Shake-off in the ^{164}Er neutrinoless double-electron capture and the dark matter puzzle

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Traditionally neutrinoless double-electronic capture is considered as a resonance process. Degeneracy of the initial and daughter nuclei is the main factor mastering the decay rate. We have fulfilled shake-off probability calculations. Allowance for the shake-off loosens the need for resonance, leading to a radical increase of the capture rate in the nonresonance nuclei. In the case of ^{164}Er, the contribution of the new mechanism increases the capture rate by a factor of 5.6. It also increases the probability of electron capture from higher shells. The influence of the shake-off is also expected to manifest itself in the other β processes which are used in the studies of the neutrino nature, its mass and role in the dark matter puzzle.

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I. INTRODUCTION

An active discussion of the problems of hypothetical dark matter, presumably composing, together with hypothetical dark energy, 95% of the Universe, stimulates the development of theories beyond the standard model. As a rule, they include violation of the lepton quantum number, unless special restrictions are introduced. This attracts great interest in the study of double-β processes, including the $2e$ decay of a nucleus, and the capture of two orbital electrons by it [1]. Of the two processes, the $2e$ decay has the highest decay rate. To date, the lifetimes of 2β decay are measured in 14 nuclei [2]. They range from several units times 10^{18} (^{100}Mo, ^{150}Nd) to 10^{24} (^{128}Te) years. Within the framework of the standard model, the lepton quantum number is conserved. This excludes double-neutrinoless-β decay or e capture with the lepton quantum number violation $|\Delta L| = 2$. The latter become possible only if neutrinos have mass and if neutrinos are particles of the Majorana nature. The study of 2β decay yielded in the following constraints on the Majorana neutrino mass: $m_\nu < 0.12$–0.26 eV with the upper bound on the half-life $T_{1/2}^{0\nu} > 8.0 \times 10^{25}$ yr [3], and similar for some other nuclei: $m_\nu < 0.33$–0.62 eV with the upper bound on the half-life $T_{1/2}^{0\nu} > 1.1 \times 10^{24}$ yr [4], $m_\nu < 0.061$–0.165 eV with the upper bound on the half-life $T_{1/2}^{0\nu} > 1.07 \times 10^{26}$ yr [5], $m_\nu < 0.11$–0.50 eV with the upper bound on the half-life $T_{1/2}^{0\nu} > 1.5 \times 10^{25}$ yr [6], and others. In the near future these experiments are expected to reach the sensitivities of up to 10^{26} yr for the half-lives, which correspond to the sensitivity in terms of the effective Majorana neutrino mass in the range of 0.06 to 0.26 eV [7]. Discovery of mass in neutrinos and their oscillations has already marked the observation of processes beyond the standard model. Thus, the search for neutrinoless binary processes should answer the question about the Majorana nature of neutrinos. Furthermore, there is a motivation to search for the neutrinoless $0\nu2e$ decay and $0\nu2e$ capture owing to the potential to clarify the possible contribution of the righthanded currents to their rates [8].

At the same time, the $2e$-capture process is studied less intensively. It is characterized with longer half-lives. Thus, the XENON Collaboration claimed to have observed two-neutrino double-electron capture in ^{124}Xe with a half-life of $(1.8 \pm 0.5) \times 10^{22}$ yr. An indication of the $2\nu2e$ capture in ^{78}Kr was obtained with the proportional chamber filled with enriched ^{78}Kr in the experiment by Gavrilyuk *et al.* [9], which gives an example of the calorimetric approach. This result was confirmed recently [10] with better statistical accuracy, yielded in the half-life of $T_{1/2}^{2\nu2K} = [1.9_{0.7}^{1.3}(\text{stat}) \pm 0.3(\text{syst})] \times 10^{22}$ yr.

Detection of the neutrinoless $2e$ capture would unambiguously point out violation of the lepton number $|\Delta L| = 2$. However, this process, having a pole singularity, has traditionally been considered as a resonance process, since not a single particle is emitted as a result of nuclear transformation [11]. This circumstance leads to a hard suppression of this mode due to the Breit–Wigner factor (see below), unless the initial and final-state energies are close to degenerate. The conservation law requires the transfer of a part of the released energy to a third body. This is the electron shell of the atom. The energy conservation may be restored, in a simplest way, through emission of a fluorescence quantum. In this case its energy includes the excessive Q value. Furthermore, a satellite shift arises because of formation of the two vacancies in the places of the captured electrons. The formed electron shell is thus inflated in comparison with a normal atomic shell [12,13]. The latter shift is present in both 0ν and 2ν double-electron

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capture. But it is the neutrinoless capture amplitude which generically includes the radiative vertex. The latter vertex, together with the Breit–Wigner factor, retards the process by orders of magnitude.

Therefore, the main criterion is focused on the study of nuclei with the small resonance defect. For a correct estimate of the capture probabilities, it is necessary to know the mass difference of the initial and final atoms to within the width of the inflated state, whose typical values lie in the range of 10–50 eV. Added to this is the uncertainty in calculating the excitation energy of the daughter atom, which, however, can be neglected in the first approximation. In contrast, the old technique made it only possible to determine the masses of nuclei with an uncertainty of tens of keV. A breakthrough was due to the development of mass spectroscopy in an optical Penning trap [14,15]. This made it possible to radically clarify the list of candidates for the experiment. In particular, ^{152}Gd, ^{164}Er, and ^{180}W become included in the list among most suitable candidates for experimental research [16]. It is established that the $^{152}\mathrm{Gd} \to {}^{152}\mathrm{Sm}$ is characterized with by far the least resonance defect $\Delta = 910$ (180) eV instead of the previously adopted value of 54.6 (35) keV. In the case of ^{164}Er, $\Delta = 6.82(12)$ keV has been obtained instead of the old 23.3 (3.9) keV. The situation changed most radically for ^{180}W: from 144.4 (45) to 11.24 (27) keV as the Δ value.

Our present purpose is to bring attention to a nonresonance shake-off mechanism, by means of which the $0\nu 2e$ capture can occur. Restoration of energy conservation occurs due to ionization of the electron shell. In this case, the excessive energy is carried away by the ejected electron. For this reason, its contribution decreases with increasing the resonance defect Δ more slowly than the conventional resonance-fluorescent mechanism. As a result, account of this mechanism can enhance the rate of the neutrinoless $2e$ capture by an order of magnitude and thus become the dominant capture mode in cases with big resonance defect. Its contribution decreases in the case of small resonance defect for lack of excessive energy. However, estimations show that even in the case of the $^{152}\mathrm{Gd} \to {}^{152}\mathrm{Sm}$ decay, the enhancement can be quite significant, achieving 23 percent [17]. In this paper, we consider the $^{164}\mathrm{Er} \to {}^{164}\mathrm{Dy}$ process, with a higher value of Δ. The results confirm expectations. Account for shake-off reduces the expected half-life of the process by almost six times.

Note that shake-off cannot only occur in the $0\nu 2e$ capture, but also in other traditional processes of β decay and e capture. Some examples are discussed in the concluding section. In the next section, we recall the basic formulas. The calculation results are given in Sec. 3. Section 4 is devoted to a discussion of the results obtained in this work.

II. COMPARISON OF THE TWO MECHANISMS OF NEUTRINOLESS 2*e* CAPTURE: PHYSICAL PRINCIPLES AND FORMULAS FOR CALCULATION

In the case of $2e0\nu$ capture, the atom remains generally neutral. Therefore, the energy release is determined by the difference in the masses of neutral atoms, the initial M_1 and the daughter one M_2 (we use the relativistic system of units $\hbar = c = m_e = 1$, with m_e being the electron mass, unless otherwise noted):

$$Q = M_1 - M_2. \tag{1}$$

However, the process with the total energy release (1) only could be realized by means of the capture of the outermost, valence electrons. As a rule, the capture of internal electrons is much more probable, as their density on the nucleus is higher. Consequently, the atom always remains in an excited state with two holes in the inflated electron shell. Let the energy of a normal atom in such a configuration be E_A. Accordingly, instead of (1), the effective energy release is realized:

$$Q_{\mathrm{eff}} = M_1 - M_2 - E_A = Q - E_A. \tag{2}$$

The process is energetically possible at $Q > 0$, but Q_{eff} can also be negative: the excessive energy can be either added to or subtracted from the energy of the satellite quantum. It is Q_{eff} that acts as the resonance defect $\Delta = |Q_{\mathrm{eff}}|$.

We recall the formula for the traditional resonance-fluorescent mechanism which corresponds to the pole approximation. The $2e0\nu$ capture brings to the formation of a doorway state. For lack of degeneracy, it is out of the mass shell, as its energy is different from E_A by the Δ value, which comprises the defect of resonance. Due to the uncertainty principle, violation of the energy conservation is possible for a time of $\tau = \hbar/\Delta$. Then the doorway state undergoes a fluorescent radiative or Auger transition, the final state being on the mass shell. The energy Δ is added to the usual energy of this transition. This is a fast entire mechanism. Formally, it is described by (cf., for example, Ref. [16]) multiplying the squared amplitude of the capture itself, Γ_{2e}, by the Breit–Wigner resonance factor

$$\Gamma_{2e}^{(\gamma)} = \Gamma_{2e} B_W, \tag{3}$$

where

$$B_W = \frac{\Gamma/2\pi}{\Delta^2 + (\Gamma/2)^2}. \tag{4}$$

In Eq. (4), Γ is the width of the inflated state of the daughter atom with the two holes. In Ref. [16] it was taken as the total width of the both holes. This is not correct: one must also add the width of the final state [18]. As a result, the value of Γ at least doubles [13]. However, the decay of ^{164}Er was not considered in Ref. [13]. For simplicity, we make comparison with Ref. [16], keeping their Γ value. The shake-off contribution is independent of the Γ value. A typical value is $\Gamma \approx 30$ eV. For illustration, the scale of the variation of the B_W factor is shown in Fig. 1 *versus* the resonance defect. In the best case of ^{152}Gd—a candidate with the least of the known to date values of $\Delta = 0.91$ keV, it suppresses the rate by a factor of 3600. In the other cases, the Δ value typically varies from several keV to one or two tens keV, while the Breit–Wigner factor drops to six orders of magnitude. Shake-off is energetically possible only for positive $Q_{\mathrm{eff}} > 0$, and from the shells whose ionization potential I_i in the daughter atom (with the two vacancies in the electron shell) satisfies the condition

$$I_i < Q_{\mathrm{eff}}. \tag{5}$$

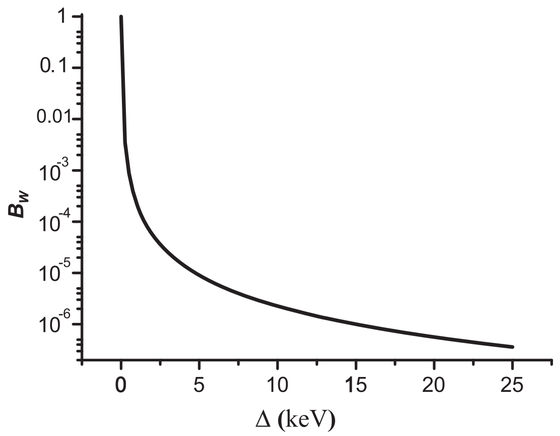

FIG. 1. Typical dependence of the Breit–Wigner factor (4) (normalized at unity for $\Delta = 0$) on the resonance defect Δ.

Then the energy of the shake-off electrons is defined by their difference as follows:

$$E_{\rm sh} = Q_{\rm eff} - I_i. \tag{6}$$

The shake-off is a consequence of the very rapid, instantaneous change in the inner-atomic electrostatic potential $V_Z(r)$ in the initial atom to the potential in the daughter atom $V_{Z-2}(r)$, see Fig. 2. Therefore, the electron wave functions of the initial and final atoms are non-orthogonal, even with the same quantum numbers. Denote the change in the potential $\Delta V(r) \equiv V_Z(r) - V_{Z-2}(r)$. And let $\phi_i(r)$ be the wave function describing ith electron in the parent atom, whereas $\psi_f(r)$—the wave function of the shake-off electron. It is calculated in the field of the daughter atom with three vacancies: two in the places of the captured electrons and one in the place of the emitted shake-off electron. Then the shake-off amplitude reads as follows [19]:

$$F_{\rm sh}(\Delta) = \langle \psi_f | \phi_i \rangle. \tag{7}$$

Similarly to (3), the full amplitude can be expressed as follows:

$$F_{2e}^{(\rm sh)} = F_{2e} F_{\rm sh}(\Delta). \tag{8}$$

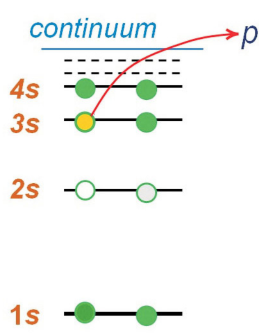

FIG. 2. Scheme of a representative shake-off process: the L_1L_1 electron capture creates two holes in the $2s$ shell. Changed instantaneously inner-atomic electrostatic potential expels the $3s$ electron into continuum with momentum p.

Now the full width of the shake-off mechanism can be represented as follows:

$$\Gamma_{2e}^{(sh)} = \Gamma_{2e} |F_{\rm sh}(\Delta)|^2. \tag{9}$$

Comparing Eq. (9) to Eq. (3), one arrives at the following expression for the relative correction to the decay probability:

$$G = \Gamma_{2e}^{(sh)} / \Gamma_{2e}^{(\gamma)} = \sum_i N_i |\langle \psi_f | \phi_i \rangle|^2 / B_W \equiv \sum_i N_i |F_{\rm sh}|^2 / B_W, \tag{10}$$

with N_j being the occupation numbers.

Within the framework of the resonance-fluorescent mechanism, the main contribution comes from the capture of the two L_1 electrons in the ^{164}Er atoms. The capture of lower electrons is energetically forbidden, that of higher ones is suppressed by the decrease in their density at the nucleus together with a decreasing Breit–Wigner factor. Contrary, in the shake-off mechanism, the decrease of the electron density, for example, in the capture from the $M1$ shell is partially compensated by an increase of the $Q_{\rm eff}$ value, since the shake-off channel from the L_1 shell gets open. This leads to the fact that, as we shall see, the probability of capture from higher shells becomes even higher than the probability of the traditional mechanism. Let ik capture occur from the higher i, k shells. Then the acceleration factor can be calculated in comparison with the most probable resonance L_1L_1 capture by means of the formula

$$G_{ik} = \frac{\rho_i(0)\rho_k(0)}{\rho_{L_1}^2(0)} \sum_j N_j \left| F_{\rm sh}^{(j)}\left(\left|Q_{\rm eff}^{(ik)}\right|\right)\right|^2 / B_W. \tag{11}$$

In Eq. (11), the summation is carried out over all shells j where shake-off is energetically allowed. $F_{\rm sh}^{(j)}(|Q_{\rm eff}^{(ik)}|)$ is still the overlap integral of the wave functions of the electron in the initial shell j and the electron in the continuum, but calculated for the actual energy release $Q_{\rm eff}^{(ik)}$ corresponding to the ik capture. In the case of the most probable L_1L_1 capture, the lowest shell where the shake-off occurs is the M shell. Alternatively, if the capture of one of the electrons occurs from the M shell, then the value of $Q_{\rm eff}^{(LM)}$ increases by the difference of the ionization potentials of the L and M shells. This automatically opens the shake-off channel from the L shell (L_1, L_2, L_3), which leads to a stepwise increase of the shake-off probability.

III. INTERPLAY BETWEEN THE SHAKE-OFF AND THE AUGER EFFECT

In the previous section, we mentioned the role of the Auger effect in the deexcitation of the doorway states. Here we emphasize the difference between the shake-off effect and the Auger effect. The latter is also accompanied by the ejection of an additional electron from the atom and creation of a hole. However, the Auger effect is due to two-electron interaction, so that the escape of one electron is induced by the transition of the other to a lower state.

For example, consider an L_1L_1 $2e0\nu$ capture accompanied with shake-off an M_2 electron. Then the atom remains in the $2s^{-2}3p^{-1}$ configuration on the mass shell. Alternatively, within the resonance-fluorescent mechanism, the mother atom may transfer to the doorway state $2s^{-2}$, which undergoes deexcitation through an $L_1M_1M_2$ Auger transition. As a result, the atom remains in the $2s^{-1}3s^{-1}3p^{-1}$ configuration, also on the mass shell. In the both cases, the daughter atom remains with three holes in the electron shell, but in the different configurations. Evidently, the energy of the Auger electron will be different from the energy of the shake-off electron. The $2e0\nu$-capture probability in the latter case is calculated by means of Eqs. (3) and (4) with the Auger width included in the Γ value.

Note that the above shake-off configuration $2s^{-2}3p^{-1}$ can, in principle, result from the Auger effect KL_1M_2, induced by two-electron KL_1 capture. The probability of this capture is small, as mentioned above, because of the large resonance defect, which in this case would be equal to $\Delta_{\rm eff} = -28.72$ keV instead of 6.82 keV.

Discussing the interplay between the Auger and shake-off mechanisms, it is worthy of mentioning the methods of the Auger spectroscopy of the hollow atoms with two vacancies in the inner orbits [20]. Knowing the precision binding energy of such configurations with the errors within 10 eV is necessary for correct estimate of the half-lives of the nuclei with respect to the $0\nu2e$ capture. By means of photoeffect one can produce a hole in the K shell. The hole can be filled by an L_1 electron, inducing a KL_1L_2 Auger effect. The photoelectron energy spectrum contains information about the single-hole excitation energies, whereas the Auger-electron energy spectrum allows for the measurement of the two-hole excitation energies of electron shells. As a result, a hollow ion is formed with two vacancies in the L shell. It differs from the neutral hollow atoms which are created in the $0\nu2e$ capture. However, in view of that the binding energy of the valence electrons does not exceed a few eV, spectroscopic investigation of the hollow ions helps to solve the problem.

Hollow atoms of ^{81}Kr with two K vacancies were studied in Ref. [10]. They were created by means of the double photoeffect on the K shell (see, e.g., Ref. [21]). The results of the spectroscopic investigation of obtained in this way hollow ions allowed the authors to draw the above conclusion concerning the observation of the $2\nu2e$ capture in ^{78}Kr.

IV. RESULTS OF CALCULATION

Calculations by means of Eqs. (10) and (11) were performed using the RAINE software package [22,23]. The one-electron wave functions and their eigenvalues were calculated by means of the self-consistent Dirac–Fock method. To better understand the physics of the process, matrix elements (7) were calculated for a number of hypothetical values of Δ from 0.05 to 20 keV for all electrons whose ionization potentials are less than the given Δ value and which, therefore, contribute to the shake-off mechanism. The total widths of the electron hole states are taken from Ref. [23].

The results are shown in Figs. 2–5, as well as in Tables I and II. Our wave functions are normalized at unity for discrete states and the δ function on the energy scale—in the continuum. Therefore, the square of the matrix element $F_{\rm sh}(\Delta)$ acquires the dimension reciprocal of the energy. The matrix elements are presented below in the relativistic system of units. The closer the shell is to the nucleus, the greater its contribution to the shake-off, if not energetically forbidden. This is illustrated in Fig. 3, which shows the $F_{\rm sh}$ matrix elements for the L_2 and L_3 subshells. The curves start from different thresholds: 9.264 and 8.358 keV, respectively. Both thresholds are higher than the effective energy release; therefore, in this case, neither of the curves contributes to shake-off in the most probable case of the L_1L_1 capture. Figure 4 shows matrix elements for the $2p_{1/2}$–$5p_{1/2}$ shells. The matrix elements for the rest of the shells are illustrated in Fig. 5.

The total acceleration factor corresponding to the total contribution to shake-off from all the electrons, relative to the resonance-fluorescent mechanism is shown in Fig. 6. The probability of this process has a pronounced stepwise character due to the fact that with increasing Q, deeper and deeper shells are switched on, and the deeper the shell lies, the greater its contribution at the threshold. As expected, the main contribution comes from the s and p electrons. It can be seen that, at small Q, the resonance mechanism dominates. At the actual value of $Q = 6.82$ keV, the contribution of the nonresonance mechanism is three times as high as that of the traditional mechanism.

Shown in Figs. 3–5, the values can be used in order to estimate the shake-off contribution in the cases of electron capture from the other, higher shells. Using the total width of the L_1 hole in the Dy atom: $\Gamma_{L_1} = 4.3$ eV [23], we obtain by means of formula (11) the total acceleration factors for capture from the L, M, and N shells. They are presented in

TABLE I. Partial gains G_{ik} (11) from the shake-off mechanism calculated for e capture in the various shells ik. $\rho(0)$ is the normalized at the L_1L_1 capture product of the densities [24] of the both captured electrons at the origin.

Shell	Δ (keV)	$\rho(0)$	G
LL	6.82	1	2.81
LM	14	0.218	1.22
MM	21	0.048	0.20
LN	15.6	0.051	0.29
MN	22.6	0.011	0.05
NN	24.3	0.003	0.01
Total:			4.58

TABLE II. Calculated half-lives of ^{152}Gd, ^{164}Er, and ^{180}W double-neutrinoless-e capture for the Majorana neutrino mass 1 eV, taking into account both mechanisms.

Nuclei	^{152}Gd $\to$ ^{152}Sm	^{164}Er $\to$ ^{164}Dy	^{180}W $\to$ ^{180}Hf
Decay channel	KL	LL	KK
Δ (keV)	0.910	6.82	12.5
Resonance half-lives (years)	10^{27}	2×10^{30}	3×10^{28}
Shake-off half-lives (years)	8×10^{26}	3.6×10^{29}	3×10^{27}

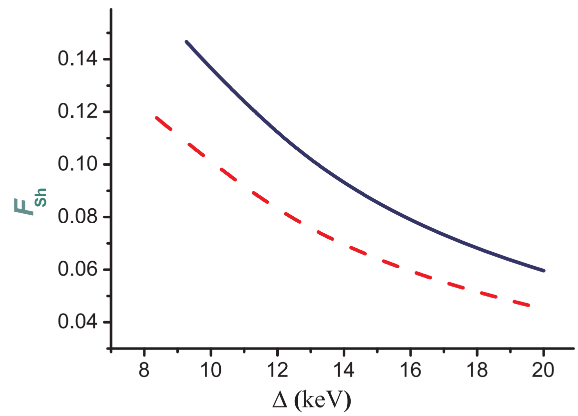

FIG. 3. Matrix elements F_{sh} for the $2p_{1/2}$- (solid curve) and $2p_{3/2}$- (dashed curve) subshells of ^{164}Dy atoms against the resonance defect Δ.

Table I. As one can see from the table, taking into account higher shells leads to an additional increase of the capture rate by 1.8 times. And the total gain is 5.6 times. Supposing that it is only the shake-off mechanism which makes $2e$ capture from higher orbits significant, one can estimate from Table I the total fraction of these captures as to be of about one third. One can easily calculate the mean shake-off probability: 82% per capture.

V. DISCUSSION OF THE RESULTS AND FUTURE PROSPECTS

Allowance for shake-off processes in the $2e0\nu$ nuclear capture generally significantly diminishes theoretical estimates for half-lives. Its peculiarity is that shake-off loosens the requirement of resonance between the initial and final atoms. It is more effective in the cases of nuclei with big Q_{eff} values, when traditional resonance-fluorescent mechanism is suppressed. Thus, taking into account the new mechanism increases the estimate of the double-capture probability by a factor of about six in the case of ^{164}Er. Taking into account an old estimate of the half-life of this nucleus as 2×10^{30} years for $m_\nu = 1$ eV [16], we obtain a refined estimate of

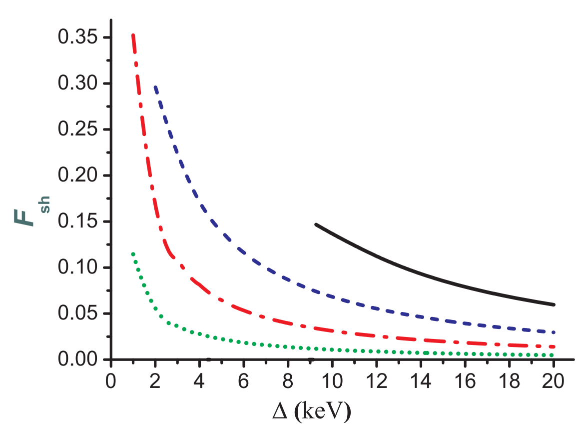

FIG. 4. Matrix elements F_{sh} for the $np_{1/2}$-subshells of ^{164}Dy atom: $n = 2$ (solid line), $n = 3$ (dashed line), $n = 4$ (dash-dotted line) and $n = 5$ (dotted line).

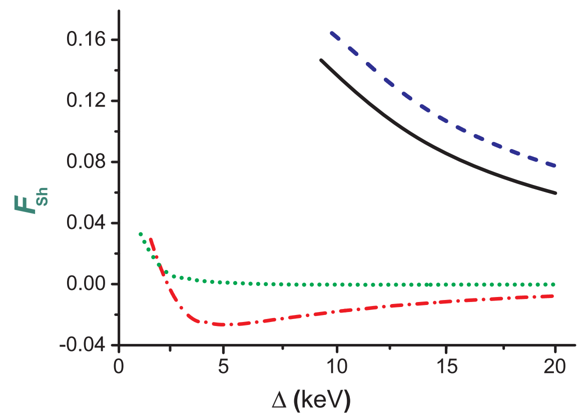

FIG. 5. Comparison of shell contributions to the shake amplitude as a function of the orbital angular momentum. Matrix elements F_{sh} for the $2s$ subshell (dashed line), $2p_{1/2}$ subshell (solid curve), $3d_{3/2}$ (dash-dotted line), and $4f_{5/2}$ (dotted line) subshells of ^{164}Dy atom.

the half-life, allowing for the shake-off mechanism, as $T_{1/2}^{0\nu} \approx 3.6 \times 10^{29}$ $(1 \text{ eV}/m_\nu)^2$ years. In the other cases of heavier nuclei with an effective energy release of $\gtrsim$10 keV, including ^{180}W, the gain achieves already a full order of magnitude. We summarize the expected results for the half-lives of the above three candidates: ^{152}Gd, ^{164}Er, and ^{180}W in Table II. Note that the presented theoretical half-lives relative to the $2e0\nu$ capture scale with $(1/m_\nu)^2$.

In view of that the half-life of another candidate for measuring the $2e0\nu$ capture of ^{152}Gd remains three orders of magnitude shorter, we can conclude that it remains a more likely candidate for setting up an experiment than ^{164}Er. At the same time, the expected lifetime of ^{180}W with respect to the $2e0\nu$ capture turns out to be only four times longer than that of ^{152}Gd.

Of course, this should not be regarded as the abolition of the degeneracy condition for the initial and final nuclei. The resonance defect of ^{152}Sm is minimal among the known candidates, remaining however to reach ≈900 eV. As one can

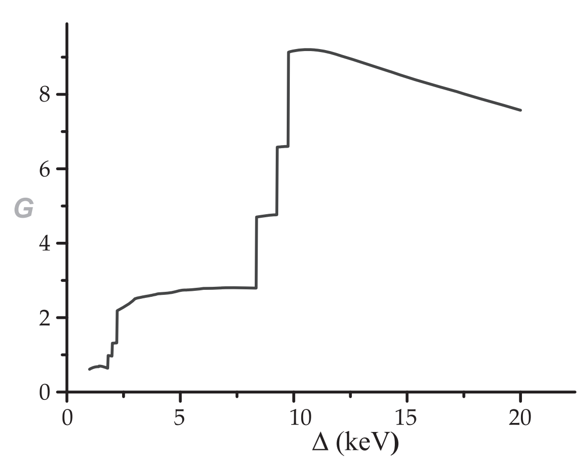

FIG. 6. The gain of the shake-off mechanism G (10) as compared with the resonance-fluorescent mechanism in the probability of double-neutrinoless-L_1L_1 capture in ^{164}Er, depending on the resonance defect Δ.

see from Fig. 1, this yet implies a suppression factor of 3600. Therefore, the degeneracy remains the main criterion in search for further candidates. There is a number of such candidates listed, e.g., in Ref. [20], whose masses are known up to several keV, however. Further advancement of the Penning-trap mass spectroscopy can help in this attitude.

Shake-off leads to a radical change of the fluorescence spectrum. As mentioned in the Introduction, the appearance of two satellites at each fluorescence line comprises a characteristic feature of 2*e* capture. First, the energies of the satellites receive an additional shift due to availability of the third vacancy on the place of the shake-off electron. Second, in the case of 2*e* capture from higher orbits, new satellites arise in the fluorescence spectrum. In the case of ^{164}Er, in one third of the cases, the capture occurs from higher orbits than L_1. Consequently, satellites fluorescence quanta appear, which correspond to the transitions of electrons to the states of the *M* and *N* shells. This new phenomenon must be taken into account in experiments. One can use it for the purpose of more reliable identification of the process and its mechanism. A more detailed analysis of the appearing satellite spectrum can be performed elsewhere.

Allowance for shake-off is also important in investigation of traditional β decay and other β processes. Such studies are carried out with the β decay of tritium [25] in the KATRIN experiment aimed at measuring the mass of an electron antineutrino and searching for sterile neutrinos. Shake-off modifies spectrum of emitted electrons near the upper bound—in the region which is most sensitive to the experimental determination of the neutrino mass. Taking shake-off into account is also important in establishing the bounds on the mass of the Majorana neutrinos in the study of double-β decay.

Similar measurements are also carried out by studying the *e* capture at ^{163}Ho, ^{159}Dy. Preference is given to these sources because of the minimum *Q* value. The lower the *Q* value, the greater the number of events falls close to the upper bound of the spectrum. In this case, the neutrino spectrum can be measured by detecting the secondary processes accompanying formation of the vacancy: fluorescence photons, Auger electrons by the calorimetric method. The calorimetric spectrum of *e* capture in ^{159}Dy to the 363.5449 keV level of ^{159}Tb, $Q = 1.14(19)$ keV was calculated in Ref. [26] with no allowance for shake-off. The calculation was performed within the Vatai approximation, in which the remaining electrons of the daughter atom inherit the quantum numbers of the parent atom. A continuous calorimetric spectrum was supposed to be created due to the width of the formed vacancy. The main contribution near the upper bound was obtained due to the N_1 capture with the formation of an excited state corresponding to the configuration [Xe]$4s^{-1}4f^{10}6s^2$. However, one can expect a significant contribution from the shake-off, for example, with the formation of a daughter atom in a configuration [Xe]$4s^{-1}5s^{-1}4f^{10}6s^2$. Then the continuity of the calorimetric spectrum is provided by the escape of the 5*s* electron into the continuum. Moreover, a significant contribution can be also expected from the electron shake-off from the N_2–N_5 and higher shells. As a result, due to various accompanying shake-off processes the capture rate can increase by several times.

Summing it up, one can conclude that the nonresonance shake-off mechanism of double-neutrinoless-*e* capture is an important example where this process, being of great interest in itself, manifests itself surprisingly clearly. Search for such surprising manifestations in other β processes looks to be a challenging task of the contemporary investigation.

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