Ionization of light atoms and ions during the nuclear $\beta^-$-decay

Alexei M. Frolov

Department of Applied Mathematics

University of Western Ontario, London, Ontario N6H 5B7, Canada

(Dated: August 5, 2014)

Abstract

Ionization of light atoms and ions during the nuclear $\beta^-$-decay is considered. To determine the final state probabilities of electron ionization we have developed a procedure based on the natural orbital expansions for the bound state wave functions of all atoms/ions involved in this process.

*E–mail address: afrolov@uwo.ca
I. INTRODUCTION

In our earlier studies (see, e.g., [1], [2], [3] and references therein) we considered atomic excitations during the nuclear $\beta^-$-decay in light, few-electron atoms and ions. In general, this process is written in the form

$$ X \rightarrow Y^+ + e^-(\beta) + \bar{\nu} $$

where the symbols $X$ and $Y$ designate two different chemical elements (isotopes) with equal (or almost equal) masses. Below, these symbols $X$ and $Y$ are used to designate the both atoms/ions and the corresponding atomic nuclei. If $Q$ is the electric charge of the incident nucleus $X$, then the nuclear charge of the final nucleus $Y$ is $Q + 1$. In Eq. (1) and everywhere below the notation $e^-(\beta)$ stands for the fast electron (or $\beta^-$-electron) emitted from the nucleus during the nuclear $\beta^-$-decay, while $\bar{\nu}$ designates the electron’s anti-neutrino. In [1] - [3] we discussed the bound-bound transitions between the incident and final states in few-electron atoms and/or ions. In [1] - [3] we assumed that the incident atom was in one of its bound state and the final ion is also formed in one of its bound states. In the case of the decay, Eq. (1), the incident atom and final ion contain the same numbers of bound electrons and this fact can be used to simplify numerical computations of the final state probabilities. In particular, in [3] we have found that $\beta^-$-decays of the $^8$Li and $^9$Li atoms in $\approx 85\%$ of all cases lead to the formation of the three-electron Be$^+$ ion

$$ Li \rightarrow Be^+ + e^-(\beta) + \bar{\nu} $$

in a variety of bound states. The final state probabilities, i.e. probabilities to form different bound states in the Be$^+$ ion during the nuclear $\beta^-$-decay of the three-electron $^8$Li and $^9$Li atoms have been accurately evaluated in [3].

Here we consider other atomic processes during the nuclear $\beta^-$-decay in atoms and ions. The most important of such processes is the ‘additional’ ionization of the final ion [4], [5]. The general equation for this process takes the form:

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

where the notation $e^-$ stands for the slow (atomic) electron formed in the unbound spectrum during the reaction, Eq. (4), while the notation $e^-(\beta)$ designates the fast $\beta^-$ electron. Note
that now the final Y$^{2+}$ ion has larger electric charge (+2), than the Y$^+$ ion formed in the reaction, Eq.(1). In the case of $\beta^-$-decay of the $^8$Li and $^9$Li atoms such an ‘additional’ ionization of the three-electron Be$^+$ ion has $\approx 15\%$ probability. The process is written in the form

$$\text{Li} \rightarrow \text{Be}^{2+} + e^- + e^-(\beta) + \nu \quad (4)$$

In some earlier works on $\beta^-$-decay in many-electron atoms the emitted atomic electrons were called and considered as the ‘secondary’ electrons, or $\delta-$electrons. Analogous processes of ‘additional’ electron ionization proceed in any $\beta^\pm-$decaying atom/ion. The corresponding probabilities of an ‘additional’ ionization of the Be$^+$ ion can be measured and used for complete description of atomic excitations during the nuclear $\beta^\pm$-decay in few-electron atoms and molecules. Further analysis shows that the secondary electron from the process, Eq.(4), can be detected in different spin states. In an ideal case we can observe such an electron either in the $\alpha-$spin state, or in the $\beta-$spin state where the notations $\alpha$ and $\beta$ are used to designate spin-up and spin-down wave functions, respectively (see, e.g., [6]). Since the total electron spin of the incident atom is conserved during the nuclear $\beta^\pm-$decay in few-electron atom (see below), we can conclude that the final Be$^{2+}$ ion arising after the reaction, Eq.(4), can be found in one of its singlet $S_e = 0$, or triplet $S_e = 1$ states. Here the notation $S_e$ stands for the total electron spin. In general, the final ion arising during the nuclear $\beta^\pm-$decay of the neutral atom is always formed in one of the two possible spin states and the difference of the spin values for such states equals unity, i.e. $\Delta S_e = 1$.

In reality, the last statement often means double ionization of the final ion arising during the nuclear $\beta^\pm$-decay. Indeed, consider, for instance, the $\beta^-$-decay of some neutral atom which has four electrons on its outer-most electron shells. Ionization during this nuclear $\beta^-$-decay leads to the formation of an ion with three electrons on its outer-most shells. The electron configuration of such an ion corresponds to either doublet spin-state (e.g., $^2S-$state), or quartet spin-state (e.g., $^4S-$state). But it is well known that all quartet spin states in ions with three bound electrons on the outer-most shells are unstable. In general, such states decay with the emission of one (additional) electron and formation of another ion with the two electrons on its outer-most shells. This simple example illustrates a general experimental situation: some final states in ions arising after the nuclear $\beta^-$-decay with additional electron ionization, Eq.(3), are unstable and they can only be stabilized by emitting one additional electron. In other words, the ionization during the nuclear $\beta^\pm$-decay
can lead, in principle, to very substantial electronic reconfiguration in the final ion. In contrast with this the process, Eq. (2), usually produces a very few minimal changes in the electronic structure of the arising ion in comparison to the incident atom.

Our main goal in this study is the analysis of electron ionization during the nuclear $\beta^-$-decay of light atoms and ions. The first problem is analytical and/or numerical calculations of the overlap integrals which are included in expressions for the probability amplitudes $M_{if}$ (see below). Formulas for these overlap integrals are discussed in the next Section. In Section III we discuss construction of accurate wave functions for few-electron atoms/ions and wave function of the free electron moving in the Coulomb field. Actual calculations of these integrals are considered in Section IV. In that Section we mention the two crucial trouble spots in such calculations. To avoid numerical problems related with these trouble spots we developed an original approach which can be used in calculations of the probability amplitudes $M_{if}$. This approach is based on the use of natural orbital expansions for the incident and final wave functions of atomic systems which take part in the $\beta^-$ decay. In Appendix, we discuss the problems related with a restricted accuracy of the sudden approximation which was applied earlier in many papers on the $\beta^\pm$-decay in atoms and molecules.

II. FINAL STATE PROBABILITIES

As is well known the velocities of $\beta^-$-electrons ($v_\beta$) emitted during the nuclear $\beta^-$-decay are significantly larger than usual velocities of atomic electrons $v_a$. In particular, in light atoms we have $v_\beta \geq 1000 v_a$. This also true for the velocities of the secondary $\delta$-electrons $e^-$ which can be emitted as 'free' particles during the reaction, Eq. (4), i.e. $v_\beta \gg v_\delta$. The inequality $v_\beta \gg v_a$ allows one to analyze the nuclear $\beta^-$-decay in light atoms by calculating the overlaps of the non-relativistic atomic wave functions. Indeed, by using the sudden approximation we can write the following expression for the final state probability of the process, Eq. (2):

$$P_{if} = |M_{if}|^2 = \int \Psi_{Li}(x_1, x_2, x_3) \Psi_{Be^+}(x_1, x_2, x_3) d^3r_1 d^3r_2 d^3r_3 ds_1 ds_2 ds_3$$

where the notation $M_{if}$ designates the probability amplitude. Here and below the four-dimensional variable $x_i$ for $i$-th electron designates combination of the three radial variables of this electron ($r_i$) and three spin variables $s_i$, i.e. $x_i = (r_i, s_i)$ for $i = 1, 2, 3$. The
notations $\Psi_{\text{Li}}(x_1, x_2, x_3)$ and $\Psi_{\text{Be}^+}(x_1, x_2, x_3)$ stand for the wave functions of the incident Li-atom and Be$^+$ ion (both these systems contain three bound electrons). The equation, Eq. (5), means that the probability amplitude $M_{if}$ equals to the overlap of the two bound state wave functions which correspond to the two different atomic systems (Li atom and Be$^+$ ion). The total number of electrons in the incident and final wave functions is exactly the same. Therefore, all calculations of the overlap integral(s), Eq. (5), are relatively simple. It does not contain any unclear moment which must be discussed in detail.

Analogously, we can write the following expression for the final state probability of the process, Eq. (4):

$$P_{if} = |M_{if}|^2 = \int \Psi_{\text{Li}}(x_1, x_2, x_3)\Psi_{\text{Be}^2+}(x_1, x_2)\psi_e(x_3)d^3r_1d^3r_2d^3r_3ds_1ds_2ds_3$$

where the notations $\Psi_{\text{Li}}(x_1, x_2, x_3)$ and $\Psi_{\text{Be}^2+}(x_1, x_2)$ designate the wave functions of the incident Li-atom and final Be$^{2+}$-ion, which contains only two bound electrons. The notation $\psi_e(x_3)$ in Eq. (6) stands for the wave function of a free electron which moves in the central, Coulomb field of the Be$^{2+}$ ion. All these wave functions can be considered as non-relativistic.

Also, without loss of generality we shall assume that all bound state wave functions arising in our equations for the amplitudes and probabilities have unit norm. Analytical and/or numerical calculation of the overlap integral, Eq. (6), is significantly more difficult problem than in the case of Eq. (5). It will be discussed in the next Section.

As mentioned above the velocity of the emitted $\beta^\pm$-electron ($v_\beta$) significantly exceeds the usual electron velocities in the both incident and final atoms. It follows from here that some conservation laws must be obeyed for any atomic transition during the nuclear $\beta^\pm$-decay of the few- and many-electron atom. In particular, the angular momentum $L$, spin $S$ and spatial parity $\pi$ of the wave function of the incident atom are always conserved during such a sudden process. For the angular momentum $L$ of the final Be$^{2+}$ ion this selection rule allows one to predict some quantum numbers of the final Be$^{2+}$ ion. For instance, if the incident Li atom was in one of its $L = 0$ states, then the angular momenta of the final Be$^{2+}$ ion and free electron must be equal to each other. In other words, if the final Be$^{2+}$ ion was formed in the bound $L$-state, then the final (or ‘free’) electron is also moving out in the $\ell$–wave, where $\ell = L$. In general, if the incident atom was in the $L_i$-state and final atom is found in one of its $L_f$-states, then the final electron is emitted in the $\ell_f$-wave, where $\ell_f$ equals one of the following numbers $|L_f - L_i|, \ldots, L_f + L_i$. From here one can derive a number of useful
selection rules which drastically simplify all numerical and analytical computations of the transitions probabilities in Eqs. (5) - (6). The total number of non-zero few-body integrals which must be evaluated numerically and/or analytically is reduced to a relatively small values.

III. WAVE FUNCTIONS

To determine the final state probability $P_{ij}$, Eq. (6), one needs to use the explicit expressions for the wave functions of the incident Li atom and final Be$^{2+}$ ion and electron which moves in the Coulomb field of the heavy Be$^{2+}$ ion. For the ground $2^2S(L = 0)$-state of the Li atom such a wave function $\Psi$ is written in the following general form (see, e.g., [7], [8])

$$\Psi(\{r_{ij}\})_{L=0} = \psi_{L=0}(A; \{r_{ij}\})(\alpha \beta \alpha - \beta \alpha \alpha) + \phi_{L=0}(B; \{r_{ij}\})(2 \alpha \alpha \beta - \beta \alpha \alpha - \alpha \beta \alpha)$$ (7)

where $\psi_{L=0}(A; \{r_{ij}\})$ and $\phi_{L=0}(B; \{r_{ij}\})$ are the two independent radial parts (= spatial parts) of the total wave function. The notations $\alpha$ and $\beta$ in Eq. (7) are the one-electron spin-up and spin-down functions, respectively (see, e.g., [9]). The notations $A$ and $B$ in Eq. (7) mean that the two sets of non-linear parameters associated with the radial functions $\psi$ and $\phi$ can be optimized independently. Note that each of the radial basis functions in Eq. (7) explicitly depends upon all six interparticle (or relative) coordinates $r_{12}, r_{13}, r_{23}, r_{14}, r_{24}, r_{34}$, where the indexes 1, 2, 3 stand for the three electrons, while index 4 means the nucleus. In modern accurate computations of bound states the radial parts of the total wave functions, e.g., $\psi_{L=0}(A; \{r_{ij}\})$ and $\phi_{L=0}(B; \{r_{ij}\})$ in Eq. (7) are usually represented by their Hylleraas series, e.g., for the $\psi_{L=0}$-functions

$$\psi_{L=0}(A; \{r_{ij}\}) = \sum_{k=1}^{N} C_k r_{23}^{n_1(k)} r_{13}^{n_2(k)} r_{12}^{n_3(k)} r_{14}^{m_1(k)} r_{24}^{m_2(k)} r_{34}^{m_3(k)} \exp(-\alpha r_{14} - \beta r_{24} - \gamma r_{34})$$ (8)

where the ‘parameters’ $\alpha, \beta$ and $\gamma$ are varied in computations, but they are the same for all basis functions in the $\psi$-expansion, Eq. (8). Three other such parameters can be found in the second term of Eq. (8), or $\phi$-expansion. The presence of six non-linear parameters in Eq. (8) increases the overall flexibility of the method. However, it is not sufficient to provide very high accuracy for three-electron atoms and ions. Briefly, this means that any accurate trial functions $\Psi(\{r_{ij}\})_{L=0}$, Eq. (7), must contain a very large number(s) $N$ of basis functions.

In order to construct a very efficient variational expansion of the wave function of the three-electron atoms and ion in our earlier work [7] we have introduced an advanced set
of radial basis functions for three-electron bound state calculations. In [7] such a basis set was called the semi-exponential, variational basis set. In general, the semi-exponential variational expansion of the radial function $\psi_{L=0}(A;\{r_{ij}\})$ is written in the form

$$
\psi_{L=0}(A;\{r_{ij}\}) = \sum_{k=1}^{N} C_k r_{23}^{n_1(k)} r_{13}^{n_2(k)} r_{12}^{m_1(k)} r_{24}^{m_2(k)} r_{34}^{m_3(k)} \exp(-\alpha_k r_{14} - \beta_k r_{24} - \gamma_k r_{34})
$$

(9)

where $\alpha_k, \beta_k, \gamma_k (k = 1, 2, \ldots, N)$ are the varied non-linear parameters. The presence of a large number of varied non-linear parameters in Eq.(9) is the main and very important difference between the traditional Hylleraas variational expansion, Eq.(8), and our variational expansion, Eq.(9).

The two-electron Be$^{2+}$ ion is the bound atomic system with the two bound electrons which are designated below as particles 1 and 2. The wave functions of such systems can accurately be approximated with the use of the exponential variational expansion in relative coordinates $r_{32}, r_{31}$ and $r_{21}$ (see, e.g., [10] and references therein). For the bound singlet $1S(L = 0)$–states in the two-electron Be$^{2+}$ ion the exponential variational expansion takes the form

$$
\Psi = \frac{1}{\sqrt{2}} \left( 1 + \hat{P}_{12} \right) \sum_{i=1}^{N} C_i \exp(-\alpha_i r_{24} - \beta_i r_{14} - \gamma_i r_{12}) (\alpha \beta - \beta \alpha)
$$

(10)

which is called the exponential variational expansion in the relative coordinates $r_{24}, r_{14}$ and $r_{21}$. The coefficients $C_i$ are the linear (or variational) parameters of the variational expansion, Eq.(10), while the parameters $\alpha_i, \beta_i$ and $\gamma_i$ are the non-linear (or varied) parameters of this expansion. In general, the total energy of the ground $1S$–state of the Be$^{2+}$ ion uniformly depends upon the total number of basis functions $N$, Eq.(10), used in calculations. The operator $\hat{P}_{12}$ is the permutation of the two identical particles (electrons). Note also that all relative coordinates $r_{ij}$, i.e. $r_{14}, r_{24}, r_{31}, r_{12}, r_{34}$ and $r_{23}$ for the three-electron atoms/ions and $r_{14}, r_{24}$ and $r_{12}$ for the two-electron atoms/ions, are translationally and rotationally invariant.

The last factor $\phi_e(r) = \phi_e(r_{34})$ in the overlap integral, Eq.(6), represents to the unbound (final) electron, which moves in the Coulomb field of the heavy Be$^{2+}$ ion. The wave function is written in the form $\phi_e(r) = \phi_{kl}(r) Y_{lm}(\mathbf{n})$, where $\phi_{kl}(r)$ is the one-electron radial function, while $Y_{lm}(\mathbf{n})$ is the corresponding spherical harmonics and $\mathbf{n} = \hat{r}$ is the unit vector associated with the vector $\mathbf{r}$. The parameter $k$ is the wave number which is uniformly related to the energy of the ‘free’ electron $k = \sqrt{\frac{2m_e E}{\hbar^2}} = \sqrt{2E}$ (in atomic units $\hbar = 1, m_e = 1, e = 1$). The
explicit formula for the radial function \( \phi_{kl}(r) = \phi_{kl}(r_{34}) \) (in atomic units) is (see, e.g., [6])

\[
\phi_{kl}(r) = \frac{C_{kl}}{(2l + 1)!} (2Qkr)^l \cdot \exp(-iQkr) \cdot \mathbf{1}_F \left[ \frac{l}{Qk} + l + 1, 2l + 2, 2iQkr \right]
\]  

(11)

where \( i \) is the imaginary unit, \( \mathbf{1}_F(a, b; x) \) is the confluent hypergeometric function (see, e.g., [11]) and \( C_{kl} \) is the following factor

\[
C_{kl} = C_{k0} \cdot \prod_{s=1}^{l} \sqrt{s^2 + \frac{1}{Q^2k^2}} = \sqrt{\frac{8\pi Qk}{1 - \exp\left(-\frac{2\pi i}{Qk}\right)}} \cdot \left\{ \prod_{s=1}^{l} \sqrt{s^2 + \frac{1}{Q^2k^2}} \right\}
\]  

(12)

In old papers the \( C_{kl} \) factor was called the Coulomb penetration factor. In these two equations the parameter \( Q \) is the electric charge of the remaining double-charged (positive) Be\(^{2+}\) ion. In our case this central atomic cluster is the Be\(^{2+}\) ion, which contains the two bound electrons, i.e. in all formulas above \( Q = 2 \) (in atomic units). In reality, this parameter can slightly be varied (around 2) to obtain better agreement with the experimental data. Such variations formally represent ionizations from different electronic shells of the incident Li atom. For \( l = 0 \) the second product in the right hand side of Eq.(12) is reduced to the unity.

With the use of Eq.(7.522.9) from [11] one finds the following expression for the overlap integral between the auxiliary orbitals \( r^n e^{-\gamma_n r} \) and the radial function \( \phi_{kl}(r) \) defined by Eq.(11):

\[
I = \frac{C_{kl}(2k)^l}{(2l + 1)!} \cdot \frac{\Gamma(n + l + 3)}{(\gamma_n - ik)^{n+l+3}} \cdot \mathbf{1}_F \left[ \frac{l}{k} + l + 1, n + l + 3; 2l + 2; -\frac{2ik}{\gamma_n - ik} \right]
\]  

(13)

The hypergeometric function in this equation can be transformed to its final form with the use of the formula, Eq.(9.131), from [11]

\[
2F_1(a, b; c; z) = (1 - z)^a \cdot 2F_1(a, b - c; c; \frac{z}{z - 1})
\]  

(14)

Finally, the formula, Eq.(13), takes the form

\[
I = \frac{C_{kl}(2k)^l}{(2l + 1)!} \cdot \frac{(n + l + 2)!}{(\gamma_n - ik)^{n+l+3}} \cdot \left( \frac{\gamma_n - ik}{\gamma_n + ik} \right)^{(\frac{l}{k} + 1)} \cdot \mathbf{1}_F \left[ \frac{l}{k} + l + 1, l - n - 1; 2l + 2; \frac{2ik}{\gamma_n + ik} \right]
\]  

(15)

As follows from Eq.(15) the expression for \( I \) is reduced to a finite sum (polynomial function), if (and only if) \( l = 0 \). In this case the computation of the corresponding hypergeometric function is simple and easy. For \( l \geq 1 \) to evaluate the hypergeometric functions at arbitrary, in principle, values of complex argument one needs to use significantly more sophisticated algorithms.
IV. CALCULATION OF THE OVELAP INTEGRALS

In this Section we discuss actual calculations of the overlap integral, Eq.(6). In particular, we analyze the two main troubles which arise during calculations of the overlap integral, Eq.(6). First of these trouble spots is directly related to the fact that the total numbers of essential (or internal) variables are different in the incident and final wave functions. Indeed, in the incident wave function of the Li-atom one finds six inter-particle coordinates, e.g., three electron-nucleus coordinates \( r_{4i} \) (\( i = 1, \ldots, 3 \)) and three electron-electron coordinates \( (r_{12}, r_{13}, r_{23}) \). In the final wave function we have three electron-nucleus coordinates \( r_{4i} \) (\( i = 1, \ldots, 3 \)) and only one electron-electron coordinate \( r_{12} \). This means that two electron-electron coordinates \( r_{13}, r_{23} \) are lost during the sudden transition from the incident to the final state in Eq.(4). It complicates the actual computations of the overlap integral, Eq.(6).

Here we cannot discuss all aspects of this interesting problem. Note only that there is an effective method which allows one to avoid problems related with different numbers of the essential variables in the incident and final wave functions. This method is based on the natural orbital expansions of all few-electron wave functions which can be found in the overlap integral, Eq.(6). Theory of natural orbital expansions has developed since the middle of 1950’s by Löwdin (see discussion and references in [12]). Below, we restrict ourselves to a very brief description of the natural orbital expansion.

In this method the radial wave functions are represented in the form of products of the natural orbitals \( \chi_k(r_i) = \chi_k(r_{iN}) \) (the symbol \( N \) stands here for the nucleus) which are some simple single-electron radial functions. In other words, we are looking for the best approximation of the actual wave functions by systems of functions which depend upon the electron-nucleus coordinates only. In our case for the three-electron Li-atom and two-electron Be\(^{2+} \) ion we can write

\[
\Psi_{L=0}(\{r_{ij}\})(\text{Li}) = \sum_{n=1}^{N_1} C_n \chi_n^{(1)}(r_1)\chi_n^{(2)}(r_2)\chi_n^{(3)}(r_3) \\
\psi_{L=0}(\{r_{ij}\})(\text{Be}^{2+}) = \sum_{k=1}^{N_2} B_k \xi_k^{(1)}(r_1)\xi_k^{(2)}(r_2)
\]

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., [13], [14]). The coefficients \( C_n \) and \( B_k \) are the coefficients of the natural orbital expansions for the Li atom and Be\(^{2+} \) ion, respectively. In general, these coefficients are determined as the solutions (eigenvectors)
of some eigenvalue problems. Note that each of these natural orbitals depends only upon the corresponding electron-nucleus coordinate \( r_i \) (or \( r_{a_i} \) in our notations). They do not include any of the electron-electron (or correlation) coordinates. By using the natural orbital expansions for the few-electron wave functions the explicit formula for the overlap integral simplifies drastically (it is represented as the product of three one-dimensional integrals). In general, application of the natural orbital expansions for few-electron atomic wave function allows one to reduce calculations of the overlap integrals to a very simple procedure, e.g., for the process, Eq. (4), one finds

\[
M_{if} = \sum_{n=1}^{N_1} \sum_{k=1}^{N_2} C_n B_k \int_0^{+\infty} \chi_n^{(1)}(r_1) \xi_k^{(1)}(r_1) r_1^2 dr_1 \int_0^{+\infty} \chi_n^{(2)}(r_2) \xi_k^{(2)}(r_2) r_2^2 dr_2 \times \\
\int_0^{+\infty} \chi_n^{(3)}(r_3) \phi_{kl}(r_3) r_3^2 dr_3
\]

where \( \phi_{kl}(r_3) \) are the functions from Eq. (11). In other words, computations of the overlap integrals are reduced to calculations of one-dimensional integer and products of such integrals. It is the main advantage of all methods based on the use of natural orbitals.

The second trouble spot follows from the fact that the explicit form of the wave functions of the bound and continuous spectra in few-electron atomic systems are substantially different. In many cases such differences lead to the appearence of integrals (see, e.g., Eq. (15)) which can be evaluated only numerically and with a number of difficulties. Furthermore, for some values of internal parameters the formulas used for such integrals become numerically unstable. This problem can be avoided with the use of different systems of basis functions to represent the actual wave functions of continuous spectrum of one-electron Coulomb problem. For instance, one can represent the radial wave function from Eq. (11) as a series of other radial functions which have a relatively simple form and set of overlap integrals between these radial functions and auxiliary orbitals \( r^n e^{\gamma_n r} \) mentioned above is written in a simple analytical form. Briefly, this means that it is better to apply different complete sets of basis radial functions to represent the actual motion of an unbound electron. In particular, we can use the following set of radial functions \( \phi_{kl}(r) = \frac{\sin kr}{r} = kj_0(kr) \), or \( \phi_{kl}(r) = \frac{\sin kr}{kr} = j_0(kr) \), where \( k = k_0, 2k_0, 3k_0, \ldots \) The ‘proper’ radial functions defined in the previous Section, Eq. (11), are represented as linear combinations (or Fourier integrals) of these ‘new’ basis radial functions and vise versa (see, e.g., [5]).
V. CONCLUSION

We have considered a number of problems which play a crucial role in calculations of the probabilities of atomic excitations during the nuclear $\beta^\pm$-decay. In contrast with our earlier studies here we discuss a possibility to observe ‘additional’ electron ionization during the nuclear $\beta^-$-decay in few-electron atoms. We investigate a few different approaches which can be applied to calculate the overlap integrals in those cases when one of the final electron is ‘free’. These overlap integrals are needed to determine the final state probabilities. It is shown that one of the best approaches to calculate such integrals is based on the use of natural orbital expansions for the bound state wave functions of the incident and final atomic systems.

Appendix

In this Appendix we discuss a few questions related to the accuracy of conservation laws for the nuclear $\beta^\pm$-decay in atomic systems. It is clear that the conservation laws for the nuclear $\beta^\pm$-decay in atomic systems mentioned in the main text are not exact, since they are based on the fact that the velocity of $\beta^-$ electron $v_\beta$ is significantly faster (in 300 - 10,000 times faster) than the average velocities of atomic electrons $v_a$. In the lowest order approximation upon the ratio $\tau = \frac{v_a}{v_\beta}$, i.e., when $\tau = \frac{v_a}{v_\beta} = 0$, these conservation laws obey rigorously. However, in the next order approximation upon $\tau$, i.e. when the ratio $\tau$ is small, but $\tau \neq 0$, these laws can only be considered as approximate. Experimental observation of possible deviations from the exact conservation laws are of great interest in some cases. In reality, one finds deviations which are related with the direct (Coulomb repulsion) and spin-spin interaction between one atomic electron and fast $\beta^\pm$-particle. Another group of deviations simply simply follows from the fact that atomic electrons and fast $\beta^-$-particle are the identical fermions. Therefore, there is a special ‘exchange’ interaction between these particles. For simplicity, below we shall consider only the $\beta^-$ nuclear decay in a few-electron atom and electron-electron interactions between atomic electrons and fast $\beta^-$-electron.

General theory of post-sudden approximation for the nuclear $\beta^-$-decays in atoms and molecules is very complex. Nevertheless, such a theory has been developed and applied to describe results of different experiments. To investigate these phenomena we wrote a detailed proposal which, however, were not welcomed by groups working in close areas. Very likely,
it is better to propose a number of simple experiments which must illustrate the importance of analysis of post-sudden approximation for the $\beta^\pm$-decay in atoms and molecules. Below we discuss three possible experiments which must detect and illustrate deviations from the sudden approximation. The first experiment is really simple and it is based on collecting a very large number of experimental results for the ‘regular’ atomic $\beta^-$-decay, Eq. (1). The main goal here is to find any possible deviation from the results predicted with the use of ‘rigorous’ conservation laws which follow from the sudden approximation. For instance, consider the $\beta^-$-decay of the $^3\text{H}^-$ ion into the $^3\text{He}$ atom [10]. Since the $^3\text{H}^-$ ion has only one bound state (the ground $1^1S^-$ state), then the final $^3\text{He}$ atom can be formed only in one of the $n^1S^-$ states of the $^3\text{He}$ atom. Suppose, however, that we have detected the final $^3\text{He}$ atom in one of its triplet states, e.g., in the $2^3S^-$ state. The formation of the triplet states in this case means an obvious deviation from the ‘rigorous’ conservation laws which follow from the sudden approximation. Our current expectation to detect these ‘non-conditional’ atomic states in experiments is unity for $\approx 10,000 - 17,000$ regular events.

Another possible experiment is even simpler. The goal is to detect fast and very fast $\delta^-$-electron (or secondary electrons) which are formed during the nuclear $\beta^-$-decay in few-electron atoms. The kinetic energy of such electrons must be significantly larger than average energies of atomic electrons. In general, these fast electrons can be formed in the result of direct transfer of momentum from the $\beta^-$-electron to the atomic electrons. The probability of ‘similar’ direct electron excitations is very small for one atomic electron ($\approx 1 \cdot 10^{-7}$), but for atoms with $N_e$ electrons such a probability is $N_e$ times larger. In any case, possible observation of the fast $\delta^-$-electron(s) will be a very interesting experimental event. The last experiment is a reliable observation of the post-decay radiation emitted during the nuclear $\beta^\pm$-decay in few- and many-electron atoms. First, note that the emitted (fast) $\beta^-$ electron undergoes an additional acceleration (or deceleration) when it leaves the atomic nucleus (see, discussion of this phenomenon in the Appendix A in [15]). However, in actual atoms and molecules one finds a small additional acceleration related with $\beta^-$-electron interactions. However, any electron acceleration means the emission of radiation which can be registered in actual experiments. For few-electron light atoms the emitted radiation which is related to the $\beta^-$-electron interaction in post-decay ions can be registered at the radio and infrared
wavelengths.

[1] A.M. Frolov and J.D. Talman, Phys. Rev. A 72, 022511 (2005).
[2] A.M. Frolov and M.B. Ruiz, Phys. Rev. A 82, 042511 (2010).
[3] M.B. Ruiz and A.M. Frolov, Adv. Quant. Chem. 67, 267 (2013).
[4] A.B. Migdal, J. Phys. (USSR) 4, 449 (1941).
[5] A.B. Migdal and V. Krainov, Approximation Methods in Quantum Mechanics, (W.A. Benjamin, New York (1969)).
[6] L.D. Landau and E.M. Lifshitz, Quantum Mechanics: non-relativistic theory, (3rd. ed. Pergamon Press, New York (1976)), Chpt. VI.
[7] A.M. Frolov, Eur. Phys. J. D 61, 571 (2011).
[8] S. Larsson, Phys. Rev. 169, 49 (1968).
[9] P.A.M. Dirac, The Principles of Quantum Mechanics, (4th ed., Oxford at the Clarendon Press, Oxford (1958)).
[10] A.M. Frolov, Phys. Rev. A 57, 2436 (1998).
[11] I.S. Gradstein and I.M. Ryzhik, Tables of Integrals, Series and Products, (6th revised ed., Academic Press, New York (2000)).
[12] R. McWeeny and B.T. Satcliffe, Methods of Molecular Quantum Mechanics, (New York: Academic Press, New York (1969)).
[13] E.R. Davidson, Adv. Quant. Chem. 6, 235 (1972).
[14] A.M. Frolov and V.H. Smith, Jr., J. Phys. B 36, 4837 (2003).
[15] A.M. Frolov, Phys. Lett. A 361, 346 (2007).