UDC 539.135

Yu. V. Dubrovskaya, O. Yu. Khetselius, A. V. Ignatenko and D. E. Sukharev

Odessa National Polytechnical University, 1, Shevchenko av., Odessa, Ukraine
Odessa State Environmental University, 15, Lvovskaya str., Odessa, Ukraine
e-mail: nucdubr@mail.ru

RELATIVISTIC AND NONRELATIVISTIC APPROACHES IN THEORY OF PERMITTED BETA-RANSITIONS: AN EFFECT OF ATOMIC FIELD ON FERMI AND INTEGRAL FERMI FUNCTIONS VALUES

Within a new optimized gauge-invariant Dirac-Fock approach it is considered a problem of computing the permitted beta transition probabilities and estimating a quality of computing the Fermi and integral Fermi functions in dependence upon the type of the atomic self-consistent field. It is shown that for small and middle values for the nuclear charge (Z <40) the difference between data obtained from other methods is low (hundredths of %). At the large Z (till Z~ 95; for example the beta decay 241Pu-241Am) calculation in a case of the HFSrel field gives 0.5% lower value for F, and respectively in a case of the GIDF field - 0.8%, compared with the non-relativistic HFSnerel value. This difference is explained by an effect of the squeezing for relativistic orbitals.

1. Introduction

In this paper we go on studying a contribution of different factors which make an influence on the permitted beta decay characteristics and consider a quality of computing the Fermi function and integral Fermi function in our consistent relativistic approach and alternative theoretical methods. Computing the b decay characteristics is traditionally of a great interest that is strengthened 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. Naturally the important topic is problem to get the renewed 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. Above important questions of theort one could note the following effects too: a). an influence of choice of atomic field model on the numerical characteristics of the beta decay, especially, it concerned the permitted beta transitions; b). changing electron wave functions as solutions of the corresponding quantum mechanical equations because of the changing atomic electric field and a difference in the valence shells occupation numbers in different chemical substances; c). A changing up limit of integration under calculating the Fermi integral function in different chemical substances [1,6].

As a rule, special tables [9] for the Fermi function and integral Fermi function are used for computing 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 our gauge invariant DF (GIDF) type approach [11-17] for computing the permitted beta transition probabilities and estimating a quality of computing the Fermi and integral Fermi functions in dependence upon the type of the atomic self-consistent field.

2. Method

The details of our approach have been presented earlier (see, for example, [10,11,17,18]), here we are limited by the key ideas. As it is well known a distribution of the b particles on energy in the permitted transitions is as follows [9]:

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

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. The key elements of the beta-decay theory for computing the b decay shape and decay half period are the Fermi function and integral Fermi function. The Fermi function F and integral Fermi function f are defined as follows:

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

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

Here f_{+l} and g_{-l} 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:

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

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

An effect of interaction in the final state between beta electron and atomic electrons with an accuracy to $(aZ/v)^2$ 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 and is derived in Ref. [1].

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_{ex} accounts for exchange inter-electron interaction. The optimization of the orbital basis's 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

The results of computing the atomic field effect of the Fermi function F values (HFS_{nonrel}, GIDF) are listed in Table 1.As the test parameter it is used the parameter:

$$\Delta_2 = \{[F^{rel}_{DIDF} (E, Z)/ F^{nonrel}_{HFS} (E, Z)]-1\}\cdot 100\%,$$

де F^{nonrel}_{HFS} is calculated in the Hartree-FockSlater (HFS) model atomic field (Harston-Pyper,1986), F^{rel}_{DIDF} – GIDF (our data). It is very inmportant to note that difference between data obtained by relativistic methods: GIDF and relativistic HFS is not significant (fractions of present) for the little and middle values of the nuclear charge Z.

Table 1

An influence of the atomic field model on the Fermi function F (E, Z) values: Δ_2 (%)

E_{kin}, keV	Z=20	Z=63	Z=95
10	-0,08	-0,24	-0,79
50	-0,06	-0,23	-0,77
100	+0,04	-0,18	-0,68
500	+0,13	-0,14	-0,61

Nevertheless, for larger Z (till Z =95) the HFS_{rel} calculation gives the value F which is less on 5% in comparison with the corresponding non-relativistic HFS_{nonrel} . For our approach this value is 0,8%. We suppose that this fact is connected with the effect of relativistic squeeze of the orbitals. In this case, the wave function (continuum) is to a greater extent screened from the charge of the atomic nucleus by a relativistic field of atomic electrons than the corresponding non-relativistic one. Further we present the results of computing function F for choosing different definitions of cited function. In the first case, the calculation of the F function is carried out using values electron wave functions on the boundary of the nucleus, in the second case - through the squares of the amplitudes of radial expansion of the wave functions $f^2_{+1}(0) + g^2_{-1}(0)$ when r→0. Here the test parameter is as follows:

$$\Delta_3 = \{[F (E, Z, R=0)) /$$

$$/F (E, Z, R=R_0]-1\}\cdot 100\%,$$

where F (E, Z, R = R0) – the function Fermi calculated the values of the wave functions on the boundary of the nucleus; F (E, Z, R = 0) - the Fermi function values calculated through the squares of the amplitudes of radial expansion of the wave functions $f^2_{+1}(0) + g^2_{-1}(0)$ when r→0. The corresponding results are presented in Table 2.

Table 2

The difference Δ_3 (%) between values of the Fermi function F (E, Z) for different definitions F (E, Z): HFS – (Band et al, 1986,2006), GIDF – our data.

E_{kin}, keV	Z=20		Z=63 GIDF	Z=95	
	HFS	GIDF		HFS	GIDF
0,1	1,35	1,39	12,72	33,9	36,8
1,0	1,37	1,42	12,84	34,1	37,2
50	1,38	1, 45	12,95	34,2	37,6
500	1,50	1,58	13,10	35,5	39,88

With the growing difference in Z values of the F function significantly increase. Similarly, the same situation takes a place with changing the integral Fermi function. In the transition from the first f definition to the second definition of the f function increases for decays:

i). ^{33}P-^{33}S (E_{bound}=249keV),^{35}S-^{35}Cl (E_{bound} =167keV) на 2-4%,

ii). ^{63}Ni-^{63}Cu (E_{bound} =65,8 keV)- на 5%,

iii). ^{155}Eu-^{155}Gd (E_{bound} =140,7 keV)-12%,

iv). ^{241}Pu-^{241}Am (E_{bound} =20,8 keV)-32%.

In literature there are different points of view on the correctness of a determination of the *F* function . We confirm more consistent and corrected definition of the *F* function through the squares of the amplitudes of radial expansion of the wave functions $f^2_{+1}(0) + g^2_{-1}(0)$ when r→0. An important issue is concerned with an area of the formation of $f(E_{bound}, Z)$.

The standard test parameter is as follows:

$$y = \int_0^x F(E,Z)\, Ep\, (E_0 - E)^2\, dE \Big/ \int_0^{E_0} F(E,Z)\, Ep\, (E_0 - E)^2\, dE$$

Ine Table 3 we present our estimates of the forming area for the integral Fermi function *f*

Table 3

The forming area for the integral Fermi function f (our estimates): t=x/E_{bound}

E_{bound} keV	β-decay	*y*, %			
		t=0,3	0,5	0,7	0,9
20,8	^{241}Pu→^{241}Am	67	89	99	100
39,4	^{106}Ru→^{106}Rh	66	88	98	100
65,8	^{63}Ni→^{63}Cu	65	87	97	100
140,7	^{155}Eu→^{155}Gd	63	84	96	100
167,4	^{35}S→^{35}Cl	58	81	95	100
249	^{33}P→^{33}S	53	78	93	100
257	^{45}Ca→^{45}Sc	52	77	91	100

Therefore, we have carried out the detailed quantitative impact assessment of the Fermi function F (E, Z) for a number permitted by beta-decays in dependence upon the choice of an atomic field in a few calculated methods such as HFS, HFS with taking into account the relativistic corrections in the Breit-Pauli approximation and our relativistic optimized DF one. It is shown that for small and middle values for the nuclear charge (Z <40) the difference between data obtained from other methods is low (hundredths of %). At the large Z (till Z~ 95; for example the beta decay ^{241}Pu-^{241}Am) calculation in a case of the HFS_{rel} field gives 0.5% lower value for F, and respectively in a case of the GIDF field - 0.8%, compared with the non-relativistic HFS_{nerel} value. This difference is in our opinion, explained by an effect of the squeezing for relativistic orbitals. In this case, the wave function (of continuum) is to a greater extent screened from the charge of the atomic nucleus by relativistic field of atomic electrons than by corresponding not- relativistic field.

References

1. Glushkov A.V., Khetselius O.Yu., Lovett L., Electron-b-nuclear spectroscopy of atoms and molecules and chemical environment effect on the b-decay parameters// Advances in the Theory of Atomic and Molecular Systems Dynamics, Spectroscopy, Clusters, and Nanostructures. Series: Progress in Theoretical Chemistry and Physics, Eds. Piecuch P., Maruani J., Delgado-Barrio G., Wilson S. (Berlin, Springer).-2009.-Vol. 20.-P. 125-172.
2. Tegen R., Beta decay of the free neutron and a (near) degenerate neutrino mass//Nucl.Phys.A.-2002.-Vol.706.-P.193-202.
3. Izosimov I. N., Kazimov A. A., Kalinnikov V. G., Solnyshkin A. A. and Suhonen J., Beta-decay strength measurement, total beta-decay energy determination and decay-scheme completeness testing by total absorption gamma-ray spectroscopy// Phys. Atom. Nucl.-2004.-Vol. 67, N10.-1876-1882.
4. Kopytin I. V., Karelin K. N., and Nekipelov A. A. Exact inclusion of the coulomb field in the photobeta decay of a nucleus and problem of bypassed elements// Phys. Atom. Nucl.-2004.-Vol. 67, N8.-P.1429-1441.

5. 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.1998-200
6. Glushkov A.V., Laser- electron-b-nuclear spectroscopy of atomic and molecular systems and chemical environment effect on the b-decay parameters: Review //Photoelectronics.-2010.-N19.-P.28-42.
7. Karpeshin F.,Trzhaskovskaya M.B., Gangrskii Yu.P.,Resonance Internal Conversion in Hydrogen-Like Ions // JETP.-2004.-Vol.99, N2.-P.286-289.
8. Kaplan I., Endpoint energy in the molecular beta spectrum, atomic mass defect and the negative $m_{\nu_e}^2$ puzzle// J.Phys.G.: Nucl.Part.Phys.-1997.-Vol.23.-P.683-692.
9. Drukarev E.G., Strikman M.I., Final state interactions of beta electrons and related phenomena// JETP.-1986. – Vol.64(10).-P.1160-1168.
10. Gelepov B.C., Zyryanova L.N., Suslov Yu.P. Beta processes.-Leningrad: Nauka, 1972.-372p.
11. Malinovskaya S.V., Dubrovskaya Yu.V., Vitavetskaya L.A., Advanced quantum mechanical calculation of the beta decay probabilities// Low Energy Antiproton Phys. (AIP).-2005.-Vol.796.-P.201-205.
12. Malinovskaya S.V., Dubrovskaya Yu.V., Zelentzova T.N., The atomic chemical environment effect on the b decay probabilities: Relativistic calculation// Kiev University Bulletin. Series Phys.-Math.–2004.-№4 .-C.427-432.
13. Glushkov A.V., Malinovskaya S.V., Dubrovskaya Yu.V., Sensing the atomic chemical composition effect on the b decay probabilities // Sensor Electr. & Microsyst. Techn.-2005.-N1.-P.16-20.
14. Dubrovskaya Yu.V., The atomic chemical environment and beta electron final state interaction effect on beta decay probabilities// Photoelectronics.-2005.-N14.-P.86-88.
15. Dubrovskaya Yu.V., The beta electron final state interaction effect on beta decay probabilities// Photoelectronics.-2006 .-N15.-P.92-94.
16. Turin A.V., Khetselius O.Yu.,. Dubrovskaya Yu.V, The beta electron final state interaction effect on beta decay probabilities for ^{42}Se nucleus within relativistic Hartree-Fock approach//Photoelectronics.-2007.-N16.-P.120-122..
17. Dubrovskaya Yu.V., Atomic chemical composition effect on the beta decay probabilities//Photoelectronics.-Vol.22.-P.124-129.
18. Dubrovskaya Yu.V., Sukharev D.E., Vitavetskaya L.A., Relativistic theory of the beta decay: Environment and final state interaction effects// Photoelectronics.-2011.-Vol.20.-P.113-116

This article has been received within 2015

UDC 539.135

Yu. V. Dubrovskaya, O. Yu. Khetselius, A. V. Ignatenko, D. E. Sukharev

RELATIVISTIC AND NONRELATIVISTIC APPROACHES IN THEORY OF PERMITTED BETA-RANSITIONS: AN EFFECT OF ATOMIC FIELD ON FERMI AND INTEGRAL FERMI FUNCTIONS VALUES

Abstract.

Within a new optimized gauge-invariant Dirac-Fock approach it is considered a problem of computing the permitted beta transition probabilities and estimating a quality of computing the Fermi and integral Fermi functions in dependence upon the type of the atomic self-consistent field. It is shown that for small and middle values for the nuclear charge (Z <40) the difference between data obtained from other methods is low (hundredths of %). At the large Z (till Z~ 95; for example the beta decay ^{241}Pu-^{241}Am) calculation in a case of the HFS_{rel} field gives 0.5% lower value for F, and respectively in a case of the GIDF field - 0.8%, compared with the non-relativistic HFS_{nerel} value. This difference is explained by an effect of the squeezing for relativistic orbitals.

Key words: the probability of beta decay, the Fermi function, model of the atomic field

УДК 539.135

Ю. В. Дубровская, О. Ю. Хецелиус, А. В. Игнатенко, Д. Е. Сухарев

РЕЛЯТИВИСТСКИЙ И НЕРЕЛЯТИВИСТСКИЙ ПОДХОДЫ В ТЕОРИИ РАЗРЕШЕННЫХ БЕТА-ПЕРЕХОДОВ: ВЛИЯНИЕ ВИДА АТОМНОГО ПОЛЯ НА ЗНАЧЕНИЯ ФУНКЦИИ ФЕРМИ И ИНТЕГРАЛЬНОЙ ФУНКЦИИ ФЕРМИ

Резюме.

В новой оптимизированной калибровочно-инвариантной теории Дирака-Фоку рассмотрена проблема вычисления вероятности разрешенных бета переходов и оценки качества вычисления функции Ферми и интегральной функции Ферми в зависимости от типа атомной поля. Проведена детальная количественная оценка влияния выбора атомного поля, генерируемого в методах Хартри-Фока-Слэтера, Хартри-Фока-Слэтера с учетом релятивистских поправок в приближении Брейта-Паули ($ХФС_{рел}$) и авторской версии оптимизированного метода Дирака-Фока (ОДФ) на функцию Ферми $F(E, Z)$ для ряда разрешенных бета распадов. Показано, что для малых и средних значений заряда ядра (Z <40) разница данных, полученных на основе всех методов является незначительной (сотые доли %). При больших Z (двигаясь к Z = 95; ^{241}Pu-^{241}Am) расчет в поле $ХФС_{рел}$ дает на 0,5% меньшую величину для F, а в поле ОДФ на 0.8%, по сравнению с нерелятивистским значением $ХФС_{нерел}$, что связано с эффектом релятивистского сжатия орбиталей.

Ключевые слова: вероятность бета распада, функция Ферми, модель атомного поля.

УДК 539.135

Ю. В. Дубровська, О. Ю. Хецеліус, Г. В. Ігнатенко, Д. Є. Сухарев

РЕЛЯТИВІСТСЬКИЙ І НЕРЕЛЯТІВІСТСКИЙ ПІДХОДИ В ТЕОРІЇ ДОЗВОЛЕНИХ БЕТА- ПЕРЕХОДІВ: ВПЛИВ ВИДУ АТОМНОГО ПОЛЯ НА ЗНАЧЕННЯ ФУНКЦІЇ ФЕРМІ І ІНТЕГРАЛЬНОЇ ФУНКЦІЇ ФЕРМІ

Резюме.

У новій оптимізованої калібрувально-інваріантній теорії Дірака-Фоку розглянута проблема обчислення ймовірності дозволених бета переходів, оцінки якості обчислення функції Фермі і інтегральної функції Фермі в залежності від типу атомної поля. Проведена докладна кількісна оцінка впливу вибору атомного поля, генеруємого у методах Хартрі-Фока-Слетеру, Хартрі-Фока-Слетеру з врахуванням релятивістських поправок у наближенні Брейта-Паулі ($ХФС_{рел}$) і авторської версії оптимізованого методу Дірака-Фоку (ОДФ) на функцію Фермі *F(E,Z)* для ряду дозволених бета розпадів. Показано, що для малих і середніх значень заряду ядра ($Z<40$) різниця даних, отриманих на основі всіх методів є незначною (соті долі %). При більших Z (рухуючись до $Z=95$; ^{241}Pu-^{241}Am) розрахунок у полі $ХФС_{рел}$ дає на 0,5% меншу величину для *F*, а в полі ОДФ на 0.8%, у порівнянні з нерелятивістським значенням $ХФС_{нерел}$, що пов'язано з ефектом релятивістського стиснення орбіталей.

Ключові слова: імовірність бета розпаду, функція Фермі, модель атомного поля