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Corrections for exchange and screening effects in low-energy beta decays

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The beta spectra of ^{241}Pu and ^{63}Ni were recently measured using metallic magnetic calorimeters. This powerful experimental technique allows theoretical beta spectra calculations to be tested at low energy with an accuracy never before achievable. Their comparison with classical beta calculations exhibits a significant deviation below 4 keV for ^{241}Pu and 8 keV for ^{63}Ni . The atomic exchange effect explains the main part of this deviation in the ^{63}Ni beta spectrum. This effect has a significant contribution, equivalent to the magnitude of the screening, in the ^{241}Pu beta spectrum.

I. INTRODUCTION

A beta spectrum is the product of a weak interaction coupling constant, a statistical phase space factor, the so-called Fermi function which corrects for the Coulomb effects, and a shape factor. The phase space factor simply reflects the momentum distribution between the electron and the neutrino. The shape factor contains all the remaining energy dependencies, such as leptonic and nuclear matrix elements or corrections for atomic effects. A program to calculate the shape of beta spectra for allowed and forbidden unique transitions has already been developed and described elsewhere [1].

Atomic effects play an important role in determining the shape of beta spectra, mainly at low energy. The precise knowledge of beta spectra shapes at low energy is of great importance in activity measurements using the Liquid Scintillation Counting technique or in deposited dose calculations, for instance. In these two examples, a beta electron of, say, 2 keV does not have the same influence as two beta electrons of 1 keV each. This fact can be easily understood through the concept of linear energy transfer [2].

Atomic electrons partially screen the nuclear charge seen by the beta electron: this is the well-known screening effect. The sudden change of the nuclear charge can induce atomic excitations or internal ionizations, which are respectively called shake-up and shake-off effects and are not expected to have a contribution higher than 0.1 %. The exchange effect is also an atomic effect. It arises from the creation of a beta electron in a bound orbital of the daughter atom corresponding to one which was occupied in the parent atom. An atomic electron from the bound

orbital simultaneously makes a transition to a continuum orbital of the daughter atom. This process cannot be distinguished from the direct decay to a final state containing one continuum electron.

Metallic magnetic calorimeters have been shown to be a powerful experimental technique to study the energy spectra of beta particles having a maximum energy of about 1 MeV. ^{241}Pu [3] and ^{63}Ni [4] beta spectra were recently measured using such detectors. The low maximum energy of each transition, coupled with the energy resolution (29 eV at 5.9 keV) and the energy threshold (300 eV for ^{241}Pu , 200 eV for ^{63}Ni) of the measurements, allow the theoretical beta spectra calculations to be tested with an accuracy never before achieved. These spectra are compared in the present work with calculations that take into account the screening and exchange effects.

II. CALCULATIONS

A. Exchange effect

As set out in detail in [5], the exchange effect is expressed as a correction factor which modifies the beta spectrum intensity I :

$$\frac{dI}{dE} = \frac{dI^{NE}}{dE} [1 + \eta_{ex}^T(E)], \quad (1)$$

where the superscript NE stands for 'no exchange', and $\eta_{ex}^T(E)$ is the total exchange factor depending on the beta electron energy E . The exchange factor involves the overlap between the electron radial wave functions of the bound and continuum orbitals.

For allowed transitions, only beta electrons created in an s bound orbital of the daughter atom take part in η_{ex}^T . Indeed, a beta transition is classified by the properties of the initial and final nuclear states: the total angular momentum change ΔJ and the parity change $\Delta\pi$. For an

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allowed transition, $\Delta J = 0, \pm 1$ and $\Delta\pi = 0$, which means that the electron-neutrino pair does not carry away any orbital angular momentum. Thus, only the ns orbitals are reachable by the beta electron.

The total exchange factor can be written in terms of the subshell contributions η_{ex}^{ns} :

$$\eta_{ex}^T(E) = \sum_n \eta_{ex}^{ns}(E) + \sum_{\substack{m,n \\ (m \neq n)}} \mu_m \mu_n, \quad (2)$$

and the exchange factor of the n -th subshell is given by:

$$\eta_{ex}^{ns}(E) = f(\mu_n^2 - 2\mu_n). \quad (3)$$

The parameters μ_n and f are expressed in terms of the bound ($f_{n,\kappa}^b, g_{n,\kappa}^b$) and continuum ($f_{\kappa}^c, g_{\kappa}^c$) electron radial wave functions evaluated at the nuclear radius R according to:

$$\mu_n = \langle Es' | ns \rangle \frac{g_{n,\kappa}^b(R)}{g_{\kappa}^c(R)}, \quad (4)$$

$$f = \frac{g_{\kappa}^c(R)^2}{g_{\kappa}^c(R)^2 + f_{\kappa}^c(R)^2}. \quad (5)$$

The quantum number $\kappa = -1$ for s orbitals. $\langle Es' | ns \rangle$ is the overlap between the bound orbital $|ns\rangle$ and the continuum orbital $\langle Es' |$ over the entire space.

Harston and Pyper [5] pointed out that the screening must distort the wave functions and can contribute significantly to the overlap. They took this effect into account using effective nuclear charges for the calculations of the wave functions involved. This does not concern the wave functions evaluated at the nuclear radius, for which the full nuclear charge has to be used. Following [5], the effective nuclear charges were determined from the mean radii of the orbitals, which were taken from [6] and [7] in the non-relativistic case (Hartree-Fock calculations), and from [8] in the relativistic case (Dirac-Fock calculations).

Finally, analytical electron radial wave functions were taken from [9] and are expressed in terms of the confluent hypergeometric function. Good accuracy on the overlap requires evaluating this special function for complex arguments of large magnitudes. Formalism of the exchange effect and consecutive calculations have already been set out in detail in [10].

B. Screening

When calculating a beta spectrum, the screening effect is generally corrected for using a constant Thomas-Fermi potential which is subtracted from the total energy of the particle [11]. This method creates a non-physical discontinuity at the minimum energy defined by the potential [1]. This minimum energy is $\lesssim 20$ keV, hence the discontinuity does not generally affect the practical use of the

spectrum. Physically the influence of the atomic electrons is expected to be significant when the beta wavelength is comparable to the atom size, thus at low energy.

As it has been shown in [10], this simple method, which allows analytical wave functions to be used, cannot be reasonable for high Z and at low energy. The usual way is to correct the Coulomb potential for the influence of the atomic electrons. Such screened potentials can be found in [12]. However, the Dirac equations for the wave functions cannot be solved analytically anymore, hence we have followed the numerical method described in detail in [13]. The electron radial wave functions are expressed locally as power series expansions, allowing the Dirac equations to be solved using recurrence relations. Special treatment is needed for the solutions relative to the regular singular point $r = 0$ and the irregular singular point $r = \infty$. Then, the calculation consists in evaluating the wave functions near $r = 0$, at a point sufficiently far away from the nucleus for a correct evaluation with the expansion near $r = \infty$, and step by step between these two points in order to reconnect each solution with the appropriate renormalisation and phase shift.

In order to be sure of our calculations, the tables from [14] of various parameters used to calculate beta spectra were recalculated. Despite a lack of precise and detailed information on the exact way these parameters had been calculated, the unscreened Coulomb functions (Table II in [14]) were perfectly reproduced, and the ratios of screened to unscreened Coulomb functions (Table III in [14]) were in very good agreement for all Z .

Beta spectra are classically calculated using the electron radial wave functions evaluated at the nuclear radius. To take the screening into account, it is not just sufficient to renormalise the wave functions and evaluate them at the nuclear radius because the screened potentials are very weak at this distance, and so, the modification is completely negligible over the entire range of the spectrum. It is, in fact, necessary to take into account the spatial extension of the wave functions. As described in [13], this can be done by evaluating the transition matrix of the corresponding beta-decay. However the calculations become very complicated because the electron wave functions are coupled with the nuclear matrix elements involved. To avoid this difficulty, we can benefit from the parameter f defined in eq. (5) for the exchange effect. This parameter represents the fraction of beta electrons which emerge in a continuum κ state if the exchange process is omitted. Instead of squared wave functions evaluated at the nucleus surface, we use the mean value of the squared radial wave functions over the entire space. That is to say:

$$\overline{g_{\kappa}^2} = \frac{1}{\Delta R} \int_{\Delta R} g_{\kappa}^2(r) dr \quad (6)$$

where ΔR is the effective integration interval. The correction factor that takes the screening into account is then:

$$C_{sc} = 1 + \frac{\Delta R_{nosc}}{\Delta R_{sc}} \cdot \frac{f_{sc} - f_{nosc}}{f_{nosc}} \quad (7)$$

where the subscript *sc* (*nosc*) means that the screened (unscreened) wave functions were used. In this way, the screening correction is physically meaningful and is correct as long as we are not dealing with forbidden non-unique transitions. Indeed, for allowed and forbidden unique transitions, the nuclear matrix elements can be factored out and have no beta energy dependence [1].

III. RESULTS

The beta spectra of ^{241}Pu [3] and ^{63}Ni [4] were recently measured using metallic magnetic calorimeters. Each source was enclosed in a gold absorber assuring a 4π solid angle and 100 % detection efficiency.

These spectra were firstly compared to classical beta calculations and a significant enhancement of the experimental spectra at low energy ($\lesssim 4$ keV for ^{241}Pu , $\lesssim 8$ keV for ^{63}Ni) could not be explained.

A. ^{63}Ni

The radionuclide ^{63}Ni decays entirely by β^- emission to the ground state of ^{63}Cu . The nature of the transition is allowed, with $Q_{\beta^-} = 66.980$ (15) keV and $T_{1/2} = 98.7$ (24) yr [15].

Calculations of the partial and total exchange factors were performed using non-relativistic effective nuclear charges, but results remain unchanged with relativistic ones. Consistently with the chemical composition of the source, we have considered a neutral Ni atom with its 1 to 4 *s* orbitals filled. The total exchange factor is in very good agreement with the one given from 5 to 67 keV in [16], where unfortunately no details of their calculations are given. Calculation of the screening correction was performed using the effective potential given in [12]. The resulting spectra are compared with the measured spectrum of [4] in figure 1.

B. ^{241}Pu

The radionuclide ^{241}Pu decays mainly by β^- emission to the ground state of ^{241}Am , and the transition probability was evaluated to be $P(\beta^-) = 99.99756$ (2) %, the remaining being α decay [17]. The nature of the transition is first forbidden non-unique, with $Q_{\beta^-} = 20.8$ (2) keV and $T_{1/2} = 14.33$ (4) yr.

In forbidden non-unique transitions, the energy dependence of the nuclear matrix elements cannot be factored out, which greatly complicates the calculations of the beta spectra shapes. However, first forbidden non-unique transitions which fulfil the assumption $2\xi = \alpha Z/R \gg E_0$

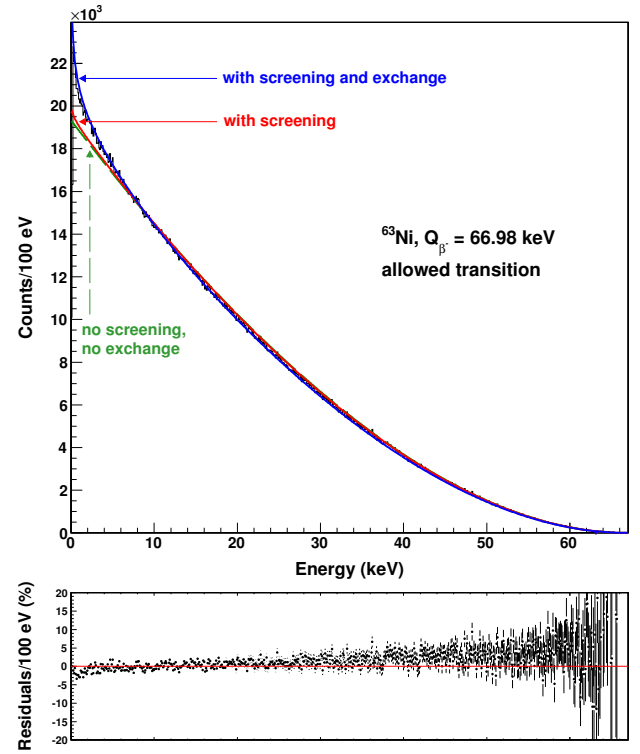


FIG. 1. Comparison between the measured beta spectrum of ^{63}Ni from [4] and three calculated spectra: a classical allowed transition without screening nor exchange, the same including screening, and a complete one including screening and exchange corrections. The corresponding residuals relative to the measured spectrum are shown just below.

can be treated as allowed ones [18], with α the fine structure constant, R the radius of the daughter nucleus, Z its nuclear charge, and E_0 the maximum energy of the transition. This approximation, also called the ξ approximation, simply means that the Coulomb energy of the beta electron at the nuclear radius must be large compared to the total decay energy. The ^{241}Pu decay is a case study for the ξ approximation because of its low Q_{β^-} compared to $2\xi \simeq 19.8$ MeV. The accuracy of the ξ approximation is $\sim E_0/\xi$, better than 0.5 % in the present case. Moreover, the theoretical shape factor of this transition was already studied through a complete calculation of the nuclear matrix elements in the framework of the Nilsson model [19]. Its influence increases linearly with the energy, but no higher than 0.3 % at the endpoint and 0.1 % below 8 keV. Therefore, this transition can be calculated as an allowed one.

Calculations for the exchange correction were initially performed within the same conditions given in [5], namely the same effective nuclear charges and considering a Pu^{3+} ion with filled *s* orbitals from 1 to 6. Our calculations are in very good agreement with the results of [5]. To be more realistic regarding the chemical composition of the source used in [3], we choose to consider a neutral Pu

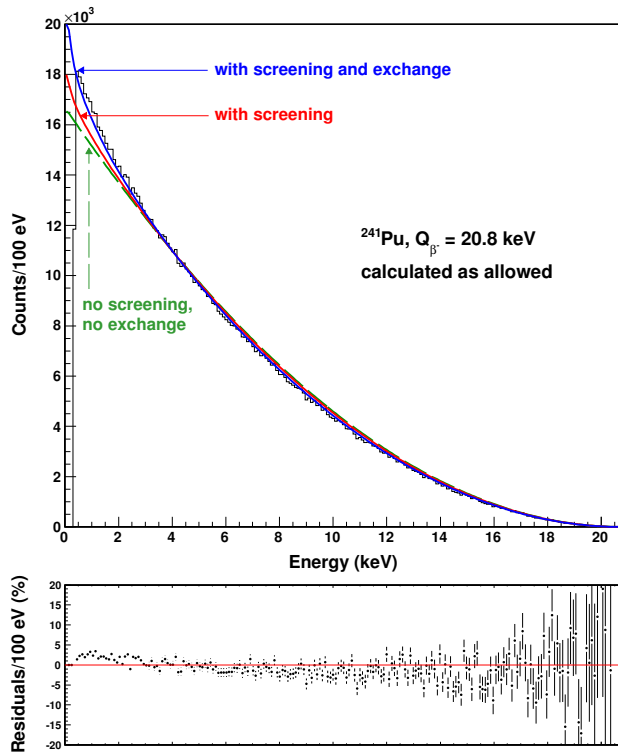


FIG. 2. Comparison between the measured beta spectrum of ^{241}Pu from [3] and three calculated spectra: a classical allowed transition without screening nor exchange, the same including screening, and a complete one including screening and exchange corrections. The corresponding residuals relative to the measured spectrum are shown just below.

atom with its $7s$ orbital also filled, which has a significant contribution below 1 keV. Obviously, relativistic effective nuclear charges are needed for this high Z nucleus.

Calculation of the screening correction was performed using the effective potential given in [12]. The resulting

spectra are compared with the measured spectrum of [3] in figure 2.

IV. DISCUSSION

Beta spectra of ^{63}Ni and ^{241}Pu are reproduced well in our calculations down to very low energies. The exchange effect is demonstrated to have a great influence on the spectrum shape within this energy range. As expected, the influence of the screening is weak for the low Z nuclide ^{63}Ni but has a significant contribution, equivalent to the magnitude of the exchange effect, for the high Z nuclide ^{241}Pu .

For ^{63}Ni , taking the exchange effect into account leads to a mean energy lower by $\sim 2.6\%$. For ^{241}Pu , the mean energy of the beta spectrum is lower by $\sim 3.5\%$ if the screening and the exchange effect are included in the calculations.

A small systematic deviation can be seen on the residuals of both transitions. It is probably due to the fact that the bound and continuum wave functions involved in the exchange effect were evaluated with analytical expressions using effective nuclear charges. Moreover, these effective charges were not determined at this stage with the same screened potentials used for the calculation of the continuum wave functions involved in the screening correction. We are now implementing a new program to calculate the exchange effect with wave functions identical to those used for the screening.

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