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Abstract. We study a new mode of the neutrinoless and two-neutrino double-beta decays in which a single electron is emitted from the atom. The other electron is assumed to occupy one of the vacant \( s_{1/2} \) or \( p_{1/2} \) subshells of the daughter ion. Such process could manifest itself through an additional background signal in the single-electron spectra, which will be accessible in the next-generation experiment SuperNEMO. We calculate the phase-space factors in terms of relativistic electron wave functions obtained as the solutions to the Dirac equation and evaluated at the nuclear radius, while taking into account the shielding effect of nuclear charge via the multiconfiguration Dirac–Hartree–Fock package \textsc{Grasp2K}. Half-lives are estimated for the most relevant double-beta-decay isotopes and experimental significance is discussed.

1. Introduction

Observation of the neutrinoless double-beta decay \((0\nu\beta\beta)\) would mark a revolution in the theory of neutrino masses and a huge step towards new physics beyond the Standard Model. It would bring us direct evidence that the massive neutrinos \( \nu_i \) \((i = 1, 2, 3)\) are in fact Majorana fermions, implying the identity of the flavor neutrinos \( \nu_\alpha \) \((\alpha = e, \mu, \tau)\) and their respective antineutrinos \( \bar{\nu}_\alpha \), and at the same time demonstrate that the total lepton number \( L \) is not strictly conserved [1]. Measurement of the \( 0\nu\beta\beta \) half-life (for which only lower bounds currently exist) would provide us with key to the absolute scale of neutrino masses \( m_i \), as well as with the possibility to infer the mechanism of leptonic CP violation required in order to explain the observed baryon asymmetry of the Universe [2]. Given the potential to answer so many fundamental questions in particle and astroparticle physics, it is understandable that in the recent decades the search for neutrinoless double-beta decay has drawn great attention of both theorists and experimentalists.

The double-beta decay is a transmutation of an even-even parent nucleus \( ^{A}\text{X} \) into a daughter nucleus \( ^{A}\text{Y} \), two electrons \( e^- \) (and a pair of antineutrinos \( \bar{\nu}_e \)), denoted \( 0\nu\beta^-\beta^- \) (\( 2\nu\beta^-\beta^- \)):

\[ ^{A}\text{Z}\text{X} \longrightarrow ^{A}\text{Z}+\text{Y} + e^- + e^- + (\bar{\nu}_e + \bar{\nu}_e). \]  

The neutrinoless mode \( 0\nu\beta^-\beta^- \) increases \( L \) by 2 units and could be discovered by revealing a monoenergetic peak at the spectrum endpoint in calorimetric measurements of the sum of electron...
energies. The two-neutrino mode $2\nu\beta^--\beta^-$ has so far been observed in 11 out of 35 isotopes for which the ordinary $\beta^-$ decay into the odd-odd intermediate nucleus is either energetically forbidden or substantially suppressed by spin selection rules. In what follows, we restrict ourselves to the dominant ground-state $0^+ \rightarrow 0^+$ nuclear transitions.

By analogy with the bound-state $\beta^-$ decay first observed about 25 years ago [3], we study the bound-state double-beta-decay modes, denoted $0\nu{\bar \nu}\beta^-$ ($2\nu{\bar \nu}\beta^-$):

$$\frac{\Lambda X}{2} \rightarrow \frac{\Lambda}{2} + Y + e^-_b + e^- + (\vec{p}_e + \vec{p}_{\nu}).$$

In these new modes, the emission of a single free electron $e^-$ is accompanied by an electron production (EP) of a bound electron $e^-_b$ in one of the available $s_{1/2}$ or $p_{1/2}$ subshells above the valence shell of the daughter $2^+$ ion. Contribution of bound states with higher angular momenta can be safely disregarded since their wave functions vanish at the origin, and hence exhibit only a minimal overlap with the nucleus; already the $p_{1/2}$ states yield only a negligible input to the decay rates. Since the free $0\nu{\bar \nu}\beta^-$ electron carries away the entire released kinetic energy $Q$, this mode could be in principle recognized as a peak near the endpoint of the single-electron spectrum which will be studied in the next-generation experiment SuperNEMO [4].

2. Calculation of phase-space factors

The double-beta decay is a 2nd-order process governed by the effective beta-decay Hamiltonian of the following $V - A$ structure [5]:

$$\mathcal{H}_\beta(x) = \frac{G_\beta}{\sqrt{2}} \bar{\psi}(x) \gamma^\mu (1 - \gamma^5) \nu_e(x) j_\mu(x) + \text{H.c.}$$

(3)

Here, $G_\beta \equiv G_F \cos \theta_C$ includes the Fermi constant $G_F$ together with the Cabibbo angle $\theta_C = 13^\circ$ due to quark mixing [6], $\bar{\psi}(x)$ and $\nu_e(x)$ are the electron and electron-neutrino fields, respectively, and the hadronic charged current $j_\mu(x) = \bar{p}(x) \gamma_\mu (g_V - g_A \gamma^5) n(x)$ couples the proton $p(x)$ and neutron $n(x)$ fields via the vector $g_V = 1$ and (unquenched) axial-vector $g_A = 1.27$ coupling constants. Due to neutrino mixing, the left-handed components of the flavor- and massive-neutrino fields are related by a unitary transformation: $\nu_{aL}(x) = \sum_i U_{ai} \nu_{iL}(x)$, where $U_{ai}$ are the elements of the PMNS matrix. The most plausible seesaw mechanism incorporates the massive neutrinos into the theory via Majorana mass terms, in which case the L-violation can be realized by a light Majorana-neutrino exchange between the two weak-interaction vertices.

The formulae for the inverse $0\nu(2\nu)\beta^-\beta^-$ half-lives [7]:

$$\left(T_{1/2}^{0\nu\beta\beta}\right)_{-1} = g_A^4 G_{0\nu\beta\beta}(Z, Q) \left| M_{0\nu\beta\beta}\right|^2 \frac{m_{\beta\beta}}{m_\nu},$$

$$\left(T_{1/2}^{2\nu\beta\beta}\right)_{-1} = g_A^4 G_{2\nu\beta\beta}(Z, Q) \left| m_\nu M_{2\nu\beta\beta}\right|^2$$

(4)
The relativistic electron wave functions $\psi(\vec{r})$ are obtained as the solutions to the Dirac equation with Coulomb potential $V(r) = -\alpha Z_{\text{eff}}/r$, where $\alpha = 1/137$ is the fine-structure constant and $Z_{\text{eff}}$ is the effective atomic number of the daughter nucleus experienced by the final-state electrons. The bispinor $\psi(\vec{r})$ with separated radial $r \equiv |\vec{r}|$ and angular $\vec{r} \equiv \vec{r}/|\vec{r}|$ variables in general takes the form [9]:

$$
\psi_{\kappa \mu}(\vec{r}) = \begin{pmatrix} f_{\kappa}(r) \Omega_{\kappa \mu}(\vec{r}) \\ i g_{\kappa}(r) \Omega_{-\kappa \mu}(\vec{r}) \end{pmatrix},
$$

where $\kappa = (l-j)(2j+1) = \pm 1, \pm 2, \ldots$ collectively labels all possible combinations of the orbital $l = 0, 1, \ldots$ and spin $s = \pm 1/2$ angular momenta, $\mu = -j, \ldots, +j$ denotes the projection of the total angular momentum $j = |l + s|$ onto the z-axis, $f_{\kappa}(r)$ and $g_{\kappa}(r)$ are the relativistic radial wave functions which further depend on the electron energy, and the two-component angular functions $\Omega_{\kappa \mu}(\vec{r})$ are known as the spinor spherical harmonics.

In the continuous spectrum, it is sufficient to consider the dominant $s_{1/2}$ term from the partial-wave expansion, in which case the free-electron wave functions are evaluated at the nuclear radius $R = 1.2 \text{ fm} A^{1/3}$ and reduced to the Fermi function [10]:

$$
F(Z, E) = f_{\frac{1}{2}}^2(E, R) + g_{\frac{1}{2}+1}^2(E, R) \approx 4 \left( \frac{1}{\Gamma(\gamma + i\nu)} \right)^2 (2pR)^{2\gamma - 2} e^{\pi \nu},
$$

where $E = \sqrt{\vec{p}^2 + m_e^2}$ is the energy of a free electron with momentum $\vec{p}$, and we have defined the parameters $\gamma = \sqrt{\kappa^2 - (\alpha Z)^2}$ and $\nu = \alpha Z E/p$ ($p \equiv |\vec{p}|$). For the free electron, the shielding effect was shown to be rather insignificant, and hence we retain the full charge of the daughter nucleus [11]: $Z_{\text{eff}} = Z + 2$.

In the discrete spectrum, the bound-electron wave functions can be approximated by the bound-state Fermi function:

$$
B_n(Z, A) = f_{n-1}^2(R) + g_{n+1}^2(R),
$$

where $n = 1, 2, \ldots$ is the principal quantum number and the two terms emerge from the inclusion of $s_{1/2}$ and $p_{1/2}$ states, respectively. For the bound electron, the shielding effect of nuclear charge has been taken into account by means of relativistic many-electron wave functions via the multiconfiguration Dirac–Hartree–Fock package GRASP2K [12].

Under the standard approximations, the bound-state double-beta-decay modes $0\nu(2\nu)\text{EP}^\beta^-$ do not alter the nuclear matrix elements: $M^{0\nu(2\nu)\text{EP}^\beta} \approx M^{0\nu(2\nu)\beta}$ and only affect the kinematical phase-space factors:

$$
G_{0\nu(2\nu)\text{EP}^\beta}(Z, Q) = \frac{G_4^4 m_e^2}{32\pi^4 R^2 \ln 2} \sum_{n=n_{\text{min}}}^{\infty} B_n(Z, A) F(Z + 2, E) E p,
$$

$$
G_{2\nu(0\nu)\text{EP}^\beta}(Z, Q) = \frac{G_4^4}{8\pi^8 m_e^2 \ln 2} \sum_{n=n_{\text{min}}}^{\infty} \int_{m_e}^{m_e+Q} dE \int_0^{m_e+Q-E} d\omega_1 \int_0^{\omega_1} d\omega_2 \int_{m_e}^{m_e+Q-E} \int_0^{\omega_2} d\omega_3 \omega_1 \omega_2 \omega_3.
$$

In both scenarios, the total released kinetic energy equals: $Q = M_i - M_f - 2m_e$, where $M_i,f$ denote the masses of the initial- and final-state nuclei and we have neglected the small neutrino masses $m_\nu$. The summation runs over all available electron shells $n$ above the valence shell of the resulting $2+$ ion, while $E$ and $\omega_{1,2}$ represent the total energies of the free electron and the two antineutrinos, respectively. Neglecting the electron binding energies and nuclear recoil, from energy conservation it follows that in $G_{0\nu(2\nu)\text{EP}^\beta}$: $E = m_e + Q$ (i.e., the single free electron carries away the entire kinetic energy released in the decay), while in $G_{2\nu(0\nu)\text{EP}^\beta}$: $\omega_2 = m_e + Q - E - \omega_1$ and the infinite sum of integrals separates into a product of the Fermi sum $\sum_{n=n_{\text{min}}}^{\infty} B_n(Z, A)$ and just one double integral independent of $n$. 

3
Table 1. $\beta^-\beta^-$-decay isotopes $\frac{A}{2}X$ with corresponding $Q$ values [13], decay-rate ratios $\Gamma^{0\nu\text{EP}}/\Gamma^{0\nu\beta\beta} \approx G^{0\nu\text{EP}}/G^{0\nu\beta\beta}$ and $\Gamma^{2\nu\text{EP}}/\Gamma^{2\nu\beta\beta} \approx G^{2\nu\text{EP}}/G^{2\nu\beta\beta}$, half-lives $T^{0\nu\text{EP}}_{1/2}$ and $T^{0\nu\beta\beta}_{1/2}$ estimated assuming $g_A = 1.27$, $|m_{\beta\beta}| = 50$ meV and nuclear matrix elements $M^{0\nu\beta\beta}$ calculated in [14, 15], and half-lives $T^{2\nu\text{EP}}_{1/2}$ extracted from measured values $T^{2\nu\beta\beta}_{1/2}$ [16].

| $\frac{A}{2}X$ | $Q$ [MeV] | $\frac{\Gamma^{0\nu\text{EP}}}{\Gamma^{0\nu\beta\beta}}$ | $\frac{\Gamma^{2\nu\text{EP}}}{\Gamma^{2\nu\beta\beta}}$ | $T^{0\nu\text{EP}}_{1/2}$ [y] | $T^{0\nu\beta\beta}_{1/2}$ [y] | $T^{2\nu\text{EP}}_{1/2}$ [y] | $T^{2\nu\beta\beta}_{1/2}$ [y] |
|---------------|-----------|-----------------|-----------------|-----------------|-----------------|-----------------|-----------------|
| $^{48}$Ca     | 4.268     | $3.51 \times 10^{-7}$ | $3.72 \times 10^{-6}$ | $1.23 \times 10^{34}$ | $4.32 \times 10^{27}$ | $1.18 \times 10^{25}$ | $4.40 \times 10^{19}$ |
| $^{76}$Ge     | 2.039     | $3.63 \times 10^{-6}$ | $3.07 \times 10^{-5}$ | $1.36 \times 10^{32}$ | $4.95 \times 10^{26}$ | $5.38 \times 10^{25}$ | $1.65 \times 10^{21}$ |
| $^{82}$Se     | 2.998     | $1.97 \times 10^{-6}$ | $1.83 \times 10^{-5}$ | $7.05 \times 10^{31}$ | $1.38 \times 10^{26}$ | $5.04 \times 10^{24}$ | $9.20 \times 10^{19}$ |
| $^{96}$Zr     | 3.565     | $7.65 \times 10^{-7}$ | $7.23 \times 10^{-6}$ | $2.46 \times 10^{32}$ | $1.88 \times 10^{26}$ | $3.18 \times 10^{24}$ | $2.30 \times 10^{19}$ |
| $^{100}$Mo    | 3.034     | $3.59 \times 10^{-6}$ | $3.29 \times 10^{-5}$ | $1.73 \times 10^{31}$ | $6.21 \times 10^{25}$ | $2.16 \times 10^{24}$ | $7.10 \times 10^{18}$ |
| $^{112}$Pd    | 2.017     | $9.69 \times 10^{-6}$ | $7.91 \times 10^{-5}$ | $1.83 \times 10^{31}$ | $1.78 \times 10^{26}$ |                          |                  |
| $^{112}$Cd    | 2.813     | $1.45 \times 10^{-6}$ | $1.28 \times 10^{-5}$ | $7.13 \times 10^{31}$ | $1.03 \times 10^{26}$ | $2.24 \times 10^{24}$ | $2.87 \times 10^{19}$ |
| $^{123}$Sb    | 2.977     | $2.11 \times 10^{-6}$ | $2.31 \times 10^{-5}$ | $1.51 \times 10^{32}$ | $4.18 \times 10^{26}$ |                          |                  |
| $^{126}$Te    | 0.867     | $1.56 \times 10^{-5}$ | $1.09 \times 10^{-4}$ | $1.36 \times 10^{32}$ | $2.13 \times 10^{27}$ | $1.84 \times 10^{28}$ | $2.00 \times 10^{24}$ |
| $^{130}$Te    | 2.528     | $2.68 \times 10^{-6}$ | $2.29 \times 10^{-5}$ | $4.33 \times 10^{31}$ | $1.16 \times 10^{26}$ | $3.02 \times 10^{25}$ | $6.90 \times 10^{20}$ |
| $^{132}$Xe    | 0.824     | $1.67 \times 10^{-5}$ | $1.15 \times 10^{-4}$ | $1.89 \times 10^{32}$ | $3.16 \times 10^{27}$ |                          |                  |
| $^{136}$Xe    | 2.458     | $2.84 \times 10^{-6}$ | $2.40 \times 10^{-5}$ | $1.24 \times 10^{32}$ | $3.52 \times 10^{26}$ | $9.12 \times 10^{25}$ | $2.19 \times 10^{21}$ |
| $^{150}$Nd    | 3.371     | $6.16 \times 10^{-7}$ | $5.61 \times 10^{-6}$ | $6.51 \times 10^{31}$ | $4.01 \times 10^{25}$ | $1.46 \times 10^{24}$ | $8.20 \times 10^{18}$ |
| $^{238}$U     | 1.145     | $2.95 \times 10^{-6}$ | $2.10 \times 10^{-5}$ |                          |                  | $9.52 \times 10^{25}$ | $2.00 \times 10^{21}$ |

3. Results and discussion

In Table 1, we present the results for the ground-state $0^+ \rightarrow 0^+$ nuclear transitions of the most relevant $\beta^-\beta^-$-decay isotopes $\frac{A}{2}X$ listed together with their respective $Q$ values [13]. The ratios $\Gamma^{0\nu\text{EP}}/\Gamma^{0\nu\beta\beta} \approx G^{0\nu\text{EP}}/G^{0\nu\beta\beta}$ and $\Gamma^{2\nu\text{EP}}/\Gamma^{2\nu\beta\beta} \approx G^{2\nu\text{EP}}/G^{2\nu\beta\beta}$ between the corresponding decay rates are independent of the nuclear matrix elements $M^{0\nu\beta\beta}$ and $M^{2\nu\beta\beta}$ as well as the effective Majorana neutrino mass $m_{\beta\beta}$, and hence free of the peculiarities of the nuclear and neutrino physics. The half-lives $T^{0\nu\text{EP}}_{1/2}$ and $T^{0\nu\beta\beta}_{1/2}$ are estimated assuming the unquenched value of the axial-vector weak coupling constant: $g_A = 1.27$, the effective Majorana neutrino mass corresponding to the top of the allowed inverted-hierarchy region: $|m_{\beta\beta}| = 50$ meV, and the nuclear matrix elements $M^{0\nu\beta\beta}$ calculated via the spherical pn-QRPA approach including the realistic CD-Bonn nucleon-nucleon potential with short-range correlations and partial isospin-symmetry restoration [14], except for the isotope $^{150}$Nd which was treated separately within the deformed pn-QRPA model [15]. On the other hand, the half-lives $T^{2\nu\text{EP}}_{1/2}$ are extracted regardless of any theoretical assumptions from the experimentally measured values $T^{2\nu\beta\beta}_{1/2}$ [16]. We observe that the $0\nu\text{EP}$-mode is strongly suppressed and out of reach of the running and near-future experiments. Conversely, its $2\nu\text{EP}$-counterpart is relatively more significant by one order of magnitude; indeed, the $2\nu\text{EP}$-half-lives are already at the level of the present $0\nu\beta\beta$-decay sensitivity. Finally, the overall suppression is mainly attributed to the presence of other electrons in the atom: the lowest-lying orbitals are already occupied, while the shielding effect of nuclear charge substantially reduces the bound-electron wave functions on the surface of the nucleus.

In figure 1, we show the calculated single-electron spectra $1/\Gamma \frac{d\Gamma}{dE} \frac{1}{dx}$ as functions of the electron kinetic energy $\epsilon = (E - m_e)/Q$ for the isotope $^{82}$Se, which will serve as the primary source isotope in the next-generation tracking-and-calorimetry double-beta-decay experiment SuperNEMO located at LSM, France [4]. The discreet $0\nu\text{EP}$ peak in principle consists of
Figure 1. Single-electron spectra $1/\Gamma \, d\Gamma/d\varepsilon$ (normalized to unity) as functions of the dimensionless portion of electron kinetic energy $\varepsilon = (E - m_e)/Q$ for the source isotope $^{82}$Se ($Q = 2.998\,\text{MeV}$) which will be studied in SuperNEMO [4], in case of the decay modes: (a) $0\nu\text{EP}\beta^-$ and $0\nu\beta^-\beta^-$, (b) $2\nu\text{EP}\beta^-$ and $2\nu\beta^-\beta^-$. For illustration, the $0\nu\text{EP}\beta^-$ peak is represented by a Gaussian with the desired energy resolution of SuperNEMO calorimeters: FWHM$/Q = 7\% / \sqrt{Q/\text{MeV}}$ and scaled by a factor of $10^4$.

an indefinite number of contributions, each shifted beyond the $Q$ value by the electron binding energy; however, these would be indistinguishable under any achievable energy resolution. In conclusion, the $2\nu\text{EP}\beta^-$ mode exhibits a different shape of the spectrum, which points to more optimistic prospects towards its observation as a background process in SuperNEMO.

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