THE NON-RESONANCE SHAKE MECHANISM OF THE NEUTRINOLESS DOUBLE ELECTRONIC CAPTURE

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Abstract

It is generally accepted that double neutrinoless electron capture is a resonance process. The calculations of the probability of shaking with the ionization of the electron shell occurring during the transformation of $^{152}$Gd and $^{164}$Er nuclei are performed below. These nuclides have the lowest resonance defect among all known nuclei, being considered as main candidates for discovering the neutrinoless mode of the transformation. The results show predominant contribution of the new mechanism for most of the candidate nuclei. The value of this amendment rapidly increases with an increasing resonance defect. Thus, in principle, double neutrinoless e-capture appears not to be a resonance process at all.

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1 Introduction

Recently, the Xenon Collaboration reported on the first ever direct observation of $2e2\nu$ capture in the $^{124}\text{Xe}$ nucleus [1]. This event was a step of paramount importance in searches for neutrinoless double electron capture. Its investigation is crucial for testing the Majorana nature of the neutrino. This process is traditionally viewed as a resonance one, since no particle is emitted upon the respective nuclear transformation [2]. Therefore, it cannot proceed on isolated nuclei even if the energy deposition is positive, $Q > 0$. The energy-momentum conservation law requires the transfer of part of energy and momentum to a third body, and the electron shell of the atom involved plays the role of this third body. The emerging vacancies are filled via fluorescence. The energy-momentum conservation law is restored after the emission of the first photon whose energy includes the excess quantity $Q$.

The probability for neutrinoless capture is maximal in the vicinity of the resonance. At the present time, interest is therefore focused primarily on nuclei characterized by a small value of $Q$. In cases where $Q$ is large, a decrease in the resonance defect is possible upon electron capture from higher lying shells, such as the $L_1$ and $M_1$ shells, or to excited states of the nucleus or atom, in which case the process is more probable than the process of capture to the ground-state level. For example, the decay process $^{152}\text{Gd} \rightarrow ^{152}\text{Sm}$ proceeds with a higher probability via the capture of $KL_1$ electrons to the ground state of the daughter $^{152}\text{Sm}$ nucleus. In that case, the resonance defect is $\Delta = 0.919$ keV. Among other candidates, the $^{164}\text{Er} \rightarrow ^{164}\text{Dy}$ transformation, for which $\Delta = 6.82$ keV, and the $^{180}\text{W} \rightarrow ^{180}\text{Hf}$ transformation, for which $\Delta = 11.24$ keV, are considered as the most probable ones [3].

In the present study, we propose an alternative, nonresonance, mechanism of neutrinoless double electron capture. Since it may come into play irrespective of the value of $\Delta$, the contribution of this mechanism decreases more slowly with increasing resonance defect than the traditional resonance-fluorescent mechanism does. Here, the restoration of the energy—momentum conservation law occurs owing to electron-shell ionization caused by the shake effect. Indeed, the $2e$ capture process is fast in relation to characteristic atomic times. Therefore, the change in
the internal atomic potential because of the change in the nuclear charge by two units and the disappearance of two electrons may be viewed as a sudden effect [2, 4]. Therefore, it may be accompanied by the shake of electron shells, with the result that one electron is emitted from the atom. It is this electron that carries away the excess of energy. Even in the case of the $^{152}\text{Gd}$ nucleus, which possesses the minimum resonance defect, the contribution of this new mechanism within the model considered below increases the decay probability by about 23% in relation to the traditional-mechanism contribution. At the same time, for the case of other candidates, characterized by higher values of the resonance defect, its contribution will prove to be dominant. Physics foundations of the nonresonance mechanism are outlined in the next section, where the respective basic relations are derived simultaneously. The results of the calculations as applied to $^{152}\text{Gd}$ and $^{164}\text{Er}$ are presented in Section 4. Section 5 is devoted to discussing the results obtained in the present study.

2 EXPRESSIONS DESCRIBING THE PROBABILITY FOR SHAKE IN DOUBLE ELECTRON CAPTURE

The newly emerging atoms have the atomic number that is smaller by two units than the atomic number of initial atoms. The former are produced as neutral atoms in a specific transition state whose shell is swollen owing to the presence of two holes in the $K$ and $L_1$ shells [5].

The energy deposition in the process of neutrinoless double electron capture is determined by the mass difference between the neutral atoms involved (the initial, $M_1$, and final, $M_2$ ones); that is,

$$Q = M_1 - M_2.$$  (1)

Even in the case of the capture of two $K$ electrons, the daughter atom is neutral.

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$^3$Unless otherwise stated, use is made here of the relativistic system of units, where $\hbar = c = m_e = 1$, $m_e$ being the electron mass.
but arises in an excited state, featuring two holes in the place of the captured electrons. This atomic state was called a swollen state [5]. Upon electron capture from higher lying shells, the excitation energy of the daughter nucleus becomes higher appropriately. We denote by $E_A$ the excitation energy of the daughter nucleus. The resonance defect can then be written as

$$\Delta = Q - E_A.$$  \hspace{1cm} (2)

If, in addition, capture occurs to an excited state of the nucleus at energy $E_N$, this leads, for quite large values of $Q$, to a further decrease in the resonance defect; that is,

$$\Delta = Q - E_A - E_N.$$  \hspace{1cm} (3)

In the case being considered, $^{152}$Gd atoms transform into $^{152}$Sm atoms via the simultaneous nuclear capture of $K$ and $L_1$ electrons. The single-electron wave functions for the initial- and final-state atoms are not orthogonal. This gives rise to various shake processes in the final nucleus via which one or several electrons go over to an excited state (shake-up) or even escape to a continuum, the latter leading to the ionization of the atom (shake-off). Let us examine in more detail the process of the second type. Suppose that, upon shake-off, the $i$th electron goes over to a continuum state $f$. We denote by $\psi_i(r)$ the wave function describing this electron in the gadolinium parent nucleus and by $\phi_f(r)$ its continuum counterpart in the field of the singly ionized samarium daughter atom with a hole in the place of the $i$th electron. The kinetic energy $E$ of the shake-off electron is determined by setting to zero the resonance defect in Eq. (2); that is,

$$E = \Delta - I_i,$$  \hspace{1cm} (4)

where $I_i$ is the ionization potential for the $i$th electron. In general, states $i$ and $f$ are not orthogonal since they are eigenfunctions of different Hamiltonians. Accordingly, we denote by $V_Z(r)$ and $V_{Z-2}(r)$ the single-electron potentials in, respectively, the parent and daughter nuclei and by $\Delta V(r) \equiv V_Z(r) - V_{Z-2}(r)$ the sudden change in the potential. The shake amplitude then assumes the form [6]

$$F_{sh} = \langle \phi_f | \psi_i \rangle.$$  \hspace{1cm} (5)
The total amplitude can be represented as the product

\[ F_{2e}^{sh} = F_{2\beta} F_{sh}, \]  

where, by \( F_{2\beta} \), we have denoted the double-electron-capture amplitude proper, which leads to the formation of the transition state of the samarium atom. For the total width, we accordingly obtain an expression in the form

\[ \Gamma_{2\beta}^{sh} = \Gamma_{2\beta} \sum_i N_i |\langle \phi_f | \psi_i \rangle|^2 = \Gamma_{2\beta} \sum_i N_i |F_{sh}|^2, \]  

where \( N_i \) is the occupation number for the \( i \)th shell.

3 FLUORESCENT NEUTRINOLESS DOUBLE ELECTRON CAPTURE

Let us now compare expression (7) with its counterpart derived for the standard resonance mechanism of neutrinoless electron capture, for example, on the basis of the model considered in [7]. The latter is obtained by multiplying the width for the formation of the doorway state, \( \Gamma_{2\beta} \), by the Breit—Wigner resonance factor; that is,

\[ \Gamma^{(\gamma)}_{2\beta} = \Gamma_{2\beta} B_W, \]  

where

\[ B_W = \frac{\Gamma/2\pi}{\Delta^2 + (\Gamma/2)^2}. \]  

In [9] \( \Gamma = \Gamma_K + \Gamma_{L_1} \) is the total width of the swollen state featuring electron holes in the \( K \) and \( L_1 \) shells and arising upon resonance 2e capture. Comparing expressions (7) and (8), we obtain the relative correction to the decay probability per unit time in a physically clear form; that is,

\[ g \equiv \Gamma_{2\beta}^{(sh)} / \Gamma_{2\beta}^{(\gamma)} = \sum_i N_i |\langle \phi_f | \psi_i \rangle|^2 / B_W \equiv \sum_i N_i |F_{sh}|^2 / B_W. \]
It should be noted that expression (5) can be recast into an equivalent form [6]; that is,

$$F_{sh} \approx I_2 = \frac{\langle \phi_f | \Delta V(r) | \psi_i \rangle}{\Delta}.$$  \hspace{1cm} (11)

In principle, shake is possible in any shell whose ionization energy is less than $Q$, but expression (11) makes it possible to understand better that it is maximal for $s$-shell electrons. Indeed, the potential $\Delta V(r)$ is restricted in space to the region in the vicinity of orbits of hole states formed upon the capture of respective electrons. Since the electron-capture probability is the highest for $s$-shell electrons, this is the region of $K$ and $L$ shells in our case. Accordingly, the potential $\Delta V(r)$ is maximal in the region of the nucleus. It decreases uniformly as the distance from the nucleus grows. As a result, the region where this potential overlaps outer electrons, especially electrons of high angular momentum, is substantially smaller than the respective overlap region for inner electrons, and this leads to a decrease in the shake probability. It should be noted that, if, in the shake potential $\Delta V(r)$, the contribution of the field of captured electrons is disregarded — that is, if it is assumed that the shake is associated only with a change of two units in the nuclear charge — the contribution of outer electrons would be overestimated.

To conclude this section, we dwell upon the question of the choice of field between that of the parent nucleus and that of the daughter nucleus in calculating the resonance energy of the emitted photon. This question was analyzed in [2, 4]. With allowance for the classic study of A.B. Migdal on the shake of an atom in beta decay [6, 8], it was found in [4] that a mathematically correct method for solving the problem in question consisted in the expanding the wave functions for the parent and intermediate atoms in the basis set of eigenfunctions for the final atom. Therefore, the resonance energy is determined by levels of the final $^{152}$Sm atom. A similar conclusion was drawn in [2]. Within the present approach, the same answer to the question of energy follows from Eq. (4): it involves the energy of precisely the final state of the atom. The same applies to the case where the traditional resonance-fluorescent mechanism is dominant: the energy-conservation law determines the first-photon energy on the basis of the balance for the final state.
of the atom.

The situation for the wave functions is different: within the accuracy of the method, one can calculate the matrix elements in Eq. (11) with the wave functions for either the initial or the final atom. For the purpose of tests, we performed calculations according to Eqs. (5) and (11) with invariable wave functions for the sake of convenience.

4 RESULTS OF THE CALCULATIONS

The calculations on the basis of Eqs. (5) and (10) were performed in the single-electron approximation by means of the RAINE code package [9]. The electron wave functions and energies were calculated by the self-consistent Dirac–Fock method. With the aim of obtaining deeper insight into underlying physics, we have calculated the matrix elements in Eqs. (5) and (11) for a number of hypothetical values of $\Delta$ between 0.05 and 10 keV for electrons whose ionization potentials are smaller than a preset value of $\Delta$ and which therefore contribute to the amplitude for the nonresonance mechanism of the process being considered.

The wave functions used are normalized to unity for discrete states and in the energy scale for continuum states. Therefore, the square of the matrix element $F_{sh}$ has the dimension of inverse energy. The matrix elements and Breit–Wigner factors are presented in the relativistic system of units. For the widths of the hole states, we used the values of $\Gamma_K = 20$ eV and $\Gamma_{L_1} = 5$ eV [10]. By employing the experimental result of $Q = 55.70(18)$ keV from the most precise measurement reported in [7], together with the calculated value of $E_A = 54.794(9)$ keV from the same article, we obtain the resonance defect of $\Delta = 0.91(19)$ keV.

The results of the calculations are given in Table I and in Fig. 1. The partial contributions of $s$ electrons from various shells are quoted in Table 1. The results in question confirm that the methods of calculations on the basis of Eqs. (5) and (11) are nearly equivalent. The respective matrix elements are somewhat different at small values of $Q \approx 0.5$ keV, but, as $\Delta$ grows, this difference decreases to a few
Figure 1: Ratio \( g \) [10] of the contributions of the nonresonance shake mechanism and the traditional resonance-fluorescent mechanism of the probability of neutrinoless double electron capture in \(^{152}\text{Gd}\) versus the resonance defect \( \Delta \).

percent, starting from \( \Delta = 0.7 \) keV.

The total contribution of the nonresonance mechanism from all electrons with respect to the resonance mechanism is shown in Fig. 1. The probability for this process has a manifest stepwise character owing to the fact that, as \( Q \) grows, ever deeper lying shells come into play; it is noteworthy that the deeper the shell, the greater its contribution at the threshold. As might have been expected, a dominant
Table 1: Results of calculations for the matrix elements $F_{\text{sh}}$ in (5) and for the relative shake-effect-induced correction $g$ in (10) to the probability for neutrinoless electron capture for s-shell electrons (also given here for the sake of comparison are the values of the sum of the squares of the matrix elements in Eqs. (5) and (11) — $\Sigma_{\text{sh}}$ and $\Sigma_2$, respectively)

| $\Delta$, keV | $F_{\text{sh}} = \langle \phi_f | \psi_i \rangle$ | $\Sigma_{\text{sh}}$ | $\Sigma_2$ | $B_W$ | $g$ |
|--------------|-----------------|-----------------|-----------------|--------------|------|
| 0.5          | 0.72 0.30 0.08  | 0.62            | 0.90            | 8.13         | 0.15 |
| 0.65         | 0.57 0.22 0.06  | 0.38            | 0.48            | 4.81         | 0.16 |
| 0.83         | 0.45 0.17 0.05  | 0.23            | 0.26            | 2.95         | 0.16 |
| 1.01         | 0.37 0.14 0.04  | 0.16            | 0.16            | 1.99         | 0.16 |
| 1.2          | 0.31 0.12 0.03  | 0.11            | 0.11            | 1.41         | 0.16 |
| 1.5          | 0.25 0.09 0.02  | 0.071           | 0.064           | 0.90         | 0.16 |

contribution comes from the 4s-, 5s- and 6s-shell electrons. The remaining shells — predominantly the $p_{1/2}$, $p_{3/2}$ and $d_{3/2}$ ones — make an additional contribution of about 30%. One can see that, at small values of $Q$, the resonance mechanism is dominant. At the real value of $Q = 0.919$ keV, the contribution of the nonresonance shake mechanism is 23%, but, at $Q = 3.43$ keV, the contributions of the two mechanisms in question would become identical. If the value of $Q$ were 10 keV, the nonresonance-mechanism contribution would have been 4.5 times as great as the resonance contribution.

This expectation is fully confirmed in the case of neutrinoless double-electron capture in $^{164}\text{Er}$ with $Q = 6.82(12)$ keV [3]. The result of calculation is presented in Fig. 2. The nonresonance mechanism turns out to be by a factor of 3 more effective than the traditional one.

5 DISCUSSION OF THE RESULTS

We have initiated the study of shake processes in neutrinoless nuclear double electron capture. As a result, we have proposed a new mechanism of neutrinoless
nuclear double electron capture. This is a nonresonance mechanism. Therefore, it is natural to expect that, it will turn out to be more probable for decay in nuclei characterized by a significant energy deposition. In the case of the neutrinoless mechanism, such cases may arise in combination with a high resonance defect.
entailing a significant decrease in the resonance-decay probability. An analysis of the nonresonance mechanism makes it possible to refine substantially the estimation of the decay half-life. The calculations performed here for $^{152}$Gd have confirmed this assumption: the inclusion of the new mechanism leads to an increase of 23% in the probability for double capture in relation to the traditional resonance-fluorescent mechanism. Taking into account the half-life of $10^{20}$ yr estimated in [7] for this nucleus with respect to the $0\nu2e$ capture mode per effective neutrino mass of $m_{\beta\beta} = 1$ eV, we obtain the refined half-life estimate of $T_{1/2}^{0\nu} \approx 8.1 \times 10^{25} \left| \frac{1\text{eV}}{m_{\beta\beta}} \right|^2$ yr. In view of the merits of $^{152}$Gd: as a candidate for measurement of $0\nu2e$ capture [7], such as a nearly nonexistent background from $2\nu2e$ capture because of the smallness of the phase space for this process and the largest value of the resonance enhancement factor in (9), this nuclide is one of most probable candidates. Next candidate is $^{164}$Er. The nonresonance mechanism shortens its lifetime by three times, thus making it also attractive candidate in searches for neutrino-less double electron capture as an indication of the Majorana nature of the neutrino.

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