langle \Psi_{in} | \sum_j^z (a_B / |r_j|) | \Psi_{in} \rangle \quad (4)$$

Here y_{in} – the wave function of atom initial state, z is a number of electrons, a_B is the Bohr radius. As method of calculation of the relativistic atomic fields and electron wave functions, we have used the GIDF approach [10,11]. The potential of Dirac equation includes also the electric and polarization potentials of a nucleus (the gaussian form of charge distribution in the nucleus was used). All correlation corrections of the PT second and high orders (electrons screening, particle-hole interaction etc.) are accounted for [5]. The GIDF equations for N-electron system are written and contain the potential: $V(r) = V(r|nlj) + V_{ex} + V(r|R)$, which includes the electrical and polarization potentials of the nucleus. The part V_{α} accounts for exchange inter-electron interaction. Note that a procedure of the exchange account in the GIDF scheme is similar to one in the usual DF

approach. Regarding the GIDKS scheme, it is similar to usual DKS scheme. The optimization of the orbital bases is realized by iteration algorithm within gauge invariant QED procedure (look its application in the beta-decay theory [5]). Approach allows calculating the continuum wave functions, taking into account fully an effect of exchange of the continuum electron with electrons of the atom. Note that this is one of the original moments of the paper. Another original moment is connected with using the consistent QED gauge invariant procedure for optimization of the electron functions basis's. Numerical calculation and analysis shows that used methods allow getting the results, which are more precise in comparison with analogous data, obtained with using non-optimized basis's. The details of the numerical procedure are presented in ref. [11-17].

3. Results and conclusions

In Table 1 we present presents our data on the atomic chemical environment effect on the probability of β decay $^{17}\text{F} \rightarrow ^{17}\text{O}$. It is easy to see that the quantitative effect of the chemical environment of part of the decay is sufficiently small.

Table 1. The atomic chemical environment effect on the β decay probability $^{17}\text{F} \rightarrow ^{17}\text{O}$; Changing the half-period $T_{1/2}$ (our data)

Decay of neutral atom		
Atom	E_{bn} , eV	$\Delta f/f$, %
$\text{F}^{(0)}$	1748000 1748100	0,006
Decay of ionized atom		
Ion	E_{bn} , eV	$\Delta f/f$, %
$\text{F}^{(-1)}$	1747900 1748000	0,006

The situation (compared ^{17}F) changes in the transition to the consideration of the decay $^{35}\text{S} @ ^{35}\text{Cl}$, $^{63}\text{Ni} @ ^{63}\text{Cu}$. In Table 2 there are presented the corresponding results for the decay $^{35}\text{S} @ ^{35}\text{Cl}$, including the value of $\Delta f/f = -\Delta T_{1/2}/T_{1/2}$. In the case of the decay of $\text{S}^{(0)}$ as the value of the boundary energy it is taken value 167450 eV,

and the decay of the ion $\text{S}^{(+2)}$ - on 30 eV less. Accordingly, in the second version, the energy calculation is based on the value of 167390 eV in the case of the decay $\text{S}^{(+2)}$, and for the decay of $\text{S}^{(0)}$ - 167420 30 eV.

Analysis for two versions of data shows that there are obtained give similar results, and, in particular, very similar values for the changing $T_{1/2}$ when the ionic parameter is changed. Regarding the value of the integral Fermi function, the characteristic value for the decay of ionized sulfur is less than in the case of neutral sulfur, respectively sulfur ionized decay is slower. The value of the Fermi function is greater for the neutral sulfur and, therefore, β -decay of the neutral sulfur is faster. As it can be seen from Table 2, the corresponding difference in the values of $T_{1/2}$ is about 0,04%. The similar data for the decay of $^{63}\text{Ni} @ ^{63}\text{Cu}$ are listed in the Table 3.

The difference in values of $T_{1/2}$ for $^{63}\text{Ni} @ ^{63}\text{Cu}$ is about $\sim 0,1\%$ (see table 3) for the twice-ionized atom of Ni in comparison with a decay of neutral nickel.

Table 2. The atomic chemical environment effect on the β decay probability $^{33}\text{P}^{(0)} \rightarrow ^{33}\text{S}$ Changing the half-period $T_{1/2}$ (our data)

Decay of neutral atom			
Atom	E_{bn} , eV	$f(E_{bn}, Z)$	$\Delta f/f$, %
$\text{S}^{(0)}$	167420 167450	1,36849(- 2) 1,36935(- 2)	0,037
Decay of ionized atom			
Ion	E_{bn} , eV	$f(E_{bn}, Z)$	$\Delta f/f$, %
$\text{S}^{(2+)}$	167390 167420	1,36798(- 2) 1,36884(- 2)	0,037

Correspondingly, the Fermi function value for for two-ionized atom of Ni is less on $\sim 0,1\%$. It means that the decay of the neutral nickel runs faster in comparison with twice-ionized atom. In conclusion let us note that our conclusions fully coincide with analysis and conclusions, presented in [1].

Despite on the relative smallness of the atomic chemical environment effect on

Table 3. **The atomic chemical environment effect on the b decay probability $^{63}\text{Ni} @ ^{63}\text{Cu}$;**

Changing the half-period $T_{1/2}$ (**our data**)

Decay of neutral atom				
Atom	E_{bn} , eV	$f(E_{bn}, Z)$	$\Delta f f.$ %	
$\text{Ni}^{(0)}$	65800	1,38463(-3)	0,095	
	65825	1,38599(-3)		
Decay of ionized atom				
Ion	E_{bn} , eV	$f(E_{bn}, Z)$	$\Delta f f.$ %	
$\text{Ni}^{(+2)}$	65777	1,38332(-3)	0,095	
	65800	1,38478(-3)		

the b decay probabilities for corresponding decays, the situation may be significantly changed under consideration of the beta decay for the heavy elements.

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Abstract

Within a new theoretical scheme for sensing the atomic chemical environment effect on the beta decay characteristics there are presented numerical results for chemical environment effect on the beta decay in the fluorine, sulphur and nickel. Despite on the relative smallness of the atomic chemical environment effect on the b decay probabilities for corresponding decays, the situation may be significantly changed under consideration of the beta decay for the heavy elements

Key words: atomic chemical composition effect, beta decay probability

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АТОМНЫЙ ЭФФЕКТ ВЛИЯНИЯ ХИМИЧЕСКОГО ОКРУЖЕНИЯ НА ВЕРОЯТНОСТЬ БЕТА РАСПАДА

Резюме

В рамках новой теоретической схемы вычисления эффекта влияния химического окружения на характеристики b распада представлены численные оценки влияния химического окружения на b распад фтора, серы, никеля. Несмотря на относительную малость влияния атомного эффекта химической связи на вероятности бета распада, ситуация может быть значительно измениться в случае бета-распада тяжелых элементов.

Ключевые слова: влияние химического окружения, вероятность бета распада.

АТОМНИЙ ЕФЕКТ ВПЛИВУ ХІМІЧНОГО ОТТОЧЕННЯ НА ІМОВІРНІСТЬ БЕТА РОЗПАДУ

Резюме

На основі нової теоретичної схеми обчислення ефекту впливу хімічного отточення на характеристики β розпаду представлені чисельні оцінки впливу хімічного отточення на β розпад фтору, сіри та нікелю. Незважаючи на відносну малість атомного ефекту хімічного середовища на ймовірності β розпаду, ситуація може бути значно змінитися у випадку бета-розпаду важких елементів

Ключові слова: вплив хімічного отточення, ймовірність бета розпаду