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FIELDS, PARTICLES, AND NUCLEI

Energy Spectrum of β Electrons in Neutrinoless Double-β Decay Including the Excitation of the Electron Shell of Atoms

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Double-β decay is accompanied with a high probability by the excitation of the electron shell of the daughter atom; as a result, the energy carried away by β electrons decreases. The mean value and standard deviation of the excitation energy of the electron shell of the daughter atom in the double-β decay of germanium $^{76}_{32}\mathrm{Ge} \to {}^{76}_{34}\mathrm{Se}^* + 2\beta^-(+2\overline{\nu}_e)$ have been determined within the Thomas–Fermi and relativistic Dirac–Hartree–Fock methods. Using the estimates thus obtained, a two-parameter model of the energy spectrum of β electrons in the neutrinoless mode has been developed including the redistribution of the reaction energy between the decay products. The shift of the total energy of β electrons does not exceed 50 eV with a probability of 90%. However, the mean excitation energy is ~400 eV, i.e., an order of magnitude higher, whereas the standard deviation is ~2900 eV, which is apparently due to a significant contribution from inner electron levels to the energy characteristics of the process. The distortion of the shape of the peak of the 0ν2β decay should be taken into account when analyzing the data of detectors with a resolution of ~100 eV or higher.

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Neutrinos play a special role in the search for physics beyond the Standard Model. Investigation of β processes sensitive to the mixing, mass, and nature of neutrinos (Dirac/Majorana) is a promising field in the search for generalizations of the Standard Model [1].

The experimental detection of the neutrinoless double-β decay (0ν2β) decay would certainly prove the existence of the Majorana neutrino mass and would significantly limit possibilities for the generalization of the Standard Model. The 0ν2β decay is detected by a narrow peak at the kinetic energy of β electrons T equal to the decay energy Q. The channels with the electron shell of the daughter atom in the ground state are not necessarily dominant in β processes [2, 3], which leads, e.g., to a noticeable increase in the probability of neutrinoless double electron capture [4–6]. Excitations of the electron shell of atoms, as well as the chemical shift of atomic levels [7] depending on the aggregate state of matter, modify the energy spectrum, in particular, spread and shift the 0ν2β peak. The peak at $T = Q$ is used as a signature of the 0ν2β decay and is sought by the CUORE [8], EXO [9], and KamLAND-Zen [10] collaborations. Multielectron modes can be detected by the SuperNEMO Collaboration [11]. The upper bound on the $^{76}_{32}\mathrm{Ge} \to {}^{76}_{34}\mathrm{Se}^* + 2\beta^-$ half-life established by the GERDA Collaboration is 5.3×10^{25} yr at a 90% C.L. [12]. The interpretation of data in terms of the Majorana neutrino mass requires control of uncertainties in the axial coupling constant of nucleons [13] and in nuclear matrix elements [14]. In this work, we study the effect of the excitation of the electron shell of atoms on the spectrum of β electrons the double-β decay.

The atomic number of the nucleus in β processes changes by $\Delta Z = \pm1, \pm2$. This charge change acts on the electron shell as a sudden perturbation, "shaking," which induces transitions of electrons of the daughter atom with a certain probability to excited levels (shake up) or to states of the continuous spectrum (shake off). The resulting energy spectrum of β electrons is determined by the contribution from the decay channel where all electrons of the final atom hold their quantum numbers and the reaction energy does not change and by the contribution from the decay channels with the excitation and ionization of the electron shell. In the latter case, the effective reaction energy decreases, which affects the shape of the energy spectrum.

To determine the energy spectrum, it is necessary to perform summation over all channels taking into account the changed reaction energy and the corresponding multiparticle amplitudes. The wavefunction

of electrons of the parent atom is projected on the wavefunction of electrons of the daughter atom in the configuration corresponding to a certain excitation of the shell. Each amplitude generally requires multiparticle numerical simulation. The number of open channels is infinite, which is a specificity of the Coulomb problem.

The mean excitation energy of the electron shell of the daughter atom and its standard deviation are quite simply calculated within the Thomas–Fermi model and in the relativistic Dirac–Hartree–Fock method. These values can then be used to construct the simplest probability distributions of the energy carried away by β electrons.

In the nonrelativistic theory, the Hamiltonian of N electrons in the atom with the atomic number Z has the form

$$\hat{H}_{Z,N} = \sum_{i=1}^{N}\left(\frac{1}{2}\mathbf{p}_i^2 - \frac{Z}{|\mathbf{r}_i|}\right) + \sum_{i<j}^{N}\frac{1}{|\mathbf{r}_i - \mathbf{r}_j|}, \qquad (1)$$

where $\mathbf{p}_i$ and $\mathbf{r}_i$ are the momentum and position vector of the ith electron, respectively. In this work, we use the atomic units, where the reduced Planck constant $\hbar$, mass of the electron m, and the elementary charge e are $\hbar = m = e = 1$ and the speed of light in vacuum is $c = 137$. The ground state is denoted as $|Z,N\rangle$. The total binding energy of electrons $E_{Z,N}$ is an eigenvalue of the Hamiltonian $\hat{H}_{Z,N}$.

The change number of the nucleus increases by two units in the 0ν2β decay. The Coulomb addition to the Hamiltonian acting as the sudden perturbation transforms the state $|Z,Z\rangle$ of the initial Hamiltonian to the superposition of states with a certain energy of the Hamiltonian

$$\hat{H}_{Z+2,Z} = \hat{H}_{Z,Z} - 2\sum_{i=1}^{Z}\frac{1}{r_i}, \qquad (2)$$

where $r_i = |\mathbf{r}_i|$. The mean energy of Z electrons forming the shell of the parent atom in the Coulomb field of the nucleus with the charge $Z+2$ is $\langle Z,Z|\hat{H}_{Z+2,Z}|Z,Z\rangle = E_{Z,Z} + 2Z^{-1}E^{\mathrm{C}}_{Z,Z}$, where

$$E^{\mathrm{C}}_{Z,Z} = -Z\sum_{i=1}^{Z}\langle Z,Z|\,\frac{1}{r_i}\,|Z,Z\rangle \qquad (3)$$

is the Coulomb interaction energy of electrons with the nucleus. The mean excitation energy of the electron shell of the daughter atom in the double-β decay is given by the expression

$$\mathcal{M} = E_{Z,Z} + 2Z^{-1}E^{\mathrm{C}}_{Z,Z} - E_{Z+2,Z}. \qquad (4)$$

The binding energies of atoms $E_{Z,Z}$ are tabulated [15–18] or can be determined using programs for the calculation of the structure of electron shells of atoms (see, e.g., [19]). The quantity $E_{Z+2,Z}$ differs from the total binding energy of electrons in the atom $E_{Z+2,Z+2}$ by the binding energy of two valence electrons, which is no more than 20 eV. The Coulomb interaction energies $E^{\mathrm{C}}_{Z,Z}$ were obtained in [18] using the relativistic Dirac–Hartree–Fock method.

The variance of the excitation energy is

$$\mathcal{D} = \langle Z,Z|\hat{H}^2_{Z+2}|Z,Z\rangle - \langle Z,Z|\hat{H}_{Z+2}|Z,Z\rangle^2. \qquad (5)$$

Taking into account Eq. (2) and that $E_{Z,N}$ are the eigenvalues of $\hat{H}_{Z,N}$, we obtain

$$\frac{1}{4}\mathcal{D} = \sum_{i=1}^{Z}\sum_{j=1}^{Z}\langle Z,Z|\frac{1}{r_i}\frac{1}{r_j}|Z,Z\rangle - \langle Z,Z|\sum_{i=1}^{Z}\frac{1}{r_i}|Z,Z\rangle^2.$$

If the exchange contributions are neglected, the off-diagonal matrix element with $i \neq j$ in the first term is factorized: $\langle Z,Z|r_i^{-1}r_j^{-1}|Z,Z\rangle \approx \langle Z,Z|r_i^{-1}|Z,Z\rangle\langle Z,Z|r_j^{-1}|Z,Z\rangle$. The factorization eliminates off-diagonal terms; as a result, the expression for the variance takes the form

$$\frac{1}{4}\mathcal{D} \approx \sum_{i=1}^{Z}\langle Z,Z|\frac{1}{r_i^2}|Z,Z\rangle - \sum_{i=1}^{Z}\langle Z,Z|\frac{1}{r_i}|Z,Z\rangle^2. \qquad (6)$$

The estimate of exchange effects using nonrelativistic wavefunctions of electrons in the Roothaan–Hartree–Fock method [17] shows that the contribution from exchange terms to the variance is below 10%.

We note that Eqs. (2)–(6) are also valid in the relativistic theory with the Dirac–Coulomb Hamiltonian as the zeroth approximation and the Breit potential describing the interaction between electrons in an order of $1/c^2$ [20].

The total binding energy and the energy of Coulomb interaction of electrons with the nucleus for the atom in the Thomas–Fermi model are given by the expressions $E_{Z,Z} = -0.764Z^{7/3}$ and $E^{\mathrm{C}}_{Z,Z} = 7E_{Z,Z}/3$ (see, e.g., [21]). The virial theorem establishes the relation between $E_{Z,Z}$ and $E^{\mathrm{C}}_{Z,Z}$. The mean excitation energy is

$$\mathcal{M} = \left(1 + \frac{14}{3Z}\right)E_{Z,Z} - E_{Z+2,Z}. \qquad (7)$$

In the double-β decay of germanium, each of two missing $4p$ electrons in selenium has a binding energy of 9.752 eV, and the sum of the first two ionization energies of selenium is 30.948 eV [22]. Taking into account the correction, $\mathcal{M} = 382$ eV.

The electron density in the Thomas–Fermi model is expressed in terms of the wavefunctions of atomic shells as

$$n(\mathbf{r}) = \sum_{i=1}^{Z} \langle Z, Z|\delta(\mathbf{r} - \mathbf{r}_i)|Z, Z\rangle. \quad (8)$$

The first term in Eq. (6) is obviously reduced to the form $\int d\mathbf{r} r^{-2} n(\mathbf{r})$. To calculate the integral, we used the parameterization of the screening function of atoms presented in [23]. The integral at small distances diverges as $\sim dr/r^{3/2}$. Furthermore, the semiclassical approximation is applicable at the distances $1/Z \lesssim r$. For numerical estimates, the electron density in the range from $r = 0$ to $r = 1/Z$ is taken to be constant equal to $n(r = 1/Z)$.

The application of the known inequality that the square of the arithmetic mean does not exceed the mean square to the second term in Eq. (6) gives

$$\frac{1}{Z}\sum_{i=1}^{Z}\langle Z, Z|\frac{1}{r_i}|Z, Z\rangle^2 \geq \left(\frac{1}{Z}\sum_{i=1}^{Z}\langle Z, Z|\frac{1}{r_i}|Z, Z\rangle\right)^2 = \left(\frac{1}{Z}\int d\mathbf{r}\frac{1}{r}n(\mathbf{r})\right)^2. \quad (9)$$

Here, the right-hand side is $(Z^{-2}E^{\mathrm{C}}_{Z,Z})^2$. This inequality determines the upper bound on the variance:

$$\frac{1}{4}\mathcal{D} \leq \frac{1}{4}\bar{\mathcal{D}} = \int d\mathbf{r}\frac{1}{r^2}n(\mathbf{r}) - Z^{-1}\left(\int d\mathbf{r}\frac{1}{r}n(\mathbf{r})\right)^2. \quad (10)$$

The variance for the double-β decay of germanium is estimated as $\bar{\mathcal{D}}^{1/2} = 2160$ eV.

The first negative moment of the probability distribution in the germanium atom calculated with the relativistic Dirac–Hartree–Fock method [15] is $\langle r^{-1}\rangle = 4.99$. The position of the ground level of the selenium atom with respect to that of germanium is determined using the RAINE software package [24, 25] implementing the relativistic Dirac–Hartree–Fock method. The substitution of the resulting values into Eq. (4) gives the mean excitation energy $\mathcal{M} = 300$ eV, which is in qualitative agreement with the Thomas–Fermi method. The substitution of the $E_{Z,Z}$ and $E^{\mathrm{C}}_{Z,Z}$ values from the table in [18] for the double-β decay of germanium into Eq. (7) yields $\mathcal{M} = 400$ eV.

The variance given by Eq. (6) is determined similarly by expressing it in terms of the first and second negative moments of the electron distribution in the germanium atom. Using the known second moments of the electron distribution in atoms [16], we determine $\mathcal{D}^{1/2} = 2870$ eV. The Thomas–Fermi value of 2160 eV is in qualitative agreement with this value.

The quantities $\mathcal{M}$ and $\mathcal{D}$ are noticeably larger than the expected values for the channels associated with the excitation of valence electrons. The contribution from discrete levels to $\mathcal{M}$ and $\mathcal{D}^{1/2}$ is obviously less than ~10 eV. The convergence of the integral over the continuous spectrum is determined by the binding energy; therefore, the contribution from the continuous spectrum to $\mathcal{M}$ and $\mathcal{D}^{1/2}$ is comparable with the contribution from the discrete spectrum. At the same time, the excitations of valence electrons dominate in the probability because the change $\Delta Z = 2$ in the atomic number of the nucleus results in a significant relative change in the screened potential at the edge of the atom.

Electrons in inner orbits are excited with a low probability but have a larger binding energy and can make a noticeable contribution to the mean excitation energy and standard deviation. Since $\Delta Z \ll Z$, perturbation theory can be used to calculate the probability of the excitation of a K electron to the continuous spectrum [26, 27] (see also [21]). The probability, mean energy, and mean square of the transition energy in the leading order are $\Delta\mathcal{P} = 0.65\Delta Z^2/Z^2$, $\Delta\mathcal{M} = 0.66\Delta Z^2$, and $\Delta\mathcal{D} = 1.87\Delta Z^2 Z^2$, respectively. In the double-β decay of germanium, $\Delta\mathcal{P} = 2.6\times10^{-3}$, $\Delta\mathcal{M} = 72$ eV, and $\Delta\mathcal{D} = (2380\ \mathrm{eV})^2$. Thus, $\Delta\mathcal{M} \sim \mathcal{M}$ and $\Delta\mathcal{D} \sim \mathcal{D}$. Consequently, the contribution from K electrons to the mean excitation energy and the standard deviation is significant.

The shell of the parent atom in β processes transits with a finite nonunity probability to the ground state of the daughter atom [2, 3, 28]. To determine the corresponding amplitude $K_Z = \langle \mathrm{Se\ III}|\mathrm{Ge}\rangle$ in the double-β decay of germanium, the wavefunctions of electrons of the germanium atom $|\mathrm{Ge}\rangle$ and the wavefunctions of the daughter selenium ion in the ground state $|\mathrm{Se\ III}\rangle$ were constructed using the Grasp-2018 package implementing the relativistic Dirac–Hartree–Fock method [19, 20]. The parameter K_Z is sensitive to the used approximations, which is due to the noticeable difference in the binding energy of electrons with the same quantum numbers on the outer shells of germanium and selenium. The calculation with the Grasp-2018 package gives the value $K_Z = 0.575$.

Taking into account energy losses to the excitation and ionization of the daughter atom, the probability distribution of the total kinetic energy of β electrons near $T = Q$ has the form

$$dF(T) = \left(K_Z^2\delta(T - Q) + (1 - K_Z^2)w(1 - T/Q)/Q)\right)dT, \quad (11)$$

where K_Z^2 is the probability that electrons of the parent atom after the decay remain in the ground state and $w(x)$ is the conditional probability density of the excitation energy $\epsilon = Q - T$ of the electron shell of the

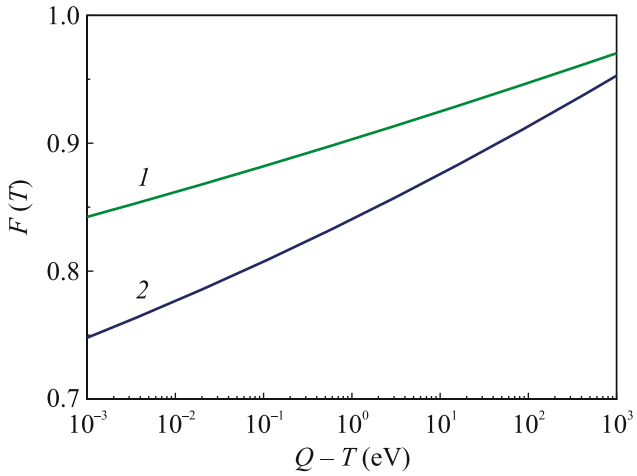

Fig. 1. Probability distribution function for the kinetic energy of β electrons T from the double-β decay of germanium with the reaction energy $Q = 2039.061(7)$ keV [12] taking into account the incomplete overlapping of electron shells of atoms according to Eq. (13). Lines *1* and *2* correspond to the mean excitation energy of the electron shell $\mathcal{M} = 300$ and 400 eV, respectively, and the square root of variance $\mathcal{D}^{1/2} = 2870$ eV.

daughter atom in units of Q; the second term leads to the spread of the peak.

The mean value, variance, and overlap amplitude K_Z are sufficient to construct the simplest two-parameter probability distribution of the energy of β electrons. Numerous problems concerning random processes involve the beta distribution [29]

$$w(x) = \frac{\Gamma(\alpha+\beta)}{\Gamma(\alpha)\Gamma(\beta)} x^{\alpha-1}(1-x)^{\beta-1} \qquad (12)$$

for the variable x in the interval [0,1], where α and β are the positive free parameters. The mean value and mean square in the beta distribution are $m = \alpha/(\alpha+\beta)$ and $m_2 = \alpha(\alpha+1)/((\alpha+\beta)(\alpha+\beta+1))$, respectively. In our case, $x = \epsilon/Q$. The relations $(1-K_Z^2)m = \mathcal{M}/Q$ and $(1-K_Z^2)m_2 = (\mathcal{D}+\mathcal{M}^2)/Q^2$ make it possible to determine the parameters α and β from the known $\mathcal{M}$, $\mathcal{D}$, and K_Z values. As an example, we consider the Ge-76 isotope used in the GERDA experiment. For the mean values $\mathcal{M} = 300$ and 400 eV and the standard deviation $\mathcal{D}^{1/2} = 2870$ eV, we obtain $\alpha = 0.016$, $\beta = 74$ and $\alpha = 0.029$, $\beta = 99$, respectively. The two-parameter gamma distribution [29] of random variables on the [0,+∞) semiaxis is also appropriate for the simulation because the condition $Q \gg \mathcal{M}, \mathcal{D}^{1/2}$ allows one to extend the integration over $x = \epsilon/Q$ to the [0,+∞) semiaxis. The beta and gamma distributions almost coincide with each other in the physical interesting region $T \sim Q$ because $\beta \gg 1$.

The probability density at $T = Q$ is singular but integrable. Figure 1 shows the following distribution function for the two above sets of the parameters α and β:

$$F(T) = K_Z^2 + (1-K_Z^2)\int_T^Q w(1-T'/Q)dT'/Q, \qquad (13)$$

which determines the probability that two β electrons have the energy differing from Q by no more than $Q - T > 0$. The energy of β electrons for $\mathcal{M} = 300$ eV deviates from Q by no more than 1 eV with a probability of 90%. The deviation for $\mathcal{M} = 400$ eV is smaller than 50 eV with the same probability. The probability increases approximately logarithmically, i.e., quite slowly, with the difference $Q - T$. Modern detectors measure the energy released in the double-β decay with an accuracy of ~1 keV, which significantly complicates the observation of effects with the excitation of electron shells. Processes of shaking of K electrons are accompanied by an energy release of ~10 keV, but these processes are highly improbable.

Thus, the electron shell of the daughter atom in β processes is excited with a high probability. The transitions of valence electrons to free discrete levels or to the continuous spectrum have dominant probabilities. In this work, the mean excitation energy of the electron shell of the daughter atom $\mathcal{M}$ and its variance $\mathcal{D}$ have been estimated in the Thomas–Fermi model and in the relativistic Dirac–Hartree–Fock method. The determined values $\mathcal{M} \sim 400$ eV and $\mathcal{D}^{1/2} \sim 2900$ eV significantly exceed the values in processes involving valence electrons. The estimated energy parameters of the transition of K electrons to the continuous spectrum indicate that the noticeable contribution to the mean energy and its variance comes from rare processes of shaking of electrons populating inner orbitals. With an increase in the resolution of detectors to ~100 eV, the distortion of the shape of the peak in the 0ν2β decay induced by the excitation of electron shells of atoms becomes significant for analysis of observational data.

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CONFLICT OF INTEREST

The authors declare that they have no conflicts of interest.

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