Role of the atomic electron shell in the double β decay

E. G. Drukarev,[1] M. Ya. Amusia,[2,3] and L. V. Chernysheva[3]
[1]*National Research Center "Kurchatov Institute," B. P. Konstantinov Petersburg Nuclear Physics Institute, Gatchina, St. Petersburg 188300, Russia*
[2]*Racah Institute of Physics, The Hebrew University, Jerusalem 91904 Jerusalem, Israel*
[3]*A. F. Ioffe Physical-Technical Institute, St. Petersburg 194021, Russia*
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We demonstrate that the limiting energy available for ejected electrons in the double-β decay is diminished by about 400 eV due to inelastic processes in the atomic electronic shell.

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I. INTRODUCTION

The double-β decay ($2\nu\beta\beta$) has been observed for eleven nuclei [1–3]. There are 35 nuclei for which the β decay is forbidden while the double β decay

$$(A,Z) \to (A,Z+2) + 2e^- + 2\bar{\nu}_e \tag{1}$$

can take place [4]. Several attempts to detect the neutrinoless double-β decay ($0\nu\beta\beta$),

$$(A,Z) \to (A,Z+2) + 2e^-, \tag{2}$$

as well as the future projects in this direction are described in the review [4]. Observation of the neutrinoless decay would mean that the electron neutrino is a Majorana particle which coincides with its antiparticle, i.e., $\nu_e \equiv \bar{\nu}_e$. In the process ($2\nu\beta\beta$), neutrinos carry the energy $M_N(Z+2) - M_N(Z) - E$ with E being the energy of the ejected electrons while $M_N(Z+2)$ and $M_N(Z)$ are the masses of the nuclei $(A,Z+2)$ and (A,Z). The ejection of the electrons with the energy $E = M_N(Z+2) - M_N(Z)$ would be a sign of the neutrinoless process ($0\nu\beta\beta$). As it stands now, neutrinoless decay has not been detected [4].

The actual experiments are carried out for the decays of atoms but not of the bare nuclei. It was claimed in the preprints [5–7] that this inserts an uncertainty of the order of 3 keV into the analysis. It was claimed also [7] that the neutrinoless decay ($0\nu\beta\beta$) actually has been detected in the experiments reported in Refs. [8,9]. This stimulated us to analyze the problem of the role of the atomic electronic shell in the double β decay. We employ the relativistic system of units with $\hbar = c = 1$.

II. DOUBLE β DECAY OF THE ATOM

Now we turn to the decay ($2\nu\beta\beta$) of the atom $\mathcal{A}_Z$ with the nucleus of the charge Z. We assume the atom $\mathcal{A}_Z$ to be in its ground state. In the main mode of the decay

$$\mathcal{A}_Z \to \mathcal{A}^{++}_{Z+2} + 2e^- + 2\bar{\nu}_e, \tag{3}$$

the doubly charged positive ion $\mathcal{A}^{++}_{Z+2}$ is also in the ground state. The masses of atom $\mathcal{A}_Z$ and that of ion $\mathcal{A}^{++}_{Z+2}$ in the ground state are $M_{At}(Z) = M_N(Z) + E_b(Z)$ and $M^{(0)}_{At}(Z+2) = M_N(Z) + E^{(0)}_b(Z+2)$, with $E_b(Z)$ and $E^{(0)}_b(Z+2)$ being the total energies of the atomic electronic shells. The upper index (0) labels that the ion $\mathcal{A}^{++}_{Z+2}$ is in the ground state. Thus, the largest energy available for the ejected electrons is

$$Q^{(0)} = Q_N + E_b(Z) - E^{(0)}_b(Z+2), \tag{4}$$

with $Q_N = M_N(Z) - M_N(Z+2)$ being the largest electron energy available in the decay of the nucleus presented by Eq. (1). One can see that $Q^{(0)} > Q_N$, i.e., the electronic shell becomes more bound. It transfers the energy to the ejected electrons. The masses of the atom $M_{At}(Z)$ and of the ion $M^{(0)}_{At}(Z+2)$ can be measured with good accuracy. Thus the limiting energy $Q^{(0)}$ is a well-established observable.

The electronic shell can be in an excited state after the decay. This can be an excited state of the ion $\mathcal{A}^{++}_{Z+2}$, also some of the Z bound electrons can be moved to continuum. This shifts the observable value of $Q^{(0)}$ to

$$Q = Q^{(0)} - \delta Q. \tag{5}$$

To obtain δQ we introduce the excitation energy $E^*_{n0} = E^{(n)}(Z+2) - E^{(0)}(Z+2) > 0$. Denoting the differential distribution of the double-β decay with excitation of the atomic electronic shell to the state n as $dW_n/d\Gamma$, we can present

$$\delta Q = \sum_n E^*_{n0} \frac{dW_n/d\Gamma}{dW_0/d\Gamma}, \tag{6}$$

with $\sum_n$ meaning the sum over the states of the discrete spectrum and integration over the continuum states. The energy of the state n should not exceed the limiting energy $Q^{(0)}$.

Note that, in the process ($2\nu\beta\beta$), the energy $Q^{(0)}$ makes several MeV [4]. A simple analysis based on estimation of the phase volume shows that both ejected electrons should be fast. Thus their velocities (in units of c) are of the order of unity. The atomic velocities are of the order $\alpha Z^{1/3}$, i.e., they are much smaller. This enables us to employ the shake-off (SO) approximation, in which the final state interactions between the beta electrons and atomic electronic shell are neglected [10]. In this approach the amplitude for the decay in which the atomic shell transfers to the state n is

$$F^{(n)} = F_N \langle \Phi_n | \Psi \rangle. \tag{7}$$

Here, F_N is the amplitude for the nuclear decay, Ψ and Φ_n are the wave functions of Z electrons in the ground state of the field of the nucleus with charge Z (the atom) and in the state

n of the field of the nucleus with charge $Z+2$. This provides

$$\delta Q = \sum_n E^*_{n0} |\langle \Phi_n | \Psi \rangle|^2. \quad (8)$$

Introducing the total change of the electronic shell energy $E_{n0} = E^{(n)}(Z+2) - E_b(Z) > 0$ and presenting $E^*_{n0} = E_{n0} + E_b(Z) - E^{(0)}(Z+2)$, we can write $\delta = \delta_1 + \delta_2$ with

$$\delta Q = \delta_1 + \delta_2, \quad \delta_1 = [E_b(Z) - E^{(0)}(Z+2)] \sum_n |\langle \Phi_n | \Psi \rangle|^2,$$

$$\delta_2 = \sum_n E_{n0} |\langle \Phi_n | \Psi \rangle|^2. \quad (9)$$

Since Eq. (9) contains only the differences of the energies we can write it in terms of the binding energies subtracting the mass terms. We can put $E_b(Z) = m_e Z + \varepsilon_b(Z)$, $E^{(0)} = m_e Z + \varepsilon^{(0)}(Z)$, and $E^{(n)}(Z+2) = m_e Z + \varepsilon^{(n)}(Z+2)$ with m_e being the electron mass at rest and $E_{n0} = \varepsilon_{n0}$. Thus, the two last equalities of Eq. (9) can be presented as

$$\delta_1 = [\varepsilon_b(Z) - \varepsilon^{(0)}(Z+2)] \sum_n |\langle \Phi_n | \Psi \rangle|^2,$$

$$\delta_2 = \sum_n \varepsilon_{n0} |\langle \Phi_n | \Psi \rangle|^2. \quad (10)$$

The squared SO matrix element $|\langle \Phi_n | \Psi \rangle|^2$ drops as ε_n^{-4} if the excitation energy ε^*_{n0} strongly exceeds the ground-state energy $|\varepsilon^{(0)}|$ [11]. Thus, the sums over n on the right-hand side of Eqs. (6) and (9) are saturated at $\varepsilon^*_{n0} \sim |\varepsilon_0| \ll Q^{(0)}$. Hence we can assume that the sum over n is carried out over all states with $\varepsilon_{n0} > 0$. If the atom is treated as a nonrelativistic system, they compose a closed set of states. This enables us to employ closure. This provides

$$\delta_1 = \varepsilon(Z) - \varepsilon^{(0)}(Z+2), \quad (11)$$

while $\delta_2 = \langle \Psi | H(Z+2) - H(Z) \Psi \rangle$ with $H(Z)$ and $H(Z+2)$ being the Hamiltonians of Z electrons in the fields of the nuclei with the charges Z and $Z+2$. Thus we obtain [11]

$$\delta_2 = \langle \Psi | \sum_{k \leqslant Z} \left(\frac{-2\alpha}{r_k} \right) | \Psi \rangle, \quad (12)$$

with the sum carried out over all electrons bound in the atom $\mathcal{A}_Z$. Both δ_1 and δ_2 can be calculated with high accuracy. Note that Eq. (9) presents the shift δE as a difference of two large values.

Corrections to the SO approximations can be obtained by inclusion of the final-state interaction (FSI) between the β electron and the bound electrons. We can write

$$\delta Q = \delta_1 + \delta_2 + \delta_{\rm FSI}. \quad (13)$$

The leading correction is proportional to the squared Sommerfeld parameter ξ of the β electron moving with the velocity v which is $\xi^2 = \alpha^2/v^2$ with $\alpha = 1/137$ being the fine structure constant. The expressions describing probability for transition of the atomic shell to any excited state with inclusion of the leading FSI terms are presented in Ref. [11]. Since the latter drop as ε_n^{-2} at large $\varepsilon_n \gg |\varepsilon_0|$, one cannot calculate the FSI contribution $\delta_{\rm FSI}$ to the shift δE by using the closure condition. Assuming that the energy transferred to the bound electrons does not exceed a certain value $\varepsilon_{\max}$ we can estimate [11]

$$\delta_{\rm FSI} = \xi^2 \sum_k \frac{a_k \langle \Psi | r_k^{-2} | \Psi \rangle}{m} \ln \frac{\varepsilon_{\max}}{|\varepsilon_k|}, \quad (14)$$

with a_k being the number of electrons in the bound state k. Note that, if the atomic electrons obtain the energy $\varepsilon_{\max}$, the energy of the β electrons cannot exceed the value $E = Q^{(0)} - \varepsilon_{\max}$.

III. NUMERICAL RESULTS

Now we carry out the numerical calculations. In actual computations the atom is presented as a system of electrons described (at least in the first step) by single-particle functions. Note that we can employ only the nonrelativistic functions since the positive-energy states compose the closed system only in nonrelativistic case. We use our Hartree–Fock computer codes [12].

Start with the double β decay of germanium ($Z = 32$) [4,8]. We find $\varepsilon(Z) = -56\,449.2$ eV and $\varepsilon^{(0)} = -65\,246.3$ eV for the ground-state energies of the atom of Ge and of the ion Se^{++} ($Z = 34$). This provides $\delta_1 = 8797.1$ eV. We obtain also $\delta_2 = -8446.1$ eV. This provides $\delta_1 + \delta_2 = 351$ eV. Note that the value of δ_1 calculated in relativistic approach (Hartri–Fock–Dirac approximation) is about 2% larger. If the relative size of relativistic correction to δ_2 is of the same order as that to δ_1, we find that relativistic corrections to δQ are also of the order 2%. The small magnitude of relativistic effects makes the nonrelativistic calculation reasonable.

In calculating the FSI contribution $\delta_{\rm FSI}$, we can put $\xi^2 = \alpha^2$ since $Q^{(0)} \approx 2$ MeV. Assuming $\varepsilon_{\max} = 3$ keV (we choose this value since such energy loss was claimed in Ref. [7]) we find that $\delta_{\rm FSI} = 0.6$ eV. Thus we obtain

$$\delta Q = 352 \text{ eV}. \quad (15)$$

For the double-β decay of xenon ($Z = 54$) [2,3,13] $\varepsilon(Z) = -19\,6714.2$ eV while for the ion Ba^{++} (Z = 56), $\varepsilon^{(0)} = -214\,419.3$ eV. Thus $\delta_1 = 17\,705.1$ eV. On the other hand $\delta_2 = -17\,292.4$ eV. This provides $\delta_1 + \delta_2 = 413$ eV. The FSI contribution is $\delta_{\rm FSI} = 1$ eV. Hence we find

$$\delta Q = 414 \text{ eV}. \quad (16)$$

The value of δ_1 calculated in the relativistic Hartree–Fock–Dirac approach provides the value which is about 1 keV larger. If the relative difference of the Hartree–Fock–Dirac and Hartree–Fock results for the value δ_2 is of the same order of magnitude as for δ_1, the uncertainty of our nonrelativistic result is of the order of 10%.

IV. SUMMARY

We carried out nonrelativistic calculations for the shift of the limiting energy available for the ejected electrons in double β decay caused by inelastic processes in the electronic shell. We demonstrated that the energy diminishes by about 400 eV. We estimated the accuracy of our calculations. Our result does not alter the earlier conclusions that the neutrinoless mode have not been observed yet.

We calculated the average energy loss of the β electrons, which is an integrated characteristic of the process. The approach is common for the processes which take place in a bound system after ejection of the fast electron. For well-studied processes such as ordinary nuclear β decay (see, e.g., Ref. [14]), it is reasonable to investigate also the differential characteristics such as the spectrum of the shake-off electrons or the probabilities of the shake-up processes. However, the very possibility of the neutrinoless double β decay is not clarified yet. Thus, calculations of differential characteristics for the $(0\nu\beta\beta)$ process are beyond the scope of our paper. Note also that calculations of differential characteristics in each process can be a subject of separate work—see, e.g., the calculations of the shake-up probabilities in the high-energy photoionization of the two-electron ions carried out in Ref. [15].

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