

Secondary electrons emitted during nuclear β^- decay in few-electron atoms

Alexei M. Frolov*

Department of Applied Mathematics, University of Western Ontario, London, Ontario N6H 5B7, Canada

David M. Wardlaw†

Department of Chemistry, Memorial University of Newfoundland, St. John's, Newfoundland and Labrador A1C 5S7, Canada

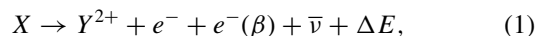
(Received 6 January 2016; published 29 June 2016)

“Additional” ionization of light atoms and ions during nuclear β^- decay is investigated. A procedure that can be used to determine the corresponding transition probabilities and the velocity/energy spectrum of secondary electrons is developed. Emission of very fast secondary electrons (δ electrons) from β^- -decaying atoms is also briefly discussed.

DOI: [10.1103/PhysRevC.93.065503](https://doi.org/10.1103/PhysRevC.93.065503)

I. INTRODUCTION

As is well known from numerous experiments, nuclear β^- decay in few- and many-electron atoms often proceeds with an “additional” atomic ionization. The general equation of this process can be written as (see, e.g., [1], [2])



where the symbols X and Y designate two chemical elements (isotopes) with almost-equal masses. The symbols X and Y in Eq. (1) are used to designate both the atoms/ions and the corresponding atomic nuclei. If Q is the electric charge of the parent (or incident) nucleus X , then the nuclear charge of the final nucleus Y is $Q + 1$. Below, the electric charge of the parent nucleus (Q) is designated by the notation Q_1 , while the electric charge of the final nucleus is denoted by the notation $Q_2 (= Q + 1)$. In Eq. (1) the notation e^- stands for the secondary (or slow) electron formed in the unbound spectrum during decay, while the notation $e^-(\beta)$ designates the primary (or fast) β^- electron and $\bar{\nu}$ denotes the electron’s antineutrino. The total energy ΔE released during the β^- decay, Eq. (1), is a given value (for each β^- decay) that cannot be changed in actual experiments. Formally, the numerical value of ΔE coincides with the maximal (kinetic) energy of the primary β^- electron emitted in Eq. (1).

Our goal in this study is the analysis of the properties of secondary electrons emitted during atomic β^- decay. In general, the properties of secondary electrons, e.g., their velocity spectra, can be used to describe the electron density distribution and electron-electron correlations in the incident atom. Moreover, by using recently developed experimental methods one can predict many interesting details on β^- decay in few-electron atoms and ions. Note that despite a number of experiments performed to investigate additional ionization of atoms during nuclear β^- decay, our current understanding of some important details of this process is still far from complete. In particular, the spectrum of the secondary electron emitted during nuclear β^- decay in atoms

has not been investigated in earlier studies. In this paper we derive a closed analytical formula for such a spectrum. Furthermore, it is crucial to explain how the electron-electron correlations in parent atoms can affect the secondary-electron spectrum. Another interesting problem discussed in this study is the formation of very fast secondary electrons (so-called δ electrons) during nuclear β^- decay in few-electron atoms/ions.

Since the first papers published in the 1950s (see, e.g., [3]), it became clear that by analyzing numerically generated spectra of the final-state probabilities during atomic β^- decay, Eq. (1), we can obtain a significant amount of useful information about the parent (or incident) atom/ion, including its atomic state and the presence of various excitations (see, e.g., [2], [4]–[7]). Furthermore, if the spectra of the final-state probabilities could be evaluated with a high accuracy (from numerical computations), then based on these spectra we would be able to predict the atom and its isotope in which nuclear β^- decay has occurred. A number of important details about electron distributions in such atoms/ions can also be accurately predicted. This conclusion is very important in applications to few- and many-electron atoms/ions with very short lifetimes. This emphasizes the importance of knowledge of the final-state probabilities for different atoms, ions, molecules, and atomic clusters.

In this study we also determine the distributions (or spectra) of the final-state probabilities of β^- -decaying atoms/ions, but our main goal is the analysis of cases where this decay proceeds with an additional atomic ionization, Eq. (1). Note that currently all calculations of the final-state probabilities for β^- -decaying atoms, ions, and molecules are performed with the use of the sudden approximation, which is based on the fact that the velocities of β^- electrons (v_β) emitted during nuclear β^- decay are significantly higher than the usual velocities of atomic electrons v_a . In particular, in light atoms we have $v_\beta \geq 50v_a - 200v_a$. This is also true for the velocities of the secondary electrons e^- , which can be emitted as “free” particles during the reaction, Eq. (1), i.e., $v_\beta \gg v_\delta$. The inequality $v_\beta \gg v_a$ allows one to apply the sudden approximation and analyze the nuclear β^- decay in light atoms by calculating the overlaps of the incident and final (nonrelativistic) atomic wave functions. The sudden approximation is based on the assumption that the wave function of the incident system does not change during the fast process, i.e., its amplitude and phase

*afrolov@uwo.ca

†dwardlaw@mun.ca

do not change. In other words, the electron density distribution in the maternal atom does not change during nuclear β^- decay (see discussions in [8] and [9]).

Our analysis of the properties of secondary electrons emitted during nuclear β^- decay in few-electron atoms begins with a general discussion of the final-state probabilities and sudden approximation, which has been extensively used in calculations of such probabilities. This problem is discussed in the next section. In Sec. III we determine the actual velocity spectrum of the secondary β^- electrons emitted during nuclear β^- decay of the one-electron tritium atom. The more general case of few-electron atoms is considered in Sec. IV, where we show explicitly that the energy/velocity spectra of secondary electrons essentially depend upon the electron-electron correlations (or interparticle correlations) in the parent few-electron atoms/ions. In Sec. V we evaluate the overall probabilities to observe very fast secondary electrons (or δ electrons) during nuclear β^- decay in few-electron atoms. Concluding remarks can be found in the last section (Sec. VI).

II. FINAL-STATE PROBABILITIES

In the sudden approximation the final-state probability of the process, Eq. (1), equals the overlap integral of the wave function of the parent atom X and wave function of the final double-charged ion Y^{2+} multiplied by the wave function of the outgoing (or “free”) electron, which has a certain momentum \mathbf{p} . The direction of the momentum \mathbf{p} in space coincides with the direction of motion/propagation of the actual free electron that is observed in experiments. Moreover, at large distances each of these free-electron wave functions must be a linear combination of a plane wave and an incoming spherical wave. Functions with such asymptotics take the form [10] (see also sec. 136 in [8])

$$\phi_p(r, \mathbf{n}_p \cdot \mathbf{n}_r) = N_f \exp\left(\frac{\pi}{2}\zeta\right) \Gamma(1 + i\zeta) {}_1F_1(-i\zeta, 1, -i(\mathbf{p} \cdot \mathbf{r} - pr)) \exp[i(\mathbf{p} \cdot \mathbf{r})], \quad (2)$$

where N_f is the normalization constant defined below, ${}_1F_1(a, b; z)$ is the confluent hypergeometric function, and $\zeta = \frac{Q_2}{a_0 p} = \frac{\alpha Q_2}{\gamma v}$, where a_0 is the Bohr radius, α is the fine-structure constant, and γ is the Lorentz γ factor [14] (see below) of the moving electron. The notations p and v stand for the momentum and velocity of the outgoing (or free) electron. Also, in this equation the two unit vectors \mathbf{n}_p and \mathbf{n}_r are defined as $\mathbf{n}_p = \frac{\mathbf{p}}{p}$ and $\mathbf{n}_r = \frac{\mathbf{r}}{r}$. There are a number of advantages in using the wave function of the free electron, which moves in the Coulomb field of the central “bare” nucleus, or a positively charged ion in the form of Eq. (2). Some of these advantages are discussed in sec. 136 of [8]. In particular, the choice of the $\phi_p(r, \mathbf{n}_p \cdot \mathbf{n}_r)$ function in the form of Eq. (2) directly leads to explicit formulas for the probability amplitudes, i.e., there is no need to perform any additional transformations of these values.

Let us consider nuclear β^- decay in actual atomic systems. First, consider the β^- -decaying hydrogen (or tritium) atom. The whole process is described by the following equation:

${}^3\text{H} = {}^3\text{He}^{2+} + e^- + e^-(\beta) + \bar{\nu}$. For simplicity, we assume that the central atomic nucleus is infinitely heavy. Also, in this study we assume that all parent (or incident) β^- -decaying atoms were in their ground 1^2s states (before β^- decay). In atomic units, where $\hbar = 1$, $m_e = 1$, and $e = 1$, the ground-state wave function of the one-electron, hydrogen-like atom/ion is $\frac{\eta\sqrt{\eta}}{\sqrt{\pi}} \exp(-\eta r)$. In the case of the β^- -decaying hydrogen/tritium atom we chose $Q_1 = Q = 1$ and $\eta = \frac{Q_1}{a_0}$, while for the final helium ion He^{2+} we have $Q_2 = Q + 1 (= 2)$ and $\zeta = \frac{Q_2}{a_0 p} = \frac{\alpha Q_2}{\gamma v}$.

The probability amplitude equals the overlap integral between the $\frac{\eta\sqrt{\eta}}{\sqrt{\pi}} \exp(-\eta r)$ function and the $N_f \phi_{kl}(r, \mathbf{n}_p \cdot \mathbf{n}_r)$ functions, Eq. (2). Calculations of similar integrals (or probability amplitudes) with the function $\phi_{kl}(r, \mathbf{n}_p \cdot \mathbf{n}_r)$, Eq. (2), are relatively simple and straightforward. There are a few steps in this procedure. First, we can write the following expression derived in [10],

$$\begin{aligned} I_1(\eta) &= 4\pi \int \exp[i(\mathbf{p} \cdot \mathbf{r} - \eta r)] \\ &\quad {}_1F_1(-i\zeta, 1, -i(\mathbf{p} \cdot \mathbf{r} - pr)) r dr \\ &= 4\pi \frac{1}{2} \left[\frac{1}{2} p^2 + \frac{1}{2} \eta^2 \right]^{\zeta-1} \left[-\frac{1}{2} p^2 + \frac{1}{2} \eta^2 - i\eta p \right]^{-i\zeta}; \end{aligned} \quad (3)$$

after a few steps of additional transformations this formula is reduced to the form

$$I_1(\eta) = 4\pi \left(\frac{\eta + ip}{\eta - ip} \right)^{i\zeta} \frac{1}{\eta^2 + p^2}. \quad (4)$$

By using the identity (see, e.g., Eq. (1.622) in [11])

$$\ln \left(\frac{\eta + ip}{\eta - ip} \right) = 2i \arctan \left(\frac{\eta}{p} \right), \quad (5)$$

we reduce the expression for the $I_1(\eta)$ integral to the form

$$I_1(\eta) = 4\pi \frac{1}{\eta^2 + p^2} \exp \left[-2\zeta \arctan \left(\frac{\eta}{p} \right) \right]. \quad (6)$$

All integrals that are needed to determine the amplitudes of the final-state probabilities can be derived by calculating partial derivatives of the $I_1(\eta)$ integral, Eq. (6), with respect to the variable $-\eta$. For instance, for our present purposes we need the integral $I_2(\eta)$, which is written in the form

$$\begin{aligned} I_2(\eta) &= 4\pi \int \exp[i(\mathbf{p} \cdot \mathbf{r} - \eta r)] \\ &\quad {}_1F_1(-i\zeta, 1, -i(\mathbf{p} \cdot \mathbf{r} - pr)) r^2 dr \\ &= -\frac{\partial I_1(\eta)}{\partial \eta} = 8\pi \frac{\eta + \zeta p}{(\eta^2 + p^2)^2} \exp \left[-2\zeta \arctan \left(\frac{\eta}{p} \right) \right]. \end{aligned} \quad (7)$$

The $I_2(\eta)$ integral, Eq. (7) (with the additional normalization factors N_f and N_H), determines the probability of the “additional” ionization of the hydrogen/tritium atom from its ground 1^2s state during nuclear β^\pm decay. The momentum of the free electron is \mathbf{p} , and $p = |\mathbf{p}|$ is its absolute value. If we want

to determine the final-state probabilities of atomic ionization during nuclear β^\pm decay of the hydrogen/tritium atom from excited s states, then higher derivatives from the $I_1(\eta)$ integral are needed. In general, all integrals $I_n(\eta)$ can be found with the use of the formula

$$I_n(\eta) = (-1)^n \left[\frac{\partial}{\partial \eta} \right]^n I_1(\eta) = 2^{n+2} \pi \frac{P_n(\eta, \zeta, p)}{(\eta^2 + p^2)^n} \times \exp \left[-2\zeta \arctan \left(\frac{\eta}{p} \right) \right], \quad (8)$$

where $P_n(\eta, \zeta, p)$ is a polynomial function of all its variables. In the derivation of formulas for the integrals $I_n(\eta)$ it is convenient to assume that these three variables, η , ζ , and p are independent of each other. However, to produce actual formulas for the probability amplitudes and final-state probabilities we have to take into account the following relation between these variables: $\frac{\eta}{p} = \frac{Q_1}{Q_2} \zeta$ or $\zeta p = \frac{Q_2}{Q_1} \eta$. This allows us to write the expression for the integral $I_2(\eta)$

$$I_2(\eta) = 8\pi \frac{\eta \left(\frac{Q_2}{Q_1} + 1 \right)}{(\eta^2 + p^2)^2} \exp \left[-2 \left(\frac{Q_2 \eta}{Q_1 p} \right) \arctan \left(\frac{Q_2 \eta}{Q_1 p} \right) \right], \quad (9)$$

where we have used the two variables η and p . However, in some cases two other variables (e.g., ζ and p) are more convenient. Note that it is possible to produce a few useful relations between $I_n(\eta)$ and $I_{n-1}(\eta)$, $I_{n-2}(\eta)$, ... $I_1(\eta)$ integrals. Such relations allow one to determine all integrals $I_n(\eta)$ without any actual computation.

III. TRITIUM ATOM

Consider nuclear β^- decay in the one-electron hydrogen/tritium atom ^3H or in some hydrogen-like ion with nuclear electric charge Q . According to the formulas derived above the probability amplitude $\mathcal{A}_{i \rightarrow f}$ is

$$\mathcal{A}_{i \rightarrow f} = 8\pi N_H N_f \frac{\eta \left(\frac{Q_2}{Q_1} + 1 \right)}{(\eta^2 + p^2)^2} \times \exp \left[-2 \left(\frac{Q_2 \eta}{Q_1 p} \right) \arctan \left(\frac{Q_2 \eta}{Q_1 p} \right) \right], \quad (10)$$

where $N_H = \sqrt{\frac{\eta^3}{\pi \alpha_0^3}}$ is the normalization constant of the hydrogen-atom wave function, while N_f is the normalization constant of the wave function which represents the “free” electron. The numerical value of this normalization constant (N_f) is determined by the equality

$$N_f^{-2} = \exp \left(\frac{\pi}{2} \zeta \right) \Gamma(1 + i\zeta) \exp \left(\frac{\pi}{2} \zeta \right) \Gamma(1 - i\zeta) = \exp(\pi \zeta) \frac{\pi \zeta}{\sinh(\pi \zeta)} = \frac{2\pi \zeta}{1 - \exp(-2\pi \zeta)}; \quad (11)$$

see, e.g., [12]. In other words, the probability amplitude $\mathcal{A}_{i \rightarrow f}$ equals

$$\mathcal{A} = 4 \sqrt{\frac{2\eta^3}{\zeta}} \left[1 - \exp \left(-2\pi \frac{Q_2 \eta}{Q_1 p} \right) \right] \frac{\eta \left(\frac{Q_2}{Q_1} + 1 \right)}{(\eta^2 + p^2)^2} \times \exp \left[-2 \left(\frac{Q_2 \eta}{Q_1 p} \right) \arctan \left(\frac{Q_2 \eta}{Q_1 p} \right) \right]. \quad (12)$$

The expression for the infinitely small final-state probability $\Delta P_{i \rightarrow f}$ takes the form

$$\Delta P_{i \rightarrow f} = |\mathcal{A}|^2 p^2 \Delta p = \frac{32\eta^3}{\zeta} \left[1 - \exp \left(-2\pi \frac{Q_2 \eta}{Q_1 p} \right) \right] \frac{p^2 \eta^2 \left(\frac{Q_2}{Q_1} + 1 \right)^2}{(\eta^2 + p^2)^4} \times \exp \left[-4 \left(\frac{Q_2 \eta}{Q_1 p} \right) \arctan \left(\frac{Q_2 \eta}{Q_1 p} \right) \right] \Delta p. \quad (13)$$

To produce the final expression which is ready for calculations we have to replace here the variables η and ζ with the expressions $\eta = \frac{Q_1}{a_0}$, $\frac{\eta}{p} = \frac{\alpha Q_1}{\gamma v}$, and $\zeta = \frac{Q_2 \eta}{Q_1 p} = \frac{\alpha Q_2}{\gamma v}$, where $Q_1 (= Q)$ is the electric charge of the incident nucleus (or central positively charged ion) and $a_0 = \frac{\hbar^2}{m_e e^2}$ is the Bohr radius. In atomic units, where $\hbar = 1$, $e = 1$, and $m_e = 1$, the Bohr radius equals unity and the ratio $\frac{\eta}{p}$ equals the ratio $\frac{\alpha Q_1}{\gamma v}$ (since $m_e = 1$), where $\alpha = \frac{\hbar^2}{m_e e^2}$ is the fine-structure constant and $v = |\mathbf{v}|$ is the absolute value of the electron's velocity (expressed in atomic units). The factor $\gamma = \frac{1}{\sqrt{1 - \frac{v^2}{c^2}}} = \frac{1}{\sqrt{1 - \alpha^2 v^2}}$ is the Lorentz γ factor [14] of the moving electron. In atomic units the electron's velocity cannot exceed the value of $c = \alpha^{-1}$ (≈ 137).

A. Velocity spectrum

From, Eq. (13), one finds the following expression for the final-state probability distribution, or $P_{i \rightarrow f}(v)$ distribution:

$$\frac{dP_{i \rightarrow f}}{dv} = \frac{32Q_1}{\alpha Q_2} \left[1 - \exp \left(-2\pi \frac{\alpha Q_2}{\gamma v} \right) \right] \frac{(Q_1^2 + Q_2^2)^2 \gamma^4 v^3}{(Q_1^2 + \gamma^2 v^2)^4} \times \exp \left[-4 \left(\frac{\alpha Q_2}{\gamma v} \right) \arctan \left(\frac{\alpha Q_2}{\gamma v} \right) \right]. \quad (14)$$

The expression on the right-hand side of this equality essentially coincides with the v spectrum of free electrons emitted during nuclear β^- decay in one-electron atoms/ions. Rigorously speaking, any spectral function must be normalized, i.e., its integral over v (from $v_{\min} = 0$ to $v_{\max} = c = \alpha^{-1}$ in a.u.) must be equal to unity. This allows one to obtain the following expression for the v spectral function (or v spectrum, for short) [13]:

$$S_e(v; Q) = \frac{32Q_1}{\mathcal{S}(Q) \alpha Q_2} \left[1 - \exp \left(-2\pi \frac{\alpha Q_2}{\gamma v} \right) \right] \frac{(Q_1^2 + Q_2^2)^2 \gamma^4 v^3}{(Q_1^2 + \gamma^2 v^2)^4} \times \exp \left[-4 \left(\frac{\alpha Q_2}{\gamma v} \right) \arctan \left(\frac{\alpha Q_2}{\gamma v} \right) \right], \quad (15)$$

where the normalization constant $\mathcal{S}(Q)$ can be obtained (for each pair $Q_1 = Q$ and $Q_2 = Q + 1$) with the use of numerical

integration. For the tritium atom $Q_1 = 1$ and $Q_2 = 2$ we have found that $\mathcal{S}(Q) \approx 196.611\ 833\ 628\ 395$. As expected, the formula, Eq. (15), contains only the absolute values of the free-electron velocity v (or momentum p) and electric charges of the atomic nuclei $Q_1 = Q$ and $Q_2 = Q + 1$. The velocity of the fast β^- electron is not included in this formula. This is a direct consequence of the sudden approximation used to derive this formula. In general, by using the known v spectral function we can evaluate the probability $p(v)$ of observing a secondary electron that moves at the velocity v (expressed in atomic units).

Note that Eq. (15) is written in a manifestly relativistic form, i.e., formally the energies of secondary electrons can be arbitrary. However, both wave functions used in our calculations of the overlap integrals are nonrelativistic. Furthermore, in applications to actual atoms and ions, the total energies of the emitted secondary electrons are nonrelativistic, e.g., $E \leq 50$ keV for arbitrary atoms and $E \leq 25$ keV for light atoms. This means we do not need to apply any relativistic, or even semirelativistic, approximation. In other words, we can always assume that $\gamma = 1$ in the formula, Eq. (15). The nonrelativistic spectral function of secondary electrons then takes the form

$$S_e(v; Q) = \frac{32Q_1}{\mathcal{S}(Q)\alpha Q_2} \left[1 - \exp\left(-2\pi \frac{\alpha Q_2}{v}\right) \right] \frac{(Q_1^2 + Q_2^2)^2 v^3}{(Q_1^2 + v^2)^4} \times \exp\left[-4\left(\frac{\alpha Q_2}{v}\right) \arctan\left(\frac{\alpha Q_2}{v}\right)\right]. \quad (16)$$

In applications to real (light) atoms the differences between these two spectral functions, defined by Eq. (15) and Eq. (16), are very small for all light atoms. This follows from the explicit form of the right-hand side of these two equations, which contains an exponential cutoff factor for high velocities/energies. In this study all computational results have been determined with the use of the spectral function, Eq. (15).

B. Calculations

In actual experiments the integral of the spectral function $S_e(v; Q)$ between the v_1 and the v_2 values ($v_2 > v_1$) gives one the probability $P(v_1; v_2)$ of detecting the free electron emitted during the process, Eq. (1), with the velocity bounded between v_1 and v_2 . This probability is normalized over all possible free-electron velocities. However, in actual experiments, in addition to such bound-free transitions we always observe a large number of bound-bound transitions. In this case the problem of determining the absolute values of probabilities of the partial bound-free transitions is reduced to calculations of the conditional probabilities. To solve this problem one needs to know the total probability of the bound-bound transitions P_{bb} during nuclear β^- decay. If this value is known, then it is easy to find the total probability of the bound-free transitions $P_{bf} = 1 - P_{bb}$ and the absolute value of the partial bound-free probability $\mathcal{P}(v_1; v_2) = P_{bf} P(v_1; v_2) = (1 - P_{bb})P(v_1; v_2)$.

Let us consider the β^- decay in the one-electron tritium atom ${}^3\text{H}$ (or T). For simplicity, here we restrict our analysis to the β^- decay of the tritium atom from its ground 1^2s state. Moreover, we assume that the atomic nucleus in the

hydrogen/tritium atom is infinitely heavy. In general, during nuclear β^- decay in such a one-electron tritium atom one can observe a large number of bound-bound transitions such as $\text{H}(1^2s) \rightarrow \text{He}^+(n^2s)$, where n is the principal quantum number of the one-electron (or hydrogen-like) He^+ ion. The sudden approximation leads to the conservation of the electron angular momentum [or $L(L+1)$ value] during nuclear β^- decays in few-electron atoms. The total electron spin [or $S(S+1)$ value] is also conserved (as well as the spatial parities $\hat{\pi}$ of the incident and final-wave functions) [2]. This means that bound-bound transitions from the 1^2s state of the tritium atom to all bound n^2s states of the one-electron helium ion (He^+) are possible. In this study the probabilities of such transitions have been determined to a high accuracy and are listed in Table I. Their numerical calculations are relatively simple, since we only need to determine the overlap of the two hydrogen-like, i.e., one-electron, wave functions. The sum of these probabilities converges to the total probability of the bound-bound transition. The convergence of the P_{bb} probability obtained with the use of the 100–1500 lowest n^2s states in the He^+ ion can be understood from Table II. The difference between unity and this probability, $P_{bb} \approx 0.973\ 727\ 35(10)$, equals the total probability $P_{bf} \approx 0.026\ 272\ 65(10)$ of the bound-free transitions for the process, Eq. (1). In other words, the P_{bf} value is the total ionization probability of the He^+ ion during nuclear β^- decay in the tritium atom. For the one-electron ${}^3\text{H}$ atom this probability ($\approx 2.627\%$) is quite low, but in many atoms the probabilities of similar processes are higher. For instance, for the β^- decay of the Li atom from its ground 2^2S state, the corresponding probability is $\approx 15\%$ [4]. In many weakly bound atomic ions, e.g., in the two-electron H^- ion [2], the overall probability of bound-free transitions is comparable to and even higher than the total probability of bound-bound transitions. Numerical calculations of the bound-bound-state probabilities for other atomic and molecular systems can be found, e.g., in [6] and [7]. Here we do not discuss such calculations, since our current goal is to investigate the bound-free transitions during nuclear β^- decay in few-electron atoms.

Convergence of the spectral integral $\mathcal{S}(Q)$ for β^- decay of a hydrogen/tritium atom with an infinitely heavy nucleus has been investigated in the following way. First, let us note that our method is based on the division of the main velocity interval between $v_{\min} = 0$ and $v_{\max} = \alpha^{-1}$ into N equal intervals $\delta = \frac{v_{\max} - v_{\min}}{N}$. To perform numerical integration each of these intervals $\delta = \frac{v_{\max} - v_{\min}}{N}$ is separated into $2^{N_s - 2} + 1$ interior subintervals which are used in the “extended” trapezoidal method in [20] and [21]. In our calculations both N and N_s values have been varied, e.g., $N = 5000, 1000, \dots$, and $N_s = 6, 8, 10, 12$. Finally, we have determined the resulting numerical value of $\mathcal{S}(Q)$ in Eq. (15) to a high accuracy: $\mathcal{S}(Q) \approx 196.611\ 833\ 628\ 395$. This value has been used in all numerical calculations of probabilities.

Table III lists numerical results for probabilities of the bound-free transitions $p_{bf}(0, v)$ during nuclear β^- decay of a hydrogen/tritium atom with an infinitely heavy nucleus. In these probabilities the velocities of the final electrons (in a.u.) are bounded between $v_1 = 0$ and $v_2 = v$. Note, again, that these probabilities [$p_{bf}(0, v)$] are the absolute probabilities of the bound-free transitions, i.e., all bound-bound transitions

TABLE I. Probabilities (in %) of ground-bound $H(1s) \rightarrow He^+(ns)$ transitions during nuclear β^- decay in the ground $1s$ state of the hydrogen/tritium atom with an infinitely heavy nucleus. n is the principal quantum number of the one-electron He^+ ion. The notation s corresponds to states in which the electron angular momentum equals 0, i.e., $\ell = 0$.

n	P_{bb}	n	P_{bb}	n	P_{bb}	n	P_{bb}
1	$0.70233196159122 \times 10^2$	26	$0.98497803948971 \times 10^{-3}$	51	$0.12974615801458 \times 10^{-3}$	76	$0.39162862050606 \times 10^{-4}$
2	$0.25000000000000 \times 10^2$	27	$0.87903331958611 \times 10^{-3}$	52	$0.12239426027150 \times 10^{-3}$	77	$0.37655868762239 \times 10^{-4}$
3	$0.12740198400000 \times 10^1$	28	$0.78776907687202 \times 10^{-3}$	53	$0.11558764797038 \times 10^{-3}$	78	$0.36225224231066 \times 10^{-4}$
4	0.38536733146295	29	$0.70872572575441 \times 10^{-3}$	54	$0.10927667532924 \times 10^{-3}$	79	$0.34866153324904 \times 10^{-4}$
5	0.17197881444822	30	$0.63992249530316 \times 10^{-3}$	55	$0.10341702481201 \times 10^{-3}$	80	$0.33574234908023 \times 10^{-4}$
6	$0.92697143554687 \times 10^{-1}$	31	$0.57975202780078 \times 10^{-3}$	56	$0.97969051544095 \times 10^{-4}$	81	$0.32345371594829 \times 10^{-4}$
7	$0.55988010386724 \times 10^{-1}$	32	$0.52690070162347 \times 10^{-3}$	57	$0.92897218340823 \times 10^{-4}$	82	$0.31175762421737 \times 10^{-4}$
8	$0.36520347436057 \times 10^{-1}$	33	$0.48028782045420 \times 10^{-3}$	58	$0.88169607495337 \times 10^{-4}$	83	$0.30061878124243 \times 10^{-4}$
9	$0.25189293972900 \times 10^{-1}$	34	$0.43901878492219 \times 10^{-3}$	59	$0.83757497787194 \times 10^{-4}$	84	$0.29000438743047 \times 10^{-4}$
10	$0.18128415546737 \times 10^{-1}$	35	$0.40234872896302 \times 10^{-3}$	60	$0.79634997068789 \times 10^{-4}$	85	$0.27988393315259 \times 10^{-4}$
11	$0.13491846662324 \times 10^{-1}$	36	$0.36965406024421 \times 10^{-3}$	61	$0.75778722345554 \times 10^{-4}$	86	$0.27022901434745 \times 10^{-4}$
12	$0.10317897096839 \times 10^{-1}$	37	$0.34041002208870 \times 10^{-3}$	62	$0.72167520551830 \times 10^{-4}$	87	$0.26101316490293 \times 10^{-4}$
13	$0.80702692482061 \times 10^{-2}$	38	$0.31417287990638 \times 10^{-3}$	63	$0.68782224288764 \times 10^{-4}$	88	$0.25221170411742 \times 10^{-4}$
14	$0.64331044013362 \times 10^{-2}$	39	$0.29056568635742 \times 10^{-3}$	64	$0.65605437674441 \times 10^{-4}$	89	$0.24380159773154 \times 10^{-4}$
15	$0.52118281754238 \times 10^{-2}$	40	$0.26926683590156 \times 10^{-3}$	65	$0.62621348192771 \times 10^{-4}$	90	$0.23576133118693 \times 10^{-4}$
16	$0.42819805426639 \times 10^{-2}$	41	$0.25000080828061 \times 10^{-3}$	66	$0.59815561042724 \times 10^{-4}$	91	$0.22807079391474 \times 10^{-4}$
17	$0.35613569395414 \times 10^{-2}$	42	$0.23253064079662 \times 10^{-3}$	67	$0.57174953004965 \times 10^{-4}$	92	$0.22071117358569 \times 10^{-4}$
18	$0.29941400117151 \times 10^{-2}$	43	$0.21665177430539 \times 10^{-3}$	68	$0.54687543276013 \times 10^{-4}$	93	$0.21366485936703 \times 10^{-4}$
19	$0.25415046800868 \times 10^{-2}$	44	$0.20218699709848 \times 10^{-3}$	69	$0.52342379084963 \times 10^{-4}$	94	$0.20691535333240 \times 10^{-4}$
20	$0.21758661045733 \times 10^{-2}$	45	$0.18898227105998 \times 10^{-3}$	70	$0.50129434216051 \times 10^{-4}$	95	$0.20044718925958 \times 10^{-4}$
21	$0.18772530302835 \times 10^{-2}$	46	$0.17690327054347 \times 10^{-3}$	71	$0.48039518821441 \times 10^{-4}$	96	$0.19424585813027 \times 10^{-4}$
22	$0.16309610499354 \times 10^{-2}$	47	$0.16583249987351 \times 10^{-3}$	72	$0.46064199130287 \times 10^{-4}$	97	$0.18829773971567 \times 10^{-4}$
23	$0.14259985577972 \times 10^{-2}$	48	$0.15566688284309 \times 10^{-3}$	73	$0.44195725848781 \times 10^{-4}$	98	$0.18259003969442 \times 10^{-4}$
24	$0.12540360783342 \times 10^{-2}$	49	$0.14631573897880 \times 10^{-3}$	74	$0.42426970206833 \times 10^{-4}$	99	$0.17711073180448 \times 10^{-4}$
25	$0.11086825104638 \times 10^{-2}$	50	$0.13769907811358 \times 10^{-3}$	75	$0.40751366744682 \times 10^{-4}$	100	$0.17184850458006 \times 10^{-4}$

are ignored. To obtain the total probabilities of the bound-free transitions the $p_{bf}(0, v)$ values from Table III must be multiplied by the factor $P_{bf} \approx 0.026\,272\,65(10)$. Then one finds for the overall probability of observing secondary (or free) electrons following nuclear β^- decay in atoms with the velocity v bounded between v_1 and v_2 values: $\overline{P}_{bf}(v_1, v_2) = P_{bf}(p_{bf}(0, v_2) - p_{bf}(0, v_1))$. For instance, in the case of nuclear β^- decay of the hydrogen/tritium atom with an infinitely heavy nucleus the overall probability of observing a secondary (or free) electron with the velocity located in the interval $0.6 \leq v \leq 3.0$ is $\overline{P}_{bf}(v_1, v_2) = P_{bf} \cdot (p_{bf}(0, v_2) - p_{bf}(0, v_1)) \approx 0.026\,272\,65 \cdot (0.901\,846\,525\,528\,880\,670 - 0.065\,985\,776\,653\,782\,145\,9) \approx 0.021\,960\,276\,9$, or 2.196 028% of all β^- decays. The first conditional probability

$p_{bf}(0, v_2)$ corresponds to $v_2 = 3.0$, while the second value $p_{bf}(0, v_1)$ has been determined for $v_1 = 0.6$. Note that for the β^- -decaying tritium atom the velocities of more than 90% of all secondary electrons are located between $v = 0.4$ and $v = 3.2$ (in a.u.) This range of velocities of secondary electrons corresponds to the maximum of the v distribution for the ${}^3\text{H} \rightarrow {}^3\text{He}^{2+} + e^- + e^-(\beta) + \bar{\nu}$ decay. Probabilities of observing secondary electrons with different velocity distributions can be evaluated analogously by using our results in Table III. In many cases it is more convenient to use the (partial) probabilities $p(v_1, v_2)$ defined for proximate numerical values of the two velocities v_1 and v_2 , rather than the probabilities $p(0, v_1)$ and $p(0, v_2)$ defined above. The corresponding numerical values of

TABLE II. Convergence of the total probabilities P_{bb} of bound-bound transitions during nuclear β^- decay of the hydrogen/tritium atom with an infinitely heavy nucleus. N is the total number of hydrogen ns states used in calculations. n is the principal quantum number, while the notation s corresponds to states in which the electron angular momentum ℓ equals 0.

N	P_{bb}	N	P_{bb}	N	P_{bb}
100	0.97371867838323	600	0.97372694486699	1100	0.97372711211312
200	0.97372504662813	700	0.97372700800983	1200	0.97372712343446
300	0.97372623196518	800	0.97372704900471	1300	0.97372713224605
400	0.97372664761376	900	0.97372707711733	1400	0.97372713923839
500	0.97372684019166	1000	0.97372709722987	1500	0.97372714487989

TABLE III. Probabilities of bound-free transitions $p_{bf}(0, v)$ during nuclear β^- decay of the hydrogen/tritium atom with an infinitely heavy nucleus. Velocities of the final electrons (in a.u.) are bounded between $v_1 = 0$ and $v_2 = v$.

v	$p_{bf}(0, v)$	v	$p_{bf}(0, v)$	v	$p_{bf}(0, v)$
0.2	$0.202955922212782602 \times 10^{-2}$	5.2	0.987931066690482215	11.0	0.999621008255497052
0.4	$0.200048139756265682 \times 10^{-1}$	5.4	0.989736091238550430	12.0	0.999752250217591601
0.6	$0.659857766537821459 \times 10^{-1}$	5.6	0.991234205230340430	13.0	0.999832921059878887
0.8	0.141004332183129327	5.8	0.992483168360981649	14.0	0.999884258264978038
1.0	0.237287332714349043	6.0	0.993528952322103761	15.0	0.999917927291765081
1.2	0.343391270067291913	6.2	0.994408306447324685	16.0	0.999940598633865546
1.4	0.448732996357998742	6.4	0.995150736609713835	17.0	0.999956223482800655
1.6	0.545899125149580895	6.6	0.995780036319943809	18.0	0.999967216325934628
1.8	0.630960454661736217	6.8	0.996315475460822611	19.0	0.999975094027025284
2.0	0.702727742898327263	7.0	0.996772726630822888	20.0	0.999980833420389250
2.2	0.761747499185994498	7.2	0.997164589802220096	21.0	0.999985077730389047
2.4	0.809452784832214921	7.4	0.997501561449582277	22.0	0.999988259111051570
2.6	0.847587005336058183	7.6	0.997792283321484132	23.0	0.999990673256248918
2.8	0.877871771087206655	7.8	0.998043897732244535	24.0	0.999992525883633287
3.0	0.901846525528880670	8.0	0.998262329974406395	25.0	0.999993962308590595
3.2	0.920812454828480454	8.2	0.998452513694625161	26.0	0.999995086624120623
3.4	0.935832170786307351	8.4	0.998618571459107597	27.0	0.999995974360824529
3.6	0.947754919518541073	8.6	0.998763959977849436	28.0	0.999996680980098227
3.8	0.957250346302898296	8.8	0.998891587348680657	29.0	0.999997247658096693
4.0	0.964842246540587289	9.0	0.999003908064542578	30.0	0.999997705279853880
4.2	0.970938568648528298	9.2	0.999103000282010388	35.0	0.999999010082609818
4.4	0.975856499673367406	9.4	0.999190628886819629	40.0	0.999999532973409329
4.6	0.979842702466459428	9.6	0.999268297146016705	50.0	0.999999875793757797
4.8	0.983089287546310995	9.8	0.999337289155711966	75.0	0.99999992734260541
5.0	0.985746248754140539	10.0	0.999398704839936441	100.0	0.99999999611764017

these probabilities $p(v_1, v_2)$ (for $v_1 \neq 0$) are listed in Table IV.

IV. β^- DECAYS IN FEW-ELECTRON ATOMS

Our original interest in the problems discussed in this study was based on the fact that in actual applications it is often important to know not only the value P_{bf} , but also the so-called partial probabilities $p_{i \rightarrow \mathbf{p}}$, where i is the incident state in the parent atom (tritium), while the notation \mathbf{p} represents the final state of the “free” electron (in momentum space) which moves in the field of the final ion (He^{2+} ion). We have developed an effective method for numerical calculations of these probabilities. This method is described in detail below. Using Eq. (14) and Eq. (15) one can determine all final-state probabilities and p and v spectra of the secondary (or free) electrons emitted during nuclear β^- decay in few-electron atoms. In general, our additional investigations of atomic ionization during nuclear β^- decay in few-electron atoms unambiguously lead to the conclusion that the spectra of secondary electrons, partial probabilities of bound-free transitions $p_{i \rightarrow \mathbf{p}}$, and total probability of such transitions P_{bf} depend upon the electron-electron correlations in the incident bound state of the maternal atom. This means that we can study electron-electron correlations in the maternal (or parent) atom by analyzing the spectra of secondary electrons emitted during its nuclear β^- decay. This conclusion is important for future experimental studies.

To illustrate the general situation with few-electron atoms and ions let us consider β^- -decaying two-electron atoms and ions, i.e., He-like atomic systems with β^- decays. Simple and very compact analytical expressions for bound-state wave functions of two-electron atoms/ions can be derived in relative and/or perimetric coordinates [5]. The exact wave functions of such atomic systems are truly correlated and depend upon all three relative coordinates r_{32} , r_{31} , and r_{21} . It is very difficult to explain in a few lines all aspects of integration in relative and/or perimetric coordinates and we do not attempt to do so here. For the purposes of this study we can operate with the following approximate analytical expression for the two-electron wave function (see, e.g, [8] and [15]):

$$\begin{aligned} \Psi &= N_1 N_2 \exp[-(Q - q)(r_{1N} + r_{2N})] \\ &= \frac{(Q - q)}{\pi a_0} \exp[-(Q - q)(r_{1N} + r_{2N})], \end{aligned} \quad (17)$$

where Q is the electric charge of the atomic nucleus ($Q \geq 2$), while $Q - q$ is the “effective” electric charge of the atomic nucleus. A small correction q ($q \leq 1$) is introduced in this equation to represent an effective contribution of electron-electron correlations. In Eq. (17) the indices 1 and 2 stand for the two atomic electrons, while the index N designates the atomic nucleus, which is assumed to be infinitely heavy. It can be shown that such a simple wave function provides a quite accurate approximation of the actual two-electron wave function. For the ground state of the He atom, the approximate wave function, Eq. (17), reproduces $\approx 98.15\%$ of its “exact”

TABLE IV. Probabilities of bound-free transitions $p_{bf}(v_1, v_2)$ during nuclear β^- decay of the tritium atom with an infinitely heavy nucleus. Calculations are performed with the use of Eq. (15), where $0 \leq v \leq \alpha^{-1}$. To obtain the absolute final-state probabilities these values must be multiplied by the additional factor $P_{bf} \approx 0.026\,272\,65(10)$.

v_1	v_2	$p_{bf}(v_1, v_2)$	v_1	v_2	$p_{bf}(v_1, v_2)$	v_1	v_2	$p_{bf}(v_1, v_2)$
0.1	0.2	$0.188748693806651259 \times 10^{-2}$	3.3	3.4	$0.707471726450662352 \times 10^{-2}$	11.4	11.5	$0.132984011459287600 \times 10^{-4}$
0.2	0.3	$0.599493924449560325 \times 10^{-2}$	3.4	3.5	$0.630325324464037966 \times 10^{-2}$	11.8	11.9	$0.108963869731728562 \times 10^{-4}$
0.3	0.4	$0.119838730486052627 \times 10^{-1}$	3.5	3.6	$0.562029109359469465 \times 10^{-2}$	12.2	12.3	$0.898231826177633474 \times 10^{-5}$
0.4	0.5	$0.191713037476076467 \times 10^{-1}$	3.6	3.7	$0.501570335101668238 \times 10^{-2}$	12.6	12.7	$0.744673944950352989 \times 10^{-5}$
0.5	0.6	$0.268148704175592575 \times 10^{-1}$	3.7	3.8	$0.448040726228595298 \times 10^{-2}$	13.0	13.1	$0.620692664989309923 \times 10^{-5}$
0.6	0.7	$0.342169825838334266 \times 10^{-1}$	3.8	3.9	$0.400629926793153534 \times 10^{-2}$	13.4	13.5	$0.519985882180620792 \times 10^{-5}$
0.7	0.8	$0.408046817645270038 \times 10^{-1}$	3.9	4.0	$0.358617903052689251 \times 10^{-2}$	13.8	13.9	$0.437716091236265067 \times 10^{-5}$
0.8	0.9	$0.461752111181489148 \times 10^{-1}$	4.0	4.1	$0.321366933187318903 \times 10^{-2}$	14.3	14.4	$0.355190209386678934 \times 10^{-5}$
0.9	1.0	$0.501069962296554854 \times 10^{-1}$	4.1	4.2	$0.288313611172121066 \times 10^{-2}$	14.7	14.8	$0.301972189121095148 \times 10^{-5}$
1.0	1.1	$0.525430066270895517 \times 10^{-1}$	4.4	4.5	$0.209661698161469378 \times 10^{-2}$	15.0	15.1	$0.268074181892024922 \times 10^{-5}$
1.1	1.2	$0.535569109220308864 \times 10^{-1}$	4.5	4.6	$0.188991759227905040 \times 10^{-2}$	15.3	15.4	$0.238503756961240852 \times 10^{-5}$
1.2	1.3	$0.533124182096042009 \times 10^{-1}$	4.6	4.7	$0.170565123472654998 \times 10^{-2}$	15.5	15.6	$0.220885480460924363 \times 10^{-5}$
1.3	1.4	$0.520239546086940725 \times 10^{-1}$	4.8	4.9	$0.139429327402048644 \times 10^{-2}$	16.0	16.1	$0.183048927501968280 \times 10^{-5}$
1.4	1.5	$0.499237380879169903 \times 10^{-1}$	5.0	5.1	$0.126289351295904078 \times 10^{-2}$	17.0	17.1	$0.127721410753661143 \times 10^{-5}$
1.5	1.6	$0.472374282113263953 \times 10^{-1}$	5.2	5.3	$0.945111931756639213 \times 10^{-3}$	18.0	18.1	$0.908492839681844620 \times 10^{-6}$
1.6	1.7	$0.441683859834397057 \times 10^{-1}$	5.4	5.5	$0.783566193490159289 \times 10^{-3}$	19.0	19.1	$0.657462602010086667 \times 10^{-6}$
1.7	1.8	$0.408893070688341261 \times 10^{-1}$	5.6	5.7	$0.652564255926359053 \times 10^{-3}$	20.0	20.1	$0.483245270914358678 \times 10^{-6}$
1.8	1.9	$0.375394578360157054 \times 10^{-1}$	5.8	5.9	$0.545847733296032050 \times 10^{-3}$	21.0	21.1	$0.360220839892367412 \times 10^{-6}$
1.9	2.0	$0.342257171222356938 \times 10^{-1}$	6.0	6.1	$0.458524742961601043 \times 10^{-3}$	22.0	22.1	$0.271967525801591057 \times 10^{-6}$
2.0	2.1	$0.310258812602125892 \times 10^{-1}$	6.7	6.8	$0.257061914585502687 \times 10^{-3}$	23.0	23.1	$0.207742414782007755 \times 10^{-6}$
2.1	2.2	$0.279930533347722332 \times 10^{-1}$	7.0	7.1	$0.203416661022484588 \times 10^{-3}$	24.0	24.1	$0.160385605407817376 \times 10^{-6}$
2.2	2.3	$0.251603010727732525 \times 10^{-1}$	7.3	7.4	$0.162215738465301014 \times 10^{-3}$	25.0	25.1	$0.125043165180335074 \times 10^{-6}$
2.3	2.4	$0.225450758213940055 \times 10^{-1}$	7.6	7.7	$0.130309358504550521 \times 10^{-3}$	27.0	27.1	$0.780383645690348706 \times 10^{-7}$
2.4	2.5	$0.201531190401666584 \times 10^{-1}$	8.0	8.1	$0.983551981869120013 \times 10^{-4}$	30.0	30.1	$0.407187063104246108 \times 10^{-7}$
2.5	2.6	$0.179817451095081113 \times 10^{-1}$	8.4	8.5	$0.750897540252961992 \times 10^{-4}$	35.0	35.1	$0.155222874488130268 \times 10^{-7}$
2.6	2.7	$0.160224922926440151 \times 10^{-1}$	8.8	8.9	$0.579397050271662135 \times 10^{-4}$	40.0	40.1	$0.662851903623728573 \times 10^{-8}$
2.7	2.8	$0.142631922581957772 \times 10^{-1}$	9.2	9.3	$0.451506651248345601 \times 10^{-4}$	45.0	45.1	$0.308047666225349931 \times 10^{-8}$
2.8	2.9	$0.126895364261496964 \times 10^{-1}$	9.6	9.7	$0.355100957492926310 \times 10^{-4}$	50.0	50.1	$0.152690469597701984 \times 10^{-8}$
2.9	3.0	$0.112862256268808421 \times 10^{-1}$	10.0	10.1	$0.281690513621917630 \times 10^{-4}$	55.0	55.1	$0.795413539717975718 \times 10^{-9}$
3.0	3.1	$0.100377863252957321 \times 10^{-1}$	10.4	10.5	$0.225258543290844444 \times 10^{-4}$	60.0	60.1	$0.430580269208474099 \times 10^{-9}$
3.1	3.2	$0.892912755022094856 \times 10^{-2}$	10.8	10.9	$0.181491361268184092 \times 10^{-4}$	70.0	70.1	$0.136754671307452372 \times 10^{-9}$
3.2	3.3	$0.794590125773871769 \times 10^{-2}$	11.0	11.1	$0.163344102596100687 \times 10^{-4}$	75.0	75.1	$0.791005569608716576 \times 10^{-10}$

total energy. The optimal value of the parameter q in Eq. (17) equals $\frac{5}{16}$ [8, 15]. On the other hand, the approximate wave function is represented in a factorized form [see Eq. (17)], which contains no mix of interelectron coordinates. Now we can repeat all calculations made in this study by using the approximate wave function, Eq. (17). Finally, we arrive at the following expression for the ν spectrum of secondary electrons emitted during the nuclear β^- decay of a two-electron atom/ion with nuclear electric charge Q :

$$S_e(\nu; Q; q) = F(Q; q) \frac{32Q_1}{S(Q; q)\alpha Q_2} \left[1 + \exp\left(-2\pi \frac{Q_2\alpha}{\gamma\nu}\right) \right] \times \frac{(Q_1^2 + Q_2^2)^2 \gamma^4 \nu^3}{(Q_1^2 + \gamma^2 \nu^2)^4} \times \exp\left[-4\left(\frac{\alpha Q_2}{\gamma\nu}\right) \arctan\left(\frac{\alpha Q_2}{\gamma\nu}\right)\right], \quad (18)$$

where $Q_1 = Q - q$, $Q_2 = Q + 1$ and the additional factor $F(Q; q)$ is written in the form

$$F(Q; q) = \frac{\sqrt{Q^3(Q-q)^3}}{(Q-\frac{q}{2})^3}. \quad (19)$$

This factor is, in fact, the probability that the second electron will stay bound (in the ground $1s$ state of the newly formed hydrogen-like ion) during nuclear β^- decay in the two-electron He-like atom/ion. As one can see from Eq. (18) the correction for electron-electron correlations [factor q from Eq. (17)] is included in the final expression for the spectral function $S_e(\nu; Q; q)$, Eq. (18), of secondary electrons. In addition to the appearance of an extra factor $F(Q; q)$ in Eq. (18), this factor also changes the effective electric charge of the nucleus in the incident atom/ion ($Q_1 = Q - q$) and produces changes in the normalization constant $S(Q; q)$ in the expression for the spectral function (or spectrum) of secondary electrons. These observations illustrate the idea that electron-electron correlations in the maternal atom directly affect the explicit

form of the spectra of secondary electrons emitted during nuclear β^- decay. For few-electron atoms this statement can be rigorously proved with the use of the natural orbital expansions for highly accurate (or truly correlated) variational wave functions for such systems (see, e.g., [18], [19]). Note, again, that in the nonrelativistic approximation we have to assume that $\gamma = 1$ in Eq. (18) and v is expressed in atomic units, where the unit velocity equals the $\frac{e^2}{\hbar} = \alpha c$ value.

In general, it is hard to determine the final-state probabilities in few-electron atoms/ions to the same accuracy as we did above for the one-electron tritium atom. The main problem is related to accurate evaluations of electron-electron correlations in such atomic systems. Another problem in actual calculations of the overlap integrals between the incident and the final wave functions follows from the fact that the total numbers of essential (or internal) variables are different in these wave functions. For simplicity, let us consider the nuclear β^- decay of the three-electron Li atom, which originally was in its ground 1^2S state. In this case Eq. (1) takes the form

$$\text{Li} \rightarrow \text{Be}^{2+} + e^- + e^-(\beta) + \bar{\nu}. \quad (20)$$

Suppose we want to use the bound-state wave functions for the incident Li atom and Be^{2+} ion. The incident wave function of the Li atom contains six interparticle coordinates, e.g., three electron-nucleus coordinates r_{4i} ($i = 1, 2, 3$) and three electron-electron coordinates r_{12}, r_{13}, r_{23} . In the final wave function, which describes the Be^{2+} ion and a free electron, one finds three electron-nucleus coordinates r_{4i} ($i = 1, 2, 3$) and only one electron-electron coordinate r_{12} . Here we assume that the free-electron wave function, Eq. (2), depends upon the $r_{43} = r_{34}$ electron-nucleus coordinate only. Briefly, this means that the two electron-electron coordinates r_{13} and r_{23} are lost during the sudden transition from the incident to the final state in Eq. (20). In atomic systems with five, six, and more electrons there are additional problems related to the appearance of the so-called unnecessary relative coordinates in the bound-state wave functions (for more details, see, e.g., [16]). For instance, there are 10 relative coordinates (since the number of combinations from 5×2 is $C_5^2 = 10$) in an arbitrary four-electron atom/ion, but only 9 of them are truly independent in three-dimensional space. Here we cannot discuss all aspects of these interesting problems and note only that each of these two problems presents significant difficulties for accurate computations of actual atoms and ions.

Finally, we have developed an approximate method which can be used to determine the final-state probabilities for all states which arise after nuclear β^- decay and which belong to the continuous spectrum of the final ion, Eq. (20). This method is based on the natural orbital expansions of all few-electron wave functions which are included in the overlap integral between wave functions of the incident and those of the final states. For the process, Eq. (20), the wave function of the incident state describes the ground 2^2S state of the three-electron Li atom. The final-state wave function is the product of the bound-state wave function of the two-electron Be^{2+} ion and the one-electron wave function of the free electron, Eq. (2), which moves in the central field of this ion. In the method of natural orbital expansions the bound-state wave functions of

few- and many-electron atoms are represented by the sums of the products of their natural orbitals $\chi_k(r_i) = \chi_k(r_{iN})$ (the symbol N stands here for the nucleus), which are some simple single-electron functions of one radial variable, $r_{iN} = r_i$, only. In other words, we are looking for the best approximation of the actual wave function of an N_e -electron atomic system by linear combinations of N_e products of functions each of which depends upon one radial electron-nucleus coordinate r_{iN} ($i = 1, \dots, N_e$) only. The natural orbital expansion is the ‘‘best’’ of all such linear combinations in Dirac’s sense [17], since the first-order density matrix is diagonal in the natural orbitals.

In our case for the three-electron Li-atom and final two-electron Be^{2+} ion we can write the natural orbital expansions

$$\Psi_{L=0}(\{r_{ij}\})(\text{Li}) = \sum_{n=1}^{N_1} C_n \chi_n^{(1)}(r_1) \chi_n^{(2)}(r_2) \chi_n^{(3)}(r_3), \quad (21)$$

$$\Psi_{L=0}(\{r_{ij}\})(\text{Be}^{2+}) = \sum_{k=1}^{N_2} B_k \xi_k^{(1)}(r_1) \xi_k^{(2)}(r_2), \quad (22)$$

respectively. Here $\chi_n(r_i)$ and $\xi_n^{(i)}(r_i)$ are the (atomic) natural orbitals constructed for the three-electron Li atom and two-electron Be^{2+} ion (see, e.g., [18], [19]). The coefficients C_n and B_k are the coefficients of the natural orbital expansions constructed for the 2^2S state of the Li atom and for the ground 1^1S state of the Be^+ ion, respectively. In general, these coefficients are determined as the solutions (eigenvectors) of associated eigenvalue problems. Note that each of these natural orbitals depends upon the corresponding electron-nucleus coordinate r_i only (or the r_{4i} coordinate in our notation). In general, the natural orbital expansions do not include any of the electron-electron (or correlation) coordinates. Use of the natural orbital expansions for the few-electron wave functions allows one to simplify drastically all calculations of the final-state probabilities. Indeed, by using the natural orbital expansions one can show that all overlap integrals are represented as the product of three one-dimensional integrals or as finite sums of such products. Briefly, we can say that application of the natural orbital expansions for few-electron atomic wave functions allows one to reduce calculations of the overlap integrals to a very simple procedure; e.g., for the process, Eq. (20), one finds for the probability amplitude M_{if} ,

$$\begin{aligned} M_{if} = & \sum_{n=1}^{N_1} \sum_{k=1}^{N_2} C_n B_k \int_0^{+\infty} \chi_n^{(1)}(r_1) \xi_k^{(1)}(r_1) r_1^2 dr_1 \\ & \times \int_0^{+\infty} \chi_n^{(2)}(r_2) \xi_k^{(2)}(r_2) r_2^2 dr_2 \\ & \times \int_0^{+\infty} \chi_n^{(3)}(r_3) \phi_{kl}(r_3) r_3^2 dr_3, \end{aligned} \quad (23)$$

where $\phi_{kl}(r_3)$ are the functions from Eq. (2). In other words, computations of the overlap integrals are now reduced to the calculation of one-dimensional integrals and products of such integrals. The total number of integrals used in Eq. (23) equals the number of bound electrons in the parent (or incident) atom/ion. In other words, in this method we do not face any problem related either to different numbers of

independent variables in the incident and final wave functions or to the existence of unnecessary relative coordinates in many-electron atomic systems. The formula, Eq. (23), can be used to determine the overall probabilities of β^- decay with the emission of a free electron during nuclear β^- decay in three-electron atoms/ions. Analogous expressions for the probability amplitudes M_{if} and final-state probabilities $P_{if} = |M_{if}|^2$ can be derived for arbitrary few- and many-electron atoms and ions.

V. FORMATION OF FAST SECONDARY ELECTRONS

In this section we briefly discuss the emission of very fast secondary electrons from β^- -decaying few-electron atoms and ions. The velocities of such “fast” secondary electrons significantly exceed the “averaged” velocities of any “secondary” electron emitted in the process, Eq. (1). In a number of books and textbooks such fast electrons are often called δ electrons. Sudden acceleration of these electrons to high velocities is related to the transfer of a large amount of momentum from a very fast, “relativistic” β^- electron to one of the atomic electrons. Formally, this process can be written in the form

$$X \rightarrow Y^{2+} + e^-(\delta) + e^-(\beta) + \bar{\nu}, \quad (24)$$

where $e^-(\delta)$ is the fast secondary electron emitted and accelerated to relatively high velocities during nuclear β^- decay. It is clear that the probability of such a process is low. In the lowest-order approximation this probability is evaluated as $P \approx \alpha^4 P_e$, where P_e is the probability of free-electron emission in the process, Eq. (24), and $\alpha = \frac{e^2}{\hbar c} \approx \frac{1}{137}$ is the dimensionless fine-structure constant, which is a small numerical value in QED. More accurate evaluation leads to a formula that contains additional factors that increase the numerical value of P . Let us derive the formula that can be used to evaluate the probability of emission of the fast δ electrons during β^- decay in few-electron atoms and ions.

In reality, a fast secondary electron arises when a substantial amount of momentum energy is transferred from the very fast β^- electron to a slow atomic electron. Therefore, we can write the following integral relation between the spectral function of primary and that of secondary electrons [22],

$$S_\delta(\gamma_2) = \int_1^{\gamma_{\max}} F(\gamma_2, \gamma_1) S_\beta(\gamma_1) d\gamma_1, \quad (25)$$

where $S_\beta(\gamma_1)$ and $S_\delta(\gamma_2)$ are the spectral functions of primary electrons (or β^- electrons) and secondary electrons (or δ electrons), respectively. In this equation the notation $F(\gamma_2, \gamma_1)$ stands for the kernel of an integral transformation, which is a real function, if both arguments are bounded between unity and α^{-1} . The explicit form of this kernel has been found in [13]. To express this kernel let us introduce the value $\Delta = \frac{\gamma_2 - 1}{\gamma_1 - 1}$, where γ_1 and γ_2 are the γ factors of the β^- and δ electrons, respectively. By using this new variable (Δ) we can write the following formula [13] for the probability of emitting one δ

electron whose γ factor equals the γ_2 value

$$\begin{aligned} P(\gamma_2) &= \int_1^{\gamma_{\max}} \left(\frac{d\sigma}{d\Delta} \right) \left(\frac{d\Delta}{d\gamma_1} \right) S_\beta(\gamma_1) d\gamma_1 \\ &= (\gamma_2 - 1) \int_1^{\gamma_{\max}} \left(\frac{d\sigma}{d\Delta} \right) S_\beta(\gamma_1) \frac{d\gamma_1}{(\gamma_1 - 1)^2}, \end{aligned} \quad (26)$$

where $\frac{d\Delta}{d\gamma_1} = \frac{\gamma_2 - 1}{(\gamma_1 - 1)^2}$ and the formula for the differential cross section $\frac{d\sigma}{d\Delta}$ is [13]

$$\begin{aligned} \frac{d\sigma}{d\Delta} &= \zeta \frac{16N_e \pi \alpha^4 a_0^2 \gamma_1^2}{(\gamma_1^2 - 1)(\gamma_1 - 1)} \left\langle \frac{a_0^2}{r_{eN}^2} \right\rangle \frac{1}{\Delta^2(1 - \Delta)^2} \\ &\quad \times \left\{ 1 - \left[3 - \left(\frac{\gamma_1 - 1}{\gamma_1} \right)^2 \right] \Delta(1 - \Delta) \right. \\ &\quad \left. + \left(\frac{\gamma_1 - 1}{\gamma_1} \right)^2 \Delta^2(1 - \Delta)^2 \right\}, \end{aligned} \quad (27)$$

where N_e is the total number of bound electrons in the parent β^- -decaying atom/ion, $\left\langle \frac{a_0^2}{r_{eN}^2} \right\rangle = \left\langle \frac{1}{r_{eN}^2} \right\rangle$ (in a.u.) is the atomic expectation value of $\frac{a_0^2}{r_{eN}^2} = \frac{1}{r_{eN}^2}$ computed for all bound (atomic) electrons, ζ is some numerical constant, and α and a_0 are the fine-structure constant and Bohr radius, respectively. Note that the formula, Eq. (27), can be considered an integral transformation of the β electron spectrum (or the spectrum of primary fast electrons). The explicit formula for the spectrum of secondary δ electrons directly follows from Eqs. (26) and (27), which must be integrated over γ_1 from 1 to $\gamma_{\max} = \frac{\Delta E}{m_e c^2}$, where ΔE is the total energy released in the nuclear β^- decay. This problem can be solved by integrating term by term in Eq. (26), where $\frac{d\sigma}{d\Delta}$ must be taken from Eq. (27).

The final step of our procedure is to find an accurate expression for the spectrum of primary β^- electrons which must be used in Eq. (25). This problem has been considered in a large number of papers [23–30]. Experimental energy spectra of the emitted primary β^- electrons can be found, e.g., in [28] and [29], where the β^- decays of ^{64}Cu and ^{210}Bi atoms were studied in detail. As follows from these studies the spectral function of primary β^- electrons can be written in the form

$$\begin{aligned} S_\beta(\gamma) d\gamma &= C_\gamma \cdot F(Q + 1, (\gamma - 1)m_e c^2) \\ &\quad \times \left[\frac{\Delta E' + m_e c^2}{m_e c^2} - \gamma - 1 \right]^2 (\gamma^2 - 1)^{\frac{1}{2}} \gamma d\gamma \\ &= C'_\gamma \cdot F(Q + 1, \gamma - 1) \left[\frac{\Delta E'}{m_e c^2} - \gamma \right]^2 (\gamma^2 - 1)^{\frac{1}{2}} \gamma d\gamma, \end{aligned} \quad (28)$$

where $\Delta E' = \Delta E - m_e c^2$. This expression almost exactly coincides with the formula, Eq. (210), derived in [30], i.e.,

$$S_\beta(\gamma) d\gamma = C'_\gamma \left[\frac{\Delta E'}{m_e c^2} - \gamma \right]^2 (\gamma^2 - 1)^{\frac{1}{2}} \gamma d\gamma. \quad (29)$$

The spectrum, Eq. (29), contains no Fermi function as introduced by Fermi in [23]. In general, the assumption that $F(Q + 1, \gamma - 1) = 1$ works well for light atoms, but for intermediate ($Q \geq 40$) and heavy ($Q \geq 75$) atoms the Fermi

TABLE V. Numerical values of the inverse normalization constants, i.e., the $N_\gamma^{-1} = (C'_\gamma)^{-1}$ value in the spectral function for primary β^- electrons, Eq. (29), as a function of the thermal effect $\Delta E'$ (in MeV) of nuclear β^- decay in light atoms.

$\Delta E'$	N_γ^{-1}	$\Delta E'$	N_γ^{-1}	$\Delta E'$	N_γ^{-1}
0.6	$0.510138920728380682 \times 10^{-3}$	2.6	$0.943534198627184360 \times 10^2$	4.6	$0.185482676760179721 \times 10^4$
0.7	$0.768274953852744202 \times 10^{-2}$	2.7	$0.115479629241228239 \times 10^3$	4.7	$0.207060009101156116 \times 10^4$
0.8	$0.365273098535936243 \times 10^{-1}$	2.8	$0.140174066944844508 \times 10^3$	4.8	$0.230589234934879363 \times 10^4$
0.9	0.110787349453086509	2.9	$0.168863421848105529 \times 10^3$	4.9	$0.256199131172405105 \times 10^4$
1.0	0.263733079531422292	3.0	$0.202006532798188682 \times 10^3$	5.0	$0.284023985445725021 \times 10^4$
1.2	0.992531073989599566	3.2	$0.283657013608144685 \times 10^3$	5.2	$0.346883961029256005 \times 10^4$
1.4	$0.271944662442253340 \times 10^1$	3.4	$0.389482828970674785 \times 10^3$	5.4	$0.420358039547922170 \times 10^4$
1.5	$0.417197363819929210 \times 10^1$	3.5	$0.452982885446960540 \times 10^3$	5.5	$0.461472909694107252 \times 10^4$
1.6	$0.616262631954181568 \times 10^1$	3.6	$0.524429148588098765 \times 10^3$	5.6	$0.505730617602198678 \times 10^4$
1.7	$0.882174671793232731 \times 10^1$	3.7	$0.604537642065602785 \times 10^3$	5.7	$0.553307240355429714 \times 10^4$
1.8	$0.122980724837757482 \times 10^2$	3.8	$0.694065721429933329 \times 10^3$	5.8	$0.604385284163182761 \times 10^4$
1.9	$0.167598801452295380 \times 10^2$	3.9	$0.793813221987212581 \times 10^3$	5.9	$0.659153799162885377 \times 10^4$
2.0	$0.223961294672658384 \times 10^2$	4.0	$0.904623606693807949 \times 10^3$	6.0	$0.717808494222105881 \times 10^4$
2.2	$0.380580798087427918 \times 10^2$	4.2	$0.116303190610637340 \times 10^4$	6.2	$0.847593242453915958 \times 10^4$
2.4	$0.612527955319830414 \times 10^2$	4.4	$0.147695449723875506 \times 10^4$	6.4	$0.995442736892640637 \times 10^4$
2.5	$0.763997524066278397 \times 10^2$	4.5	$0.165733856922900762 \times 10^4$	6.5	$0.107670505698641369 \times 10^5$

function in Eq. (28) is really needed. As follows from Eq. (29) the normalization constant C'_γ is a function of the thermal energy released during nuclear β^- decay, i.e., of the $\frac{\Delta E'}{m_e c^2}$ ratio, where $m_e = 0.511\,099\,891\,0\text{ MeV}/c^2$. Inverse values of the normalization factors $(C'_\gamma)^{-1}$ determined numerically for different $\Delta E'$ values listed in Table V. By using the formulas, Eqs. (26) and (27) and Eq. (28), one can obtain a closed analytical formula for the probabilities of emission and the energy/velocity spectrum of fast secondary electrons (or δ electrons) emitted during nuclear β^- decay in arbitrary few- and many-electron atoms/ions.

VI. CONCLUSIONS

We have considered nuclear β^- decays in few-electron atoms and ions that lead to an additional ionization of the final ion in which one of the atomic electrons becomes unbound. The procedure is developed for determining the corresponding transition probabilities and the velocity/energy spectrum of secondary electrons. Formation of fast secondary electrons (δ

electrons) during nuclear β^- decay in few-electron atoms/ions is also briefly discussed.

It should be mentioned that the important role of bound-free transitions during nuclear β^- decay in few-electron atoms has been emphasized since earlier works by Migdal (see, e.g., [8], [9], and references therein). In this study we have chosen the proper wave functions to describe the unbound (or “free”) electron that is emitted during nuclear β^- decay. This allows us to solve a number of long-standing problems, e.g., to derive the explicit formulas for the velocity/energy spectra of secondary electrons emitted during nuclear β^- decay. Furthermore, now it is absolutely clear that the spectra of emitted secondary electrons have different forms for different few-electron atoms/ions, since these spectra strongly depend upon the electron-electron correlations in the bound state of the parent atom/ion. From there one finds the “similarity law” between the velocity spectra of secondary electrons emitted during nuclear β^- decay of two different atoms/ions that have the same (or similar) electron configurations. We also describe an approach that can be useful for derivation of the velocity/energy spectrum of very fast secondary electrons (δ electrons) which are observed during nuclear β^- decays in few- and many-electron atoms/ions.

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