SENSING THE ATOMIC CHEMICAL COMPOSITION EFFECT ON THE β DECAY PROBABILITIES

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Abstract

SENSING THE ATOMIC CHEMICAL COMPOSITION EFFECT ON THE BETA DECAY PROBABILITIES

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New theoretical schemes for sensing the atomic chemical environment effect on the beta decay characteristics are proposed. As method of calculation of the relativistic atomic fields and electron wave functions, the gauge invariant Dirac-Fock type and Dirac-Kohn-Sham approaches are used. The numerical results for atomic chemical environment effect on the beta decay in the sulfur and plutonium are presented.

Key words: sensing, atomic chemical composition influence, beta decay probability

Анотація

ДЕТЕКТУВАННЯ ЕФЕКТУ ВПЛИВУ ХІМІЧНОГО ОТТОЧЕННЯ НА ІМОВІРНІСТЬ β РОЗПАДУ

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Запропоновані нові теоретичні схеми детектування та пояснення ефекту впливу хімічного отточення на характеристики β розпаду. Як метод розрахунку релятивістських атомних полів і електронних хвильових функцій використані калібровочно-інваріантні схеми типу Дірака-Фока та Дірака-Кона-Шема. Представлені чисельні оцінки впливу хімічного отточення на β розпад сіри та плутонія.

Ключові слова: детектування, вплив хімічного отточення, імовірність β розпаду.

Аннотация

ДЕТЕКТИРОВАНИЕ ЭФФЕКТА ВЛИЯНИЯ ХИМИЧЕСКОГО ОКРУЖЕНИЯ НА ВЕРОЯТНОСТЬ β РАСПАДА

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Предложены новые теоретические схемы детектирования и объяснения эффекта влияния химического окружения на характеристики β распада. В качестве метода расчета релятивистских атомных полей и электронных волновых функций использованы калибровочно-инвариантные схемы типа Дирака-Фока и Дирака-Кона-Шэма. Представлены численные оценки влияния химического окружения на β распад серы и плутония.

Ключевые слова: детектирование, влияние химического окружения, вероятность β распада.

1. Introduction

Paper is devoted to carrying out new scheme for sensing an influence of the chemical environment on the β decay characteristics with using new theoretical scheme for calculation of the β decay characteristics (c. f. [1-10]).. In last years a calculating the β decay processes and sensing an influence of the chemical environment on the beta β ccharacteristics attracts a great interest especially due to the new experimental studies of the β decay for a number of nuclei [1-3]. A number of experimental and theoretical papers appeared where the different aspects of the β 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 β-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. [4]) 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. [2-6], 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. 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 energy 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 [5,6] for the Fermi function and integral Fermi function is used for calculating the beta spectrum shape. In ref. [5] calculation scheme is based on the non-relativistic Hartree-Fock-Slater approach, but the finite size of nucleus is taken into account. In ref. [6], the latter was taken into account as correction to the Coulomb scheme calculation result and the screening effect was calculated within the atomic Hulten potential. In paper [3] 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. In ref. [11-14] there were developed new ab initio schemes to calculating spectra, wave functions basis's of the heavy elements with account of relativistic, correlation, nuclear, QED effects, based on the gauge-invariant QED perturbation theory (PT) [10,15-18]: gauge invariant DF (GIDF) type and Dirac-Kohn-Sham (GIDKS) approaches. We use these schemes as basic in the problem of sensing an influence of the chemical environment on the β decay characteristics.

2. The beta decay calculation method and the atomic chemical composition effect

As it is well known a distribution of the β particles on energy in the permitted transitions is as follows [5,6]:

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

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 β 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:

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

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

Here f_{+1} and g_{-1} are the relativistic electron radial functions; the indexes $\pm l = \chi$, where $\chi = (l-j)/(2j+1)$. 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. [5]); ii). the values of these functions in the zero are used (see ref. [6]). The half decay period can be defined as follows:

$$T_{1/2} = 2\pi^3 \ln2/[G^2 |M|^2 f(E_0, Z)].$$

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

$$g_l(r) > r^{-1}[(E+1)/E]^{1/2} \sin(pr + \delta_l), \qquad (3a)$$

$$f_l(r) > r^{-1}(l/|l|) [(E-1)/E]^{1/2} \cos(pr + \delta_l). \qquad (3б)$$

As method of calculation of the relativistic atomic fields and electron wave functions, we have used the GIDF and GIDKS approaches [11-14]. 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 [5,6]. New approaches were earlier used in calculation of spectra, relativistic and radiation corrections, hyperfine structure parameters etc. for some heavy and super heavy ions, the beta-decay probabilities, laser-electron-nuclear and meso-atomic processes [10-18]. We set the charge distribution in the nucleus by the Gaussian function:

$$\rho(r|R) = \left(4\gamma^{3/2}/\sqrt{\pi}\right)\exp\left(-\gamma r^2\right).$$

Here $\gamma = 4/\pi R^2$; R is an effective nucleus radius, defined as: $R = 1,60 \cdot 10^{-13} Z^{1/3}$ (cm). The Coulomb potential for spherically symmetric density $\rho(r|R)$ is:

$$V_{nucl}(r|R) = -\left((1/r)\int_0^r dr' r'^2 \rho(r'|R) + \int_r^\infty dr' r' \rho(r'|R)\right).$$

The GIDF or GIDKS 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_{ex} accounts for exchange inter-electron inter-action. 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 rest of the exchange-correlation effects are accounted for in the first two QED perturbation theory orders by the total inter-electron interaction. The optimization of the orbital basises is realized by iteration algorithm within gauge invariant QED procedure [10].

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 basises. 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 basises. The details of the numerical procedure are presented in ref. [9-18].

3. Results and discussion

In order to study sensing the atomic chemical environment effect on the β decay, we have considered the following β decays: $^{35}S \rightarrow ^{35}Cl$ and $^{241}Pu \rightarrow ^{241}Am$. The first transition is allowed; the transition $^{241}Pu \rightarrow ^{241}Am$ is non-unique of the first forbidding. Comparison of the Fermi function values is carried out for different approximations of the exchange account, calculation with using wave functions on the boundary of the charged spherical nucleus and with using squires of the amplitudes of expansion of these functions near zero. The results of our calculation are presented in the table 1.

For the boundary energy under decay of the $S^{(0)}$ it was accepted the value 167450eV. Analogously the value 167420eV was used under decay of the $S^{(+2)}$ in the first variant of calculation. The pair of the energy values: 167420eV and 167390eV has been chosen in the second variant of calculation correspondingly. The experimental value for E_{bn} is as follows: 167400±100eV. Two versions of calculation give practically the same values for changing half decay period under changing the ionic feature: $\Delta f/f = 0,037$ % (GIDF scheme) and $\Delta f/f = 0,039\%$ (GIDKS scheme). Here the following notation is used: $\Delta f/f$ is the relative changing probability of the decay (the integral Fermi function), which is equal to relative changing the decay half period $-\Delta T_{1/2}/T_{1/2}$.

For comparison let us give the value, obtained in the usual DF scheme: $\Delta f/f = 0,03\%$ (DF scheme) [4]. At the same time many applications of the considered theoretical schemes in the atomic calculations have shown the using optimized atomic functions gives more precise results than the non-optimized ones (c. f. [2,4,9-12,17,18]).

Table 1.

The atomic chemical environment effect on the β decay probability

Decay of neutral atom			Decay of ionized atom			Calculation Scheme
Atom	E_{bn}, eV	$f(E_{bn},Z)$	Atom	E_{zp}, eV	$f(E_{bn},Z)$	
$S^{(0)}$	167420	1,36849(-2)	$S^{(2+)}$	167390	1,36798(-2)	GIDF
	167450	1,36935(-2)		167420	1,36884(-2)	
$S^{(0)}$	167420	1,37982(-2)	$S^{(2+)}$	167390	1,37927(-2)	GIDKS
	167450	1,38069(-2)		167420	1,38014(-2)	

Calculation for the $^{35}S \rightarrow ^{35}Cl$ transition showed that the integral Fermi function was less for decay of the ionized sulfur and, as result, decay of the ionized sulfur runs more slowly and, other versa, the Fermi function is more for neutral sulfur and its decay runs more quickly. However, the corresponding difference in values of the half decay period $T_{1/2}$ is a little value. This is agreed with known data (c. f. [4-6]). Naturally, these data are accepted for the sulfur compounds, where the bond can be treated as ionic one.

Another situation, namely, the significant changing of the $T_{1/2}$ value, occurs for the ^{241}Pu. According to our calculation, the Fermi function under double ionization is less on 0,25-0,48%. It means, naturally, that the decay of ^{241}Pu runs more slowly. The typical example of the Pu compounds is pair PuO_2 and PuO [4-6]. The detailed analysis shows [13] that an account of the possible channel of the β decay with occupying external atomic orbitals, in our opinion, gives a reasonable explanation of dependence of the plutonium half decay period upon the chemical composition than version without account of this channel. In any case, using the calculation schemes [11-14] allows to make theoretically a sensing the atomic chemical environment effect on the β decay characteristics with the most physically reasonable result (see also [14,15]).

So, we have proposed new theoretical schemes for sensing the atomic chemical environment effect on the β decay and presented the results, showing the influence of the chemical environment on the β decay characteristics for the sulfur and plutonium.

References

1. Izosimov I. N., Kazimov A. A., Kalinnikov V. G., Solnyshkin A. A. and Suhonen J., β-Decay Strength Measurement, Total β-Decay Energy Determination and Decay-Scheme Completeness Testing by Total Absorption γ-ray Spectroscopy// Phys. Atom. Nucl. — 2004. — Vol. 67. — P. 1876-1882.
2. Kopytin I. V., Karelin K. N., and Nekipelov A. A. Exact Inclusion of the Coulomb Field in the Photo-beta Decay of a Nucleus and Problem of Bypassed Elements// Phys. Atom. Nucl. — 2004. — Vol. 67, N8. — P. 1429-1441.
3. Karpeshin F. F., Trzhaskovskaya M. B., Gangrskii Yu. P.,Resonance Internal Conversion in Hydrogen-Like Ions //JETP. — 2004. — Vol. 99, N2. — P. 286-289.
4. Band I. M., Listengarten M. A., Trzhaskovskaya M. B., Possibility of beta decay in model of atom of the Hartree-Fock-Dirac and influence of chemical composition on the beta decay// Izv. AN USSR. — 1987. — Vol. 51,N11. — P. 1998-2000.
5. Gelepov B. C., Zyryanova L. N., Suslov Yu. P. Beta processes. — L., 1990. — 372p.
6. Behrens H., Janske J. Landolt-Berstein. New series. Group 1. V. 4. Berlin-N-Y.:Spriner, 1999.
7. Tegen R. Beta decay of the free neutron and a (near) degenerate neutrino mass// Nucl. Phys. A.: Nucl. and Hadr. Phys. — 2002. — Vol. 706. — P. 193-202.
8. Goldansky V. I., Letokhov V. S. On problem of g laser on nuclear transitions//JETP. — 1974. — Vol. 67. — P. 513-524.
9. Ivanov L. N., Letokhov V. S. Spectroscopy of autoionization resonances in heavy elements atoms// Com. Mod. Phys. D.:At. Mol. Phys. — 1985. — Vol. 4. — P. 169-184.
10. Glushkov A. V., Ivanov L. N. Radiation Decay of Atomic States: atomic residue and gauge non-invariant contributions // Phys. Lett. A. — 1992. — Vol. 170,N1. — P. 33-37.
11. Glushkov A. V., Malinovskaya S. V., Co-operative laser nuclear processes: border lines effects// In: New projects and new lines of research in nuclear physics. Eds. G. Fazio and F. Hanappe, Singapore : World Scientific. — 2003. — P. 242-250.

12. Glushkov A. V., Malinovskaya S. V., Svinarenko A. A., Chernyakova Yu. G., QED Calculation of Electron Satellites Spectra in Intense Laser Field in Multicharged Ion//Int. J. Quant. Chem. — 2004. — Vol. 99,N5. — P. 673-678.

13. Malinovskaya S. V., Dubrovskaya Yu. V., Electron re-arrangement resulting from beta decay: New relativistic quantum-mechanical approach// Proc. Intern. Nuclear Physics Conference, Geteborg (Sweden), 2004. — P. 131.

14. Glushkov A. V., Dubrovskaya Yu. V. Consistent quantum mechanical calculation of beta decay probabilities and effect of chemical environment on beta decay// Proc. Intern. Nuclear Physics Conference, Geteborg (Sweden), 2004. — P. 135.

15. Glushkov A. V. Negative Ions of inert Gases// Pis'ma to JETP. — 1992. — T. 55,N2- C. 104-107; JETP Lett. — 1992. — Vol. 55,N2. — P. 97-100.

16. Glushkov A. V., Ivanova E. P. Theoretical Study of Multicharged Ions Spectra of Ne-and F- isoelectronic sequences// J. Quant. Spectr. Rad. Transfer. — 1986. — Vol. 36, N2. — P. 127-145.

17. Glushkov A. V., Rusov V. D., Ambrosov S. V., Loboda A. V., Resonance states of compound super-heavy nucleus and EPPP in heavy nucleus collisions // New Projects and New Lines of research in Nuclear physics. Eds. Fazio G.,Hanappe F. — Singapore : World Sci., 2003. — P. 142-154.

18. Glushkov A. V., Ambrosov S. V., Loboda A. V., et al, QED calculation of the super heavy elements ions: energy levels, radiative corrections and hfs for different nuclear models// Nucl. Phys. A.: Nucl. and Hadr. Phys. — 2004. — Vol. 734. — P. 21-24.