PHYSICAL REVIEW A **82**, 042511 (2010)

Atomic excitations during the nuclear β^- decay in light atoms

Alexei M. Frolov[1] and María Belén Ruiz[2]
[1]*Department of Chemistry, University of Western Ontario, London, Ontario N6H 5B7, Canada*
[2]*Department of Theoretical Chemistry, Friedrich-Alexander-University Erlangen-Nürnberg, Egerlandstraße 3, D-91058 Erlangen, Germany*
(Received 27 July 2010; published 22 October 2010)

Probabilities of various final states are determined numerically for β^--decaying He, Li, and Be atoms. In our evaluations of the final-state probabilities we have used the highly accurate atomic wave functions constructed for each few-electron atom or ion. We also discuss an experimental possibility to observe negatively charged ions which form during the nuclear β^+ decays. Corrections on direct interaction between atomic electrons and fast β electrons or positrons are considered. It is shown that for our results obtained for $\beta^\pm$ decays in few-electron atoms with the use of the sudden approximation such corrections are very small ($\approx\alpha^4$) and can be neglected.

DOI: 10.1103/PhysRevA.82.042511 PACS number(s): 36.10.Dr, 13.35.Bv, 14.60.Ef

I. INTRODUCTION

In this study we consider atomic excitations which arise during the nuclear β^- decay in light few-electron atoms. Our main goal is to determine numerically the corresponding final-state probabilities or, in other words, the absolute probabilities of formation of the final system(s) in certain bound and/or unbound states which arise after the nuclear β^- decay in light few-electron atoms. A basic theoretical analysis of atomic excitations during the nuclear β^- decay has been performed in our earlier works [1,2]. In this study we do not repeat all steps and arguments from those works. Instead, we bring our attention to some new problems which have not been solved in earlier studies. Note only that our analysis and computations of atomic excitations are based on the sudden approximation [3,4]. In turn, the sudden approximation follows from the well-known experimental fact that the velocities of the emitted β^- electrons are significantly larger than the usual velocities of atomic electrons. In many actual cases such velocities are close to the speed of light in vacuum (i.e., $v_\beta \approx c$). It follows from here that the emitted β^- electron leaves the external shells of an atom for a time which is approximately $\tau_\beta \approx a_0/c = \alpha\tau_a = \alpha\hbar/(e^4 m_e)$, where $\alpha \approx \frac{1}{137}$ is the fine-structure constant, $\hbar$ is the reduced Planck constant, m_e is the electron mass (at rest), a_0 is the Bohr radius, c is the speed of light in vacuum, and $\tau_a = \hbar/(e^4 m_e) \approx 2.418\,884 \times 10^{-17}$ s is the atomic time. For internal atomic or electron shells, one also finds that $\tau_\beta \ll \tau_a$, since the passing time τ_β for β^- electrons decreases with the radius of the electron shell.

The general equation of the β^- decay can be written in the form

$$Q \rightarrow (Q+1)^+ + e^- + \nu, \tag{1}$$

where Q is the nuclear charge of the incident nucleus, while e^- and ν are the emitted (fast) electron and neutrino, respectively. The emitted electron is usually very fast and its Lorentz γ factor ($\gamma = E/m_e c^2$) is bounded between 2 and 15–18. In all actual cases, the nuclear β^- decay proceeds in many-electron atoms or ions, rather than in bare nuclei. The arising atomic system with the nuclear charge $(Q+1)^+$ is also a many-electron ion (or atom). Our main goal in this study is to determine the final-state probabilities for this newly arising atomic system. Suppose that the incident atom was in one of its bound states, for example, in the A state. The final ion is formed in one of its states (bound or unbound), for example, in the B state. The aim of theoretical analysis of nuclear $\beta^\pm$ decays in atomic systems is to evaluate the corresponding transition amplitude $\mathcal{A}_{AB} = |\langle A \mid B\rangle|$ and final-state probability $p_{AB} = \mathcal{A}^2_{AB} = |\langle A \mid B\rangle|^2$.

This problem has attracted significant theoretical attention (see, e.g., Refs. [1,5–7]), since various β^--decaying nuclei are of great interest in various applications to modern technology, scientific research, nuclear medicine, and so on. For instance, the β^--decaying isotope iodine-131 (^{131}I, so-called radioiodine) is extensively used in nuclear medicine both diagnostically and therapeutically. Examples of its use in radiation therapy include the treatment of thyrotoxicosis and thyroid cancer. Diagnostic tests exploit the mechanism of absorption of iodine by the normal cells of the thyroid gland. ^{131}I can be used to destroy thyroid cells therapeutically. Other β^--decaying isotopes of iodine are used (mainly as radioactive labels) in modern biology, and in physical and organic chemistry [8].

Another well-known β^--decaying isotope is strontium-90 (^{90}Sr). It finds extensive use in medicine and industry, as a radioactive source for thickness gauges and for superficial treatment of some cancers. Controlled amounts of ^{90}Sr can be used in the treatment of bone cancer. The radioactive decay of ^{90}Sr generates a significant amount of heat. Strontium fluoride of strontium-90 (^{90}SrF$_2$) is widely used as a heat source in many remote thermoelectric generators, since it is much cheaper and less dangerous than the alternative source based on plutonium-238 (^{238}Pu). ^{90}Sr is also used as a radioactive tracer in medicine and agriculture. The isotope ^{90}Sr can be found in significant amounts in spent nuclear fuel, in radioactive waste from nuclear reactors, and in nuclear fallout from nuclear tests. It is interesting to note that the fission product yield of ^{90}Sr sharply depends upon the type of explosive nuclear (fission) device. A relatively large output of ^{90}Sr in nuclear fallout is a strong indication that the original nuclear explosive device was made from uranium-233 (or uranium-235) rather than from ^{239}Pu. Advanced nuclear explosive devices which contain substantial amounts of ^{245}Cm and ^{247}Cm and/or ^{249}Cf and ^{251}Cf produce significantly smaller yields of ^{90}Sr than analogous devices made from ^{239}Pu. A brief discussion of different applications of other β^--decaying atoms can be found, for example, in Ref. [1] (see also Ref. [8]). Note that for ^{131}I, ^{90}Sr, and for many other β^--decaying isotopes or atoms our knowledge about the final (or postdecay) atomic states is far from complete, since in almost all cases we cannot determine the final-state probabilities. Currently, for some of the β^--decaying atoms we can only predict approximate probabilities to find the final ions or atoms in their ground state(s). Analogous evaluations of the probability to form the first excited (bound) states and for the total probability of electron ionization are very approximate. Probabilities to form other excited states, including various unbound states, in the final atomic systems have never been evaluated (even approximately) for $\geqslant$99.9% of all β^--decaying atoms. The goal of this and following studies is to correct such a situation, at least for some light atoms. In general, the results of experiments, in which the final-state probabilities for $\beta^{\pm}$-decaying atoms and molecules are measured, can be considered a very serious quantitative test for the modern theory of electron density distribution in atoms and molecules.

Formally, the current theory of β^- decay in atoms (and molecules) is self-consistent and it does not include any unsolved problems. All troubles of the current theoretical evaluations are mainly related to the relatively low accuracy of the wave functions used in calculations. For instance, in [1] we have calculated a large number of probabilities for the "ground-state to ground-state" transitions. In fact, such probabilities are now known for all atoms from He up to Ar [1]. However, analogous calculations of the "ground-state to excited-states" probabilities are significantly more difficult to perform, since for many atoms or ions we do not have sufficiently accurate wave functions of the excited states. Finally, the computed values of final-state probabilities for the excited states are not accurate. Furthermore, these values often oscillate if the number of basis functions increases.

Analogous computations for the β^+ decays in atoms are even more complicated. In particular, it is very hard to determine the final-state probabilities accurately if a negatively charged ion is formed as a result of the atomic β^+ decay. In such cases one needs to use highly accurate methods which are specifically designed for accurate computations of the negatively charged ions. In this study we have developed such a method, and this allows us to determine the final-state probabilities in those cases when negatively charged ions are formed after the nuclear β^+ decays in some few-electron atoms and ions. The probabilities to form bound negatively charged ions, which are computed below, have not been determined in earlier studies. Another interesting problem is the emission of the fast secondary electrons during nuclear $\beta^{\pm}$ decays in many-electron atoms and molecules.

The present work has the following structure. In the next section we discuss a few numerical methods which are used to determine the bound-state wave functions of the incident and final states in few-electron atoms and ions. Section III contains a brief discussion of the final-state probabilities computed for some β^--decaying light atoms. Here we consider the He, Li, and Be atoms. Our present analysis is extensive and it includes a few excited states in each of the final ions. In Sec. IV we determine the ground-state to ground-state and excited-state to ground-state transition probabilities for the β^+ decay in some light atoms. The final atomic system in this case is a negatively charged ion. Emission of the fast, secondary electron (or δ electrons) during the nuclear $\beta^{\pm}$ decay in atoms are considered in Sec. V. The concluding remarks can be found in the last section.

II. METHOD

Let us assume that we have an N-electron atom which is described by its bound-state wave function Ψ_i, that is, $H_0\Psi_i = E_i\Psi_i$, where H_0 is the atomic Hamiltonian (see, e.g., [9]), E_i is the corresponding eigenvalue (or total energy, for short), and Ψ_i is the eigenfunction of the incident bound state which has a finite norm, that is, $\mid \Psi_i \mid^2 = 1$. Consider now a sudden change of the Hamiltonian of the atomic system. By sudden change we mean that the change in the original Hamiltonian H_0 occurs in a time which is very short compared with the periods of (atomic) transitions from the given state i to other states. The electron density distribution and the corresponding wave function cannot change for such a short time and remain the same as before perturbation. This means that after such a process we find the new atomic system with the new Hamiltonian H_f, but with the old electron density distribution. Such an electron density distribution is described by the old wave function Ψ_i. The new Hamiltonian H_f has a complete system of eigenfunctions; that is, $H_f\Phi_f^{(k)} = E_k\Phi_f^{(k)}$. Therefore, at the final stage of the process we have only states with the wave functions $\Phi_f^{(k)}$. The incident wave function Ψ_i is now represented in the form of an expansion $\Psi_i = \sum_k A_k\Phi_f^{(k)}$, where the coefficients A_k can be considered the transition (probability) amplitudes. The corresponding probabilities $p_k = |A_k|^2$ determine the probability to detect the final system in its state $\Phi_f^{(k)}$, if the initial state of the system was described by the wave function Ψ_i. Note that the system of notations used here corresponds to the case of the discrete spectra in both the incident and final atomic systems. In general, the expansion $\Psi_i = \sum_k A_k\Phi_f^{(k)}$ must contain different parts which represent the discrete and continuous spectra, respectively.

Thus, to determine the probability amplitudes A_k we need to compute the overlap integrals between two N-electron wave functions Ψ_i and $\Phi_f^{(k)}$ functions for different k, that is,

$$A_k = \int \Psi_i^*(\mathbf{r}_1,\ldots,\mathbf{r}_N)\Phi_f^{(k)}(\mathbf{r}_1,\ldots,\mathbf{r}_N)d^3\mathbf{r}_1\cdots d^3\mathbf{r}_N. \quad (2)$$

In general, this value is complex, but the corresponding probabilities $p_k = |A_k|^2$ are always real and their values are bounded between 0 and 1. As follows from Eq. (2), any of the final states must have the same L and S quantum numbers as the incident state. Here and in what follows, the notation L designates the angular (electron) momentum of the atom, while the notation S denotes the total electron spin. Note that the L and S quantum numbers are used in the nonrelativistic LS classification scheme which is appropriate for light atoms and ions. Briefly, we can say that the angular (electron) momentum of the atom and its total electron spin are conserved during the nuclear β^- decay. This means that the original problem of determining the final-state probabilities in the case of β^- decay in atoms is reduced to the construction of highly accurate wave functions for the incident and final states with the same L and S quantum numbers. This means the angular momentum $\mathbf{L}$ and total electron spin $\mathbf{S}$ are conserved during the nuclear β^- decay in many-electron atoms. In addition to these two quantum numbers the spatial parity of the incident wave function is also conserved.

The conservation of the angular (electron) momentum L and total electron spin S of the atom during the nuclear β^- decay follows directly from perturbation theory. In fact, these conservation rules are not fundamental; that is, they are obeyed only in the lowest-order approximations upon $\alpha = \frac{e^2}{\hbar c} \approx \frac{1}{137}$, where α is the fine-structure constant. It can be shown that in higher-order approximations upon α the L and S quantum numbers are not conserved (see discussion in Sec. V). The leading correction to the nonrelativistic results (i.e., to the final-state probabilities) is $\approx\alpha^2(\alpha Q)^2$, where Q is the electric nuclear charge (in atomic units). In light atoms such a correction is very small ($\approx\alpha^4$) and can be ignored. In heavy atoms with $Q \approx 100$, the overall contribution of this correction is substantially larger, but these atoms are not considered in this work.

A. Variational wave functions

Numerical evaluations of the overlap integral, Eq. (2), require the knowledge of highly accurate wave functions of the incident and final atomic systems. To determine such wave functions for the ground and excited states of different atoms and ions, in this work we perform extensive calculations of few-electron atomic systems. Then, by using our accurate wave functions, we determine the corresponding transition amplitudes and the final-state probabilities. This is the second step of our procedure. In this section we discuss the methods used to construct highly accurate wave functions of few-electron atoms and ions. In general, the wave functions of the excited states which have the same symmetry as the ground state can be found as the solutions of the corresponding eigenvalue problem.

The energies of the different bound states are calculated by optimizing the orbital exponents of the corresponding root of the eigenvalue equation. Furthermore, our wave functions are simultaneously the eigenfunctions of the angular momentum and spin operators, $\hat{L}^2$ and $\hat{S}^2$, respectively. Therefore, these eigenfunctions can be used in numerical calculations of various bound-state properties. The Slater orbitals are the natural basis for all atomic calculations. In this study we also use the basis of radial functions constructed from Slater orbitals.

To perform numerical computations of few-electron atoms and ions in this study we apply the Hylleraas–configuration-interaction (Hy-CI) method and the configuration-interaction (CI) method with Slater orbitals. Both these methods are included in our package of computer codes. The Hy-CI method, introduced by Sims and Hagstrom [10,11], combines the use of orbitals with higher angular momentum (as in the regular CI procedure) and inclusion of the interelectronic distance r_{ij} into the wave function (as for Hylleraas-type trial wave functions). The Hy-CI and CI wave functions for an n-electron systems are defined as

$$\Psi = \sum_{k=1}^{N} C_k \Phi_k, \quad \Phi_k = \hat{O}(\hat{L}^2)\hat{\mathcal{A}}\phi_k \chi, \tag{3}$$

where Φ_k are symmetry-adapted configurations, N is the number of configurations, and the constants C_k are determined variationally. The operator $\hat{O}(\hat{L}^2)$ projects over the proper spatial space, so that every configuration is an eigenfunction of the square of the angular momentum operator $\hat{L}^2$. $\hat{\mathcal{A}}$ is the n-particle antisymmetrization operator, and χ is the spin eigenfunction:

$$\chi = [(\alpha\beta - \beta\alpha)\cdots(\alpha\beta - \beta\alpha)\alpha], \tag{4}$$

where for even electron systems the last α spin function is omitted. The spatial part of the basis functions are Hartree products of Slater orbitals:

$$\phi_k = r_{ij}^{\nu} \prod_{i=1}^{n} \phi_i(r_i,\theta_i,\varphi_i), \tag{5}$$

where the power ν takes the value 0 or 1. For $\nu = 0$, the wave function reduces effectively to a CI wave function. The basis functions ϕ_k are the products of Slater orbitals defined as follows:

$$\phi(\mathbf{r}) = r^{n-1} e^{-\alpha r} Y_l^m(\theta,\phi), \tag{6}$$

where $Y_l^m(\theta,\phi)$ are the spherical harmonics. The phases used in our definition of $Y_l^m(\theta,\phi)$ correspond to the choice made by Condon and Shortley [12]:

$$Y_l^m(\theta,\phi) = (-1)^m \left[\frac{2l+1}{4\pi}\frac{(l-m)!}{(l+m)!}\right]^{1/2} P_l^m(\cos\theta) e^{im\phi}, \tag{7}$$

where $P_l^m(\cos\theta)$ are the associated Legendre functions.

The integrals occurring in our calculation are up to four-electron integrals in the Hy-CI method and two-electron integrals in the CI method. Expressions for all these integrals are given in Refs. [13–15]. The calculation of the overlap between the wave functions of bound states requires only the usual two- and three-electron integrals.

Currently, the nonrelativistic total energy of the ground state of a helium atom is known to very high accuracy (up to 45 decimal digits) [16]. Many excited S, P, D, F, ... states in two-electron helium atoms have also been computed to high numerical accuracy (see, e.g., Refs. [17–19]). The ground $1\,{}^1S$ state of the heliumlike Li$^+$ ion (or ${}^\infty$Li$^+$ ion) has been determined to high accuracy [20,21], while the $2\,{}^1S, \ldots, 7\,{}^1S$ states in the Li$^+$ ion are known to significantly less accuracy [22–24]. Highly accurate calculations of the excited S states in the Li$^+$ ion higher than $7\,{}^1S$ have never been performed.

As a reference calculation in the case of heliumlike two-electron atoms, we start with a Hy-CI energy of the ${}^\infty$He atom $-2.903\,724\,376\,99$ a.u. This energy was obtained with the use of 820 configurations and a basis set which included the s, p, d, and f Slater orbitals [$18s,16p,16d,16f$]. This total energy has uncertainty which is less than 1×10^{-9} a.u. The "optimal" exponent $\alpha = 2.9814$ has been obtained by optimizing 404 configurations constructed with a smaller basis [$11s,11p,11d,11f$]. The best Hy-CI energy obtained with a single exponent for the ground state of the He atom with the infinitely heavy nucleus is $-2.903\,724\,377\,01$ a.u. (974 configurations). All these calculations have been performed with the use of quadruple precision, or 30 decimal digits per computer word. Some special measures have been taken to avoid any linear dependence for this basis set.

The total energies of different bound $n\,{}^1S$ states in the Li$^+$ ion are shown in Table I. In calculations of the overlap, which

TABLE I. The transition amplitudes and final-state probabilities for the nuclear β^- decay from the ground $1\,^1S$ state of the helium atom into various (bound) states of the Li$^+$ ion. All calculations for this table have been performed with the use of Hylleraas configuration interaction wave functions with s, p, d, and f Slater orbitals. The He atom wave function ($1\,^1S$ state) used in these calculations corresponds to the energy −2.903 724 376 99(10) a.u. with 820 configurations. Reference energies: nonrelativistic total energy of the helium atom (ground state): −2.903 724 377 034 119 583 110 34 a.u. (variational) and −2.903 724 377 034 119 583 112 0(7) a.u. (asymptotic) [25]. The best-to-date nonrelativistic energy for the He atom contains over 45 stable decimal digits, −2.903 724 377 034 119 598 311 159 245 194 404 446 696 925 310 5 a.u. [16].

State of Li$^+$	N	Amplitude	Probability	Energy Li$^+$ (a.u.)	Ref. Ener. (a.u.)	Ref.
$1\,^1S$	820	0.841 794 254(4)	0.708 617 6(3)	−7.279 913 407 46	−7.279 913 412 67[a]	[21]
$2\,^1S$	820	0.386 502 7(8)	0.149 384(4)	−5.040 876 743 8(2)	−5.040 876 731 01	[22]
$3\,^1S$	820	0.136 30(4)	0.018 579(3)	−4.733 755 81(4)	−4.733 732	[23]
$4\,^1S$	820	0.079 01(5)	0.006 243(3)	−4.629 783 49(3)	−4.629 778	[24]
$5\,^1S$	820	0.053 68(7)	0.002 882(5)	−4.582 421 93	−4.582 424	[24]
$6\,^1S$	820	0.040 17(2)	0.001 614(2)	−4.556 877 65	−4.556 951	[24]
$7\,^1S$	820	0.032 87(9)	0.001 081(3)	−4.540 877	−4.541 692	[24]
$8\,^1S$	820	0.043 20(2)	0.001 866(1)	−4.528 507		

[a] The computed energy is −7.279 913 412 669 305 96 a.u. [21]. The lowest computed energy is −7.279 913 412 669 305 964 919 459 221 006 611 682 a.u. [20].

involve the wave functions of the He atom and Li$^+$ ion, we have used the wave functions for atom and ion with the same number of terms. The orbital exponents of different states were always different. In fact, the orbital exponents of every excited state have been optimized at several stages and used for the larger basis (for more detail, see Table II). The optimal values of exponents are shown in Table II. Every time a new exponent has been introduced in a series of calculations, a complete reoptimization has been made. Currently, our best calculations have been performed with 820 configurations, but the optimal exponents have been obtained in calculations with a smaller basis [$14s$,$14p$,$14d$,$14f$] (680 Hy-CI configurations). The use of a single exponent (considering double occupancy of the orbitals) for all configurations has been sufficient to obtain highly accurate energies. The total energies obtained in this study for the $2\,^1S$, $3\,^1S$, and $4\,^1S$ states of the Li$^+$ ion are the lowest values obtained to date.

Note that our resulting wave functions derived after optimization are not orthogonalized. Therefore, the overlaps between configurations must be determined. In turn, this problem is reduced to a numerical calculation of the overlap integrals. The symmetry-adapted configurations have been constructed for S symmetry as $s(1)s(2)$, $s(1)s(2)r_{12}$, $p(1)p(2)$, $p(1)p(2)r_{12}$, $d(1)d(2)r_{12}$, $f(1)f(2)$, and $f(1)f(2)r_{12}$. Using the short notation [e.g., $p_0(1)p_0(2) = p_0p_0$, $p_1(1)p_{-1}(2) = p_1p_{-1}$, etc.], we can write the symmetry-adapted configurations pp, dd, and ff in the form

$$\begin{aligned} pp &= p_0p_0 - p_1p_{-1} - p_{-1}p_1, \\ dd &= d_0d_0 - d_1d_{-1} - d_{-1}d_1 + d_2d_{-2} + d_{-2}d_2, \qquad (8) \\ ff &= f_0f_0 - f_1f_{-1} - f_{-1}f_1 + f_2f_{-2} + f_{-2}f_2 \\ &\quad - f_{-3}f_3 - f_{-3}f_3. \end{aligned}$$

In Table II we also show the convergence of the energy with respect to several truncated wave-function expansions. The exponents used in every calculation are given explicitly for each state. It was observed that for the determination of higher excited states the diffuse functions are needed and the wave-function expansions become larger. The total energies of the first four excited states can be determined to an accuracy better than ±1 × 10^{-6} a.u. However, such an accuracy rapidly decreases for the highly excited states. The value of the calculated overlap integral, which includes the excited states of Li$^+$ and the ground state of the He atom, substantially depends upon the overall accuracy of the calculated energy. For low-lying states, we have determined the overlaps with overall accuracy ≈4–5 stable decimal digits. For higher states such an accuracy decreases, but the absolute values of overlaps become very small and tend to zero.

In calculations of the Li and Be atoms and corresponding isoelectronic ions Be$^+$ and Li$^-$, we have used the wave functions constructed with the use of the L-S CI method. In the CI calculations we have used double precision, which was sufficient for our purposes. It was checked by performing analogous calculations with quadruple precision. Calculations with double precision are significantly faster. The method used for calculations and optimization of the orbital exponents is very similar to the method used above for two-electron systems.

For the three-electron systems Li and Be$^+$, we use the full configuration-interaction method. In such cases, therefore, there are no configurations which have been either selected or eliminated. We have used a set of s, p, and d Slater orbitals and two exponents, considering double occupancy of the orbitals. The exponents are the same for all configurations. We have optimized the exponents for the smaller basis used (i.e., $n = 3$ [$3s$,$2p$,$1d$] or $n = 4$) and employed them in the calculations with the larger basis sets $n = 5,6$. Eventually, the exponents in larger calculations are also optimized. The configurations are symmetry adapted and are constructed by combining the two-electron configurations of Eq. (8) with one s orbital. These configurations are sss, spp, pps, sdd, and dds. The obtained energies have been determined with ≈1 × 10^{-3} a.u. accuracy for the ground and excited states of the Li atom and Be$^+$ ion. They are shown in Table III. The overlaps between the wave functions of the ground state of the Li atom and the ground and excited states of Be$^+$ have been calculated numerically (see Table III). The values converge adequately and the overlaps rapidly decrease for higher excited state.

TABLE II. Convergences for the transition amplitudes, final-state probabilities, and total energies for different $n\,^1S$ states of the Li^+ ion.

State of Li^+	N	Expt.	Energy (a.u.)	Ref. Ener. (a.u.)	Amplitude	Probability
$1\,^1S$	365	2.520 933	−7.279 913 387 92		0.841 782 679 5	0.708 598 08
$1\,^1S$	631	2.520 933	−7.279 913 407 02		0.841 782 675 8	0.708 598 07
$1\,^1S$	820	2.520 933	−7.279 913 407 46	−7.279 913 412 7	0.841 794 254 4	0.708 617 57
$2\,^1S$	365	2.310 125	−5.040 876 708 8		0.386 495 74	0.149 378 96
$2\,^1S$	631	2.310 125	−5.040 876 743 7		0.386 495 69	0.149 378 92
$2\,^1S$	820	2.310 125	−5.040 876 743 8(2)	−5.040 876 7	0.386 502 78	0.149 384 40
$3\,^1S$	365	1.914 217	−4.733 628 80		0.136 714	0.018 691
$3\,^1S$	433	1.914 217	−4.733 711 18		0.136 463	0.018 622
$3\,^1S$	631	1.914 217	−4.733 751 12		0.136 323	0.018 584
$3\,^1S$	820	1.703 409	−4.733 755 81(4)	−4.733 732	0.136 304	0.018 579
$4\,^1S$	365	1.821 455	−4.618 380 12		0.096 628	0.009 337
$4\,^1S$	433	1.728 693	−4.625 609 11		0.087 485	0.007 654
$4\,^1S$	463	1.728 693	−4.627 503 63		0.084 276	0.007 103
$4\,^1S$	631	1.728 693	−4.628 588 58		0.082 097	0.006 740
$4\,^1S$	722	1.307 501	−4.629 770 02		0.078 972	0.006 237
$4\,^1S$	820	0.978 434	−4.629 783 49(3)	−4.629 778	0.079 015	0.006 243
$5\,^1S$	463	1.544 017	−4.564 019 93		0.078 132	0.006 105
$5\,^1S$	548	1.544 017	−4.564 139 29		0.078 035	0.006 089
$5\,^1S$	631	1.544 017	−4.570 249 51		0.072 624	0.005 274
$5\,^1S$	722	1.307 501	−4.579 562 74		0.060 734	0.003 689
$5\,^1S$	792	1.307 501	−4.581 541 66		0.059 914	0.003 590
$5\,^1S$	820	0.891 026	−4.582 421 93	−4.582 424	0.053 687	0.002 882
$6\,^1S$	548	1.610 647	−4.454 802 11		0.093 882	0.008 814
$6\,^1S$	631	1.610 647	−4.478 052 26		0.088 051	0.007 753
$6\,^1S$	722	1.399 839	−4.516 489 83		0.075 639	0.005 721
$6\,^1S$	792	1.399 839	−4.542 488 52		0.057 221	0.003 274
$6\,^1S$	820	0.891 026	−4.555 784 89		0.044 220	0.001 955
$6\,^1S$	820	0.691 701	−4.556 877 65	−4.556 951	0.040 172	0.001 614
$7\,^1S$	548	1.518 309	−4.343 051		0.096 978	0.009 405
$7\,^1S$	631	1.518 309	−4.383 434		0.091 388	0.008 352
$7\,^1S$	722	1.307 501	−4.452 212		0.079 887	0.006 382
$7\,^1S$	820	0.885 885	−4.529 541		0.049 684	0.002 469
$7\,^1S$	820	0.655 102	−4.540 877	−4.541 692	0.032 879	0.001 081
$8\,^1S$	631	1.610 647	−4.160 498		0.099 804	0.009 961
$8\,^1S$	722	1.399 839	−4.292 650		0.092 109	0.008 484
$8\,^1S$	792	1.307 501	−4.405 691		0.077 831	0.006 058
$8\,^1S$	820	0.885 885	−4.489 693		0.059 589	0.003 551
$8\,^1S$	820	0.564 485	−4.528 507		0.043 202	0.001 866

For four-electron atomic systems, we optimize the orbital exponents using a small basis, $n = 4$ (this means $[4s3p2d1f]$), and use those exponents in larger calculations with $n = 5,6$. The configurations are grouped in blocks for a given n and according to the type (i.e., *ssss*,*sspp*,*ppss*, *spps*, ...). Then the blocks of configurations have been filtered with a threshold of average single configuration contribution of $\approx 1 \times 10^{-3}$ a.u. All blocks of configurations with small contribution to the total energy have been eliminated after being tested. This could not produce any substantial loss in the total energy. In reality, the corresponding error was $\leqslant 1 \times 10^{-3}$ a.u. In addition, all configurations in our calculations have been ordered according to their orbitals (s, p, d, and f orbitals), and within these groups by approximately energetic order.

As the ground state of the Be atom is also an ^1S state, the configurations can be constructed combining the two-electron symmetry-adapted configurations of Eq. (8). Resulting configurations are *ssss*, *sspp*, *spps*, *ppss*, *pppp*, *ssdd*, *sdds*, *ddss*, *sppd*, *dpps*, *sdpp*, *ppdd*, *pddp*, *ddpp*, *ssff*, *ddff*, and *ffff*. A set of two exponents (double occupancy of the shells) has been used. With this restriction, the configurations shown above represent all possible cases that can be formed. Nevertheless, the configurations *ddff* and *ffff* have been eliminated because their contributions were less than the threshold. An additional configuration type of S symmetry, *sppd*, and its permutations, *dpps* and *sdpp*, contribute considerably to the energy calculations on four-electron systems, but not in three-electron ones, where they contribute $\leqslant 1 \times 10^{-4}$ a.u. This configuration is somehow

TABLE III. Transition amplitudes and final-state probabilities for the nuclear β^- decay from the ground ^2S state of the Li atom into the ground and excited $n\,^2S$ states ($n = 1, \ldots, 5$) of the Be$^+$ ion.

State of Be$^+$	N	Amplitude	Probability	Energy (a.u.)	Ref. Ener.[a]	Ref.
$1\,^2S$	33	0.766 353	0.587 297	−14.310 171 49	−14.324 763 176 790 43(22)	[26]
$1\,^2S$	98	0.747 147	0.558 228	−14.318 058 14		
$1\,^2S$	216	0.758 931	0.575 976	−14.321 184 01		
$1\,^2S$	403	0.757 726	0.574 148	−14.322 215 55		
$1\,^2S$	est.[b]	0.757 7(12)	0.574(2)			
$2\,^2S$	98	0.525 207	0.275 842	−13.916 544 22	−13.922 789 268 544 2	[27]
$2\,^2S$	216	0.521 907	0.272 387	−13.918 261 03		
$2\,^2S$	403	0.522 474	0.272 980	−13.919 197 76		
$2\,^2S$	est.	0.522 4(5)	0.272 9(6)			
$3\,^2S$	98	0.094 836	0.008 994	−13.790 756 54	−13.798 716 57	[28]
$3\,^2S$	216	0.078 840	0.006 216	−13.795 237 09		
$3\,^2S$	403	0.087 985	0.007 741	−13.795 761 22		
$3\,^2S$	est.	0.088(7)	0.007(5)			
$4\,^2S$	216	0.047 017	0.002 211	−13.725 530 23	−13.744 630 6	[29]
$4\,^2S$	403	0.033 557	0.001 126	−13.735 270 47		
$4\,^2S$	est.	0.03(7)	0.001(5)			
$5\,^2S$	403	0.017 717	0.000 314	−13.701 527 00	−13.716 286 24	[28]
$5\,^2S$	est.	0.02(3)	0.000 3(1)			

[a] The reference energies employed here for the Li ground state wave functions are −7.470 554 44, −7.473 000 00, −7.475 065 44, and −7.475 819 45 a.u. for $n = 3$, 4, 5, and 6 wave functions, respectively. The best ground-state energy for neutral Li is −7.478 060 323 910 10(32) a.u. [26].

[b] The estimate of uncertainties.

more complex:

$$\begin{aligned} sppd = {} & sp_0p_0d_0 + sp_1p_1d_{-2} + sp_{-1}p_{-1}d_2 + sp_1p_{-1}d_0 \\ & + sp_{-1}p_1d_0 - sp_1p_0d_{-1} - sp_{-1}p_0d_1 \\ & - sp_0p_1d_{-1} - sp_0p_{-1}d_1. \end{aligned} \tag{9}$$

Table IV contains the probability amplitude and final-state probability for the β^+ decay of the four-electron Be atom into the four-electron Li$^-$ ion. In this case, in numerical calculation of the overlap, we follow the same method of calculation used above for two-electron systems. However, for four-electron atomic systems, no Hy-CI terms have been included. We plan to include such terms in future studies. Since the computed CI energies are known to an accuracy of $\pm 1 \times 10^{-3}$ a.u., then here we restrict our calculations to the lowest three S states in the incident Be atom. The calculated ground-state energy of the Li$^-$ ion is −7.498 913 85 a.u. (for 2155 CI configurations), and it is close to the best-to-date value −7.500 582 50 a.u. [30] known in the literature for this system. The calculated total energy of the ground state of the Be atom, −14.665 206 19 a.u., is very close to the best results of recent calculations, −14.667 356 49 a.u. [31]. This value agrees very well with the value −14.665 445 00 a.u. calculated by Bunge with approximately the same basis [32]. As expected, the excited states of the Be atom can be determined with less accuracy than the ground state. The calculated total energies together with the overlaps between wave functions of the ground or excited states of the Be atom and the ground state of the Li$^-$ ion can be found in Table V.

TABLE IV. Transition amplitude and final-state probability for the nuclear β^+ decay from the ground $1\,^1S$ state of the Be atom into the ground $1\,^1S$ state of the Li$^-$ ion.

N	Amplitude	Probability	Energy (a.u.)	Ref. Ener. (a.u.)
572	0.465 191	0.216 403	−7.497 066 19	−7.500 582 500[a]
1001	0.453 986	0.206 103	−7.498 521 37	
2155	0.454 427	0.206 504	−7.498 913 85	
est.[b]	0.454 4(5)	0.206 5(4)		

[a] Reference [30].

[b] The estimate of uncertainties.

Finally, the "ground-state to ground-state" transition probability for the β^--decaying Be atom (to B$^+$ ion) can be found in Table VI. The reference ground-state energies for the Be atom are given in Table V. Note that our ground-state energy of the B$^+$ ion has an overall accuracy which is better than $\pm 1 \times 10^{-3}$ a.u.

III. RESULTS FOR β^--DECAYING LIGHT ATOMS

As we mentioned earlier, we consider the β^- decays in a number of few-electron atoms: He, Li, and Be. In all our calculations, we assume that before the nuclear β^- decay each of the atoms was in its ground state (except for calculations shown in Table V). Furthermore, the probability of direct electron ionization during β^- decay was assumed to be small. Its contribution is essentially ignored in this study. Numerical evaluation of the corresponding small correction can be found in Sec. V. Briefly, this means that all ions which are formed after the nuclear β^- decay contain the

TABLE V. Transition amplitudes and final-state probabilities for the nuclear β^+ decay from the ground and excited $n\,^1S$ states ($n = 1,2,3$) of the Be atom into the ground $1\,^1S$ state of the Li$^-$ ion.

State of Be	N	Amplitude	Probability	Energy (a.u.)	Ref. Ener. (a.u.)[a,b]
$1\,^1S$	572	0.465 191	0.216 403	−14.662 921 18	−14.667 356 486
$1\,^1S$	1001	0.453 986	0.206 103	−14.664 823 14	
$1\,^1S$	2155	0.454 427	0.206 504	−14.665 185 12	
$1\,^1S$	est.[c]	0.454 4(5)	0.206 5(4)		
$2\,^1S$	572	0.605 389	0.366 495	−14.407 342 75	−14.418 240 328
$2\,^1S$	1001	0.594 124	0.352 983	−14.414 113 24	
$2\,^1S$	2155	0.595 986	0.355 199	−14.415 257 47	
$2\,^1S$	est.	0.595 9(9)	0.355 2(10)		
$3\,^1S$	572	0.000 057	0.000 000	−14.359 487 53	−14.370 087 876
$3\,^1S$	1001	0.000 089	0.000 000	−14.361 620 61	
$3\,^1S$	2155	0.000 098	0.000 000	−14.361 786 13	
$3\,^1S$	est.	0.0	0.0		

[a] The reference energies employed here for the Li$^-$ ground-state wave functions are −7.497 066 19 a.u. for 572, −7.498 521 37 a.u. for 1001, and −7.498 913 85 a.u. for 2155 configurations, respectively. The best energy is −7.500 582 500 a.u. [30].

[b] Reference [31].

[c] The estimate of uncertainties.

same number of electrons as the original atoms. In other words, all final-state probabilities can be determined with the use of Eq. (2), where the overlap integral contains two N-electron wave functions. For instance, the nuclear β^- decay of the He atom produces the two-electron Li$^+$ ion. If the incident He atom was in its ground $1\,^1S$ ($L = 0$) state, then, in keeping with the conservation rules formulated above, the final two-electron Li$^+$ ion will be in one of its bound $n\,^1S$ ($L = 0$) states, where $n = 1,2,3,\ldots,$ or in an unbound state. In this study, we consider the bound $n\,^1S$ ($L = 0$) states in the Li$^+$ ion up to $n = 8$. The transition amplitudes $A_{g\to n}$ and corresponding probabilities $p_{g\to n} = |A_{g\to n}|^2$ for the nuclear β^- decay of the He atom can be found in Table I. Table I also contains the total energies of all $n\,^1S$ ($L = 0$) states (for $n = 1,2,\ldots,8$) in the Li$^+$ ion. These energies indicate, in principle, the overall quality of the bound-state wave functions used in our calculations of the overlap integrals, Eq. (2). The wave function of the ground $1\,^1S$ ($L = 0$) state in the incident He atom corresponds to the energy $E = -2.903\,724\,377\,01$ a.u., which is very good for the Hy-CI wave function with $N \leqslant 974$ terms.

Note that there are a few simple rules which must be obeyed, in principle, for any distribution of the final-state probabilities $p_{g\to n}$ obtained in numerical calculations. For simplicity, let us restrict ourselves to the cases when all final states are also bound and each of these states is labeled with the integer quantum number n ($n \geqslant 0$). This quantum number n is often called the "excitation number" or "index of excitation." The value $n = 0$ corresponds to the ground state in a few-electron atom (i.e., $n = g$). The first rule for probability distribution is simple and states that the numerical values of such probabilities rapidly decrease if the excitation number n increases; that is, it must be $p_{g\to n} > p_{g\to(n+1)}$ for an arbitrary n ($n \geqslant 0$). In reality this inequality is even stronger: $p_{g\to(n+1)} \ll p_{g\to n}$. In some actual calculations, one can find an opposite inequality for the final-state probabilities. Usually, it is directly related to very slow convergence rate(s) for the wave functions of the incident and final atomic systems. Numerical values of these final-state probabilities cannot be used in actual applications. They must be improved in future calculations with better convergent basis sets. The only expectation from this rule can be found in those cases when the ground-state wave function of the incident system and the trial wave function of one of the excited states of the final ion are almost orthogonal to each other. The final-state probability is a very small value for such an excited state. In many cases, it directly follows from an additional symmetry of the basis functions used to construct the variational wave functions.

The second rule states that the sum of all partial probabilities must converge to the value which exceeds ≈0.75 (if the initial system was a neutral atom), but always less than

TABLE VI. Transition amplitudes and final-state probabilities for the nuclear β^- decay from the ground $1\,^1S$ state of the Be atom into the ground $1\,^1S$ state of the B$^+$ ion. Convergence of the calculations is shown with the increasing basis set.

State of B$^+$	N	Amplitude	Probability	Energy (a.u.)	Ref. Ener.
$1\,^1S$	572	0.751 759	0.565 142	−24.344 002 96	−24.348 884 446[a]
$1\,^1S$	1001	0.749 761	0.562 141	−24.345 883 91	
$1\,^1S$	est.[b]	0.749 7(10)	0.562 1(7)		

[a] Reference [33].

[b] The estimate of uncertainties.

unity. In fact, the difference

$$P_{\text{ion}}(g) = 1 - \sum_{n=1}^{N_{\max}} p_{g\to n} \tag{10}$$

is the total probability of electron ionization (from the ground state g) during the nuclear β^- decay in a neutral atom. Ionization means that after β^- decay the total number of bound electrons decreases by unity. It is clear that the sum in Eq. (10) must be infinite (i.e., $N_{\max} = \infty$). In actual computations, however, there is a problem of slow convergence for the wave functions of highly excited bound states. This means that in actual cases the sum Eq. (10) is usually finite. The actual maximal value of N in Eq. (10), $N_{\max}$, is determined by the first rule mentioned above; that is, in the sum of Eq. (10) we can use only those bound states for which the inequality $p_{g\to n} > p_{g\to(n+1)}$ is obeyed. The approximate value of P_{ion} determined for the nuclear β^- decay in the He atom with the use of our results from Table I is $P_{\text{ion}} \approx 0.108$. In other words, the one-electron Li^{2+} ions are formed in ≈10.8% of all β^- decays of the He atoms. In actual experimental conditions these ions can be observed in the β^- decays of the ^{6}He atoms. The half-life of the ^{6}He atom against such a β^- decay is ≈0.82 s.

In general, the method described above can be used to determine the total probability of ionization during the nuclear β^- decay in any neutral atom. It is very simple and has many advantages in comparison with the so-called direct methods. In these direct methods the wave functions of the outgoing electron and double-charged final ion must be explicitly constructed. Then one needs to compute the overlap integral between the product of these two wave functions and the wave function of the incident atom. This step corresponds to the sudden approximation used above. However, in actual calculations we cannot assume that the outgoing electron is always in the s wave. Briefly, this means that we need to include many configurations in which the final (free) electron moves in the $p, d, f, \ldots$ waves, while the double-charged final ion is in one of its $P, D, F, \ldots$ states, respectively. If the incident atom was in one of its S states, then only the $sS, pP, dD, \ldots$ configurations for the final system must be used in calculations. The total energies some of these configurations are close to each other. To reach a "realistic" accuracy one needs to consider a very large number (up to few dozens) of different configurations (with different L) in the final system. In general, each of these computations is not easy to conduct with relatively high accuracy. This significantly complicates all direct calculations of the ionization probabilities.

An interesting and actual question is the convergence of computational results obtained for the transition amplitudes and transition probabilities. Recently, a number of papers have been published about nuclear β^- decay in different atoms and ions. In all these works it was assumed that the determined transition amplitudes and corresponding probabilities are "exact;" that is, they will not change noticeably in similar future calculations. In many cases, however, the following calculations show that such results were not exact, and overall changes in some cases are relatively large. In particular, all calculations of the transition amplitudes and transition probabilities performed with the use of Hartree, Hartree-Fock, and Hartree-Fock-CI methods cannot be considered very accurate unless some additional measures have been taken. In this study we decided to analyze this problem in detail. The result of our analysis can be found in Table II, where various transition amplitudes and transition probabilities are determined with the different number(s) of basis functions.

As follows from Table II, our method provides a very good convergence rate for the ground and low-excited $n\,^1S$ $(L = 0)$ states in the Li^+ ion. For the excited $n\,^1S$ $(L = 0)$ states with $n \geqslant 6$ the overall convergence rate drops drastically. In such cases, to keep the overall accuracy of our calculations of the corresponding overlap integrals we need to use larger numbers of basis functions. In general, it is very hard to compute transition probabilities for highly excited (bound) states of the final atomic system. On the other hand, the numerical values of these probabilities decrease rapidly when the "excitation number" n increases. Therefore, by using a few known transition probabilities into the lowest bound states of the final system, we can accurately evaluate the total "ground-state to bound-states" probability and total ionization probability for an arbitrary β^--decaying atom.

Our results obtained for the atomic transition amplitudes and corresponding transition probabilities for the nuclear β^- decay in the Li atom can be found in Table III. In these calculations we assume that the original Li atom was in its ground (doublet) $1\,^2S$ state. Due to the conservation of the L and S quantum numbers, the final Be^+ ion will be in one of its bound (doublet) $n\,^2S$ states. The final-state probability amplitudes and corresponding probabilities have been computed with the use Eq. (2). The "ground-state to ground-state" probability and the corresponding transition amplitude for the β^--decaying B atom are shown in Table VI. Note that for all elements discussed in this study our computed "ground-state to ground-state" probabilities coincide well with the corresponding results from Ref. [1]. However, if the final ion is in one of its excited states, then our current results have substantially better accuracy. This is directly related to the better overall accuracy of our current wave functions.

The knowledge of the final-state probabilities allows one to predict the excitations of the final atomic fragment (i.e., in the final atom or ion). In general, any excited state in a few-electron atom decays with the emission of a few optical quanta. These transitions produce a unique spectrum of postdecay optical radiation. By using the computed final-state probabilities we can estimate the spectrum and intensity of the postdecay optical radiation which is observed for some time τ (usually $\tau \approx 1 \times 10^{-9}$ to 1×10^{-2} s) after the nuclear β^- decay. In the case of the β^--decaying ^{6}He atom (from its ground state), the postdecay optical radiation corresponds to the chain of optical transitions from the final $n\,^1S$ state of the Li^+ ion into its ground $1\,^1S$ state. For instance, for the $3\,^1S$ state in the Li^+ ion this chain of dipole transitions is $3\,^1S \to 2\,^1P \to 1\,^1S$. Various collisions between Li^+ ions and He or Li atoms and possible electron capture by the Li^+ ion must also be taken into account. The arising (optical) spectrum of postdecay radiation is very complex, but it can be studied, in principle, with the use of theoretical and current experimental methods.

IV. FORMATION OF THE NEGATIVELY CHARGED IONS DURING β^+ DECAY IN FEW-ELECTRON ATOMS

Formation of the negatively charged ions (or anions) during the nuclear β^+ decay in many-electron atoms is a very interesting experimental problem. On the other hand, it is very interesting to evaluate the corresponding final-state probabilities by using our computational methods described above. It is clear *a priori* that such probabilities can be found with the use of the sudden approximation (exactly as it was made above for the nuclear β^- decay). Formally, in the case of the nuclear β^+ decay in many-electron atoms, one needs to determine the same overlap integral, Eq. (2), between the incident and final N-electron wave functions. This is exactly the same procedure as described above for the nuclear β^- decay, but actual computations of the overlap integrals, Eq. (2), is a significantly more complicated problem in those cases when the negatively charged ions are involved. The first complication follows from the experimental fact that many atoms do not form stable negatively charged ions. However, if such negatively charged ions are stable, then the construction of highly accurate variational wave function(s) for these ions is a very hard problem. Briefly, this means that the final-state probabilities obtained for the nuclear β^+ decay in many-electron atoms are not very reliable if they have been determined for the negatively charged ions.

Nevertheless, in this study we have determined probabilities for the ground-state (atom) to ground-state (negative ion) transition for the nuclear β^+ decay in some light atoms. Note that each of the negatively charged atomic ions have either one bound (ground) state, or no bound states at all. In particular, we consider the possibility of forming the ^{7}Li$^-$ ion during the nuclear β^+ decay of the ^{7}Be nucleus. It should be mentioned that more than 99% of all ^{7}Be nuclei decay by the electron capture. If K-electron capture in the ^{7}Be atom occurs, then the Li$^-$ ion cannot be formed. However, any experimental observation of the Li$^-$ ions from decaying ^{7}Be nuclei will be an actual indication of the competing β^+ decay. As follows from Table IV, the total probability to form the bound Li$^-$ ion during such a decay is evaluated as ≈ 0.2065. This means that the Li$^-$ ions will form in $\approx 20.65\%$ of all nuclear β^+ decays of Be atoms; that is, in one of five such decays we can observe the negatively charged Li$^-$ ion. Another interesting result can be found in Table V. As follows from that table, the probability to form the bound Li$^-$ ion is larger $\approx 35.5\%$ in those cases, when the incident Be atom was in its excited $2\,^1S$ state. It indicates clearly that the distribution of the final-state probabilities in those cases when the negatively charged ions are formed is very different from the known distributions of β^--decaying neutral atoms.

Another interesting β^+-decaying atomic system with a small number of electrons is the ^{11}B$^-$ ion. This ion arises during the nuclear β^+ decay of the ^{11}C atom [$\tau_{\beta^+}(^{11}\mathrm{C}) \approx 20.4$ min]. It is very likely that the formation of the ^{11}B$^-$ ion will be the first actual experiment which can confirm the direct formation of the negatively charged ions during the nuclear β^+ decay.

The formation of negatively charged ions during the nuclear β^+ decay has a great theoretical interest, since the probability to form such ions is directly related to the change in distribution of the outermost electron(s). Furthermore, the density distributions of the outermost electron(s) for all negatively charged ions are very similar to each other. As is well known (see, e.g., Ref. [34]), the radial wave function $R(r)$ of an arbitrary N-electron atomic system with the nuclear charge Q at large r has the following asymptotic form:

$$R^Q(r) \sim r^{b-1}\exp(-tr) = r^{\frac{Q^*}{t}-1}\exp(-tr), \tag{11}$$

where $t = \sqrt{2I}$, $b = Q^*/t$, and $Q^* = Q - N + 1$, and the notation I stands for the first ionization potential. For negatively charged ions, $Q^* = Q - N + 1 = 0$ and $R^Q(r) = \frac{1}{r}\exp(-tr)$; that is, it does not depend explicitly upon Q. This substantially simplifies all following evaluations and makes them universal for all negatively charged ions. In particular, we can expect that the total probabilities of negative ion formation will accurately be represented by one relatively simple formula which contains only a few parameters. This means that, if we know such probabilities for some of the negatively charged ions, then we can accurately predict analogous values for other similar ions.

V. EMISSION OF THE FAST δ ELECTRONS DURING THE NUCLEAR β^- DECAY IN ATOMS

The sudden approximation used above allows one to determine the final-state probabilities for the $\beta^\pm$ decays in many-electron atoms. Briefly, the analysis of atomic excitations is reduced to the description of changes in electron density distribution produced by a sudden change of the nuclear electric charge $Q \rightarrow Q \pm 1$. The electronic or positronic nature of the $\beta^\pm$ decay is not critically important for our method. However, the sudden approximation is true only in the lowest-order approximations upon the fine-structure constant α. This means that, if we are interested in highly accurate results for the final-state probabilities, then we need to consider and evaluate the corresponding correction(s). The leading contribution comes from the lowest-order correction on electron-electron scattering, which is $\approx \alpha^2(\alpha Q)^2$. In heavy atoms with $Q \approx 100$, such a correction is relatively large ($\approx \alpha^2$), but in light, few-electron atoms it is significantly smaller ($\approx \alpha^4$). Nevertheless, this correction describes the new phenomenon (i.e., the emission of the fast secondary electrons), which are traditionally called the δ electrons. Let us discuss this phenomenon in detail. As is well known from quantum electrodynamics (see, e.g., Refs. [35,36]), the differential cross section of the electron-electron scattering is written in the form

$$d\sigma = 2\pi\alpha^4 a_0^2 \frac{dx}{\gamma^2 - 1} \times \left[1 + \frac{(\gamma-1)^2\gamma^2}{x^2(\gamma-1-x)^2} - \frac{2\gamma^2+2\gamma-1}{x(\gamma-1-x)}\right], \tag{12}$$

where a_0 is the Bohr radius, γ is the γ factor of the β electron emitted from the nucleus, and the parameter x is the energy lost by the β electron (or gained by the atomic electron a),

$$x = \frac{\epsilon_\beta - \epsilon'_\beta}{m_e c^2} = \frac{\epsilon'_a - \epsilon_a}{m_e c^2}, \tag{13}$$

where the prime designates the particle after the process. It is usually assumed that one of the two electrons (atomic electron in our case) was at rest before electron-electron collision or scattering (i.e., $\epsilon_a = m_e c^2$).

Equation (12) is the closed expression for the differential cross section of electron-electron scattering which depends upon the parameter x, Eq. (13), and γ factor of the β^- electron. As follows from Eq. (12), the probability to observe or produce a fast δ electron during the nuclear β^--decay is very small in comparison with "regular" atomic processes, since it contains an additional factor $\alpha^4 \approx 2.83 \times 10^{-8}$. Note also that Eq. (12) is derived for a free electron which is located at a distance a_0 from atomic nucleus. The actual K electrons in heavy atoms are significantly closer to the nucleus than electrons from outer electron shells. The effective radius of the K-electron shell is smaller than a_0 in $\approx Q^2$ times. This means that the factor $2\pi\alpha^4 a_0^2$ in Eq. (12) must be multiplied by an additional factor Q^2. For light atoms considered in our study the overall probability to observe the emission of the fast δ electrons during the nuclear β^- decay is very small. The situation changes for heavy atoms with $Q \approx 90$–100, but such atoms are not discussed here.

The emission of the fast δ electrons can also be observed during the nuclear β^+ decay in many-electron atoms. In such a case, the formula for the cross section of electron-positron scattering takes the form [35,36]

$$d\sigma = 2\pi\alpha^4 a_0^2 \frac{dx}{\gamma^2 - 1}\left[\frac{\gamma^2}{x^2} - \frac{2\gamma^2 + 4\gamma + 1}{(\gamma + 1)x} + \frac{3\gamma^2 + 6\gamma + 4}{(\gamma + 1)^2} - \frac{2\gamma}{(\gamma + 1)^2}\Delta + \frac{1}{(\gamma + 1)^2}\Delta^2\right], \qquad (14)$$

where γ is the γ factor of the positron emitted from the nucleus, while all other notations are the exactly same as in Eq. (12). Note again that in light atomic systems the cross section, Eq. (14), is very small. In heavy atoms the situation changes and in one of $\approx$17 000 nuclear β^+ decays we can also observe the emission of the fast δ electron.

VI. DISCUSSION AND CONCLUSION

We have considered atomic excitations arising during the nuclear β^- decay. For some light few-electron atoms, such final-state probabilities and the total ionization probabilities have been determined numerically to a very good numerical accuracy. Our interest in light atoms is directly related to the fact that currently the highly accurate wave functions of the ground and six to eight low-lying excited states can only be constructed for some few-electron atoms and ions. Consideration of the six to eight bound states in the final atomic system allows us to perform a complete analysis of atomic excitations during the nuclear β^- decay. We also consider the formation of negatively charged ions during the nuclear β^+ decay. By using our highly accurate wave functions for the negatively charged ions, we have determined the "ground-state to ground-state" probabilities for some nuclear β^+ decays in which such negatively charged ions are formed (or can be formed).

It should be mentioned that atomic excitations during the nuclear $\beta^\pm$ decay were observed for the first time in 1912 (all earlier references on this matter can be found, e.g., in Refs. [3,5–7]). In general, atomic and molecular excitations arising during the nuclear $\beta^\pm$ decay have many interesting aspects for theoretical study and experimental investigation. Analysis of the direct atomic excitations in earlier studies was substantially restricted by the use of nonaccurate atomic wave functions. In this study, we have applied highly accurate wave functions for all few-electron atoms and ions. The overall accuracy of our predictions for many excited states has increased significantly. In future studies we want to extend our analysis to atomic systems with more electrons. A separate goal is a consideration of different atomic (and molecular) excitations, analysis of the postdecay radiation, and so on.

Note that the final-state probabilities determined above for a number of β^--decaying light atoms can also be used as important numerical tests for other similar values needed in the analysis of various nuclear reactions in few-electron atoms or ions. For instance, for exothermic nuclear $(n;t)$, $(n;p)$, and $(n;\alpha)$ reactions in few-electron atoms or ions [37] one needs to determine the numerical value of the following integral:

$$A_k(\mathbf{V}) = \int \Psi_i^*(\mathbf{r}_1,\ldots,\mathbf{r}_N)\exp\left[\imath\mathbf{V}\cdot\left(\sum_{i=1}^{N}\mathbf{r}_i\right)\right] \times \Phi_f^{(k)}(\mathbf{r}_1,\ldots,\mathbf{r}_N)d^3\mathbf{r}_1\ldots d^3\mathbf{r}_N, \qquad (15)$$

where N is the total number of bound electrons (here we assume that N does not change during the nuclear reaction), while $\mathbf{V}$ is the nuclear velocity in the final state (i.e., after the nuclear reaction). Note that in the limit $\mathbf{V} \rightarrow \mathbf{0}$ the value $A_k(\mathbf{V})$ from Eq. (15) converges to the A_k value from Eq. (2). This explains why the final-state probabilities determined by Eq. (2) are often considered the "nucleus-at-rest" limit of atomic probabilities obtained for more general nuclear reactions.

In conclusion, we want to note that this work opens a new avenue in the analysis of atomic excitations during the nuclear $\beta^\pm$ decay in atoms and molecules. Currently, many aspects of this problem are of significant experimental and theoretical interest. In particular, the study of atomic excitations arising in the nuclear $\beta^\pm$ decay can improve our understanding of many atomic and QED processes. Furthermore, the complete and accurate analysis of atomic excitations during various nuclear reactions and processes is a complex problem which requires an extensive development of new numerical methods and algorithms. It should be mentioned that a sudden change of the electric charge of an atomic nucleus and following changes in the electron density distribution during the nuclear β^- decay must be of great interest for the density functional theory of atoms and molecules. Note also that analysis of possible molecular excitations arising during the nuclear β^- decay in molecules is a significantly more complicated problem than an analogous problem for atoms. Nevertheless, some useful conclusions about different excitations in molecular systems can be made and corresponding probabilities can be evaluated numerically. In fact, in the last five to seven years, we have achieved a remarkable progress in the understanding of atomic excitations during various nuclear processes, reactions, and decays. Unfortunately, except for a very few experimental papers published as a rule years ago (see, e.g., Refs. [38–40]), the current theory of atomic excitations during various nuclear reactions has no experimental support. This is a very strange situation, since all required (atomic) experiments are very easy to perform. Currently, we can only hope that our work will stimulate some experimental activity in the area.

ACKNOWLEDGMENTS

It is a pleasure to thank James S. Sims (NIST) for fruitful discussions on the Hy-CI method. One of us (A.M.F.) wants to thank the University of Western Ontario and Professor D. M. Wardlaw for financial support. M.B.R. would like to thank Carlos Bunge for advice on the CI method and Professor Peter Otto of the University Erlangen-Nürnberg for supporting this project.

[1] A. M. Frolov and J. D. Talman, Phys. Rev. A **72**, 022511 (2005).
[2] A. M. Frolov, Phys. Rev. A **58**, 4479 (1998).
[3] A. B. Migdal, J. Phys. (USSR) **4**, 449 (1941).
[4] A. B. Migdal and V. Krainov, *Approximation Methods in Quantum Mechanics* (W. A. Benjamin, New York, 1969).
[5] E. L. Feinberg, J. Phys. (USSR) **4**, 423 (1941).
[6] G. A. Skorobogatov, Theor. Exp. Chem. **2**, 20 (1967).
[7] H. W. Schwartz, J. Chem. Phys. **21**, 45 (1953).
[8] M. Hassinski and J.-P. Adlow, *Radiochemical Survey of the Elements* (Elsevier, Amsterdam, 1969).
[9] L. D. Landau and E. M. Lifshitz, *Quantum Mechanics (Non-Relativistic Theory)*, 3rd ed. (Pergamon, Oxford, 1977).
[10] J. S. Sims and S. A. Hagstrom, J. Chem. Phys. **55**, 4699 (1971).
[11] J. S. Sims and S. A. Hagstrom, Phys. Rev. A **4**, 908 (1971).
[12] E. U. Condon and G. H. Shortley, *The Theory of Atomic Spectra* (Cambridge University Press, Cambridge, England, 1967).
[13] M. B. Ruiz, J. Math. Chem. **46**, 24 (2009).
[14] M. B. Ruiz, J. Math. Chem. **46**, 1322 (2009).
[15] J. S. Sims and S. A. Hagstrom, J. Phys. B **37**, 1519 (2004).
[16] C. Schwartz, Int. J. Mod. Phys. E **15**, 877 (2006); e-print arXiv:math-ph/0605018.
[17] H. Nakashima, Y. Hijikata, and H. Nakatsuji, J. Chem. Phys. **128**, 154108 (2008).
[18] G. W. F. Drake and Z.-C. Yan, Chem. Phys. Lett. **229**, 486 (1994).
[19] J. S. Sims and W. C. Martin, Phys. Rev. A **37**, 2259 (1988).
[20] H. Nakashima and H. Nakatsuji, J. Chem. Phys. **127**, 224104 (2007).
[21] A. M. Frolov, J. Chem. Phys. **124**, 224323 (2006).
[22] C. L. Pekeris, Phys. Rev. **126**, 143 (1962).
[23] A. W. Weiss, J. Res. Natl. Bur. Stand. Sect. A **71**, 163 (1967).
[24] J. F. Perkins, Phys. Rev. **151**, 80 (1966); Y.-K. Kim and M. Inokuti, Phys. Rev. A **1**, 1132 (1970).
[25] A. M. Frolov, J. Chem. Phys. **126**, 104302 (2007).
[26] M. Puchalski, D. Kedziera, and K. Pachucki, Phys. Rev. A **80**, 032521 (2009).
[27] M. Puchalski and K. Pachucki, Phys. Rev. A **78**, 052511 (2008).
[28] F. W. King, J. Phys. Chem. A **113**, 4110 (2009).
[29] Z.-W. Wang, X.-W. Zhu, and K. T. Chung, Phys. Rev. A **46**, 6914 (1992).
[30] A. M. Frolov and D. M. Wardlaw, Phys. Rev. A **78**, 042506 (2008).
[31] M. Stanke, J. Komasa, S. Bubin, and L. Adamowicz, Phys. Rev. A **80**, 022514 (2009).
[32] C. F. Bunge, Phys. Rev. A **14**, 1965 (1976).
[33] S. Bubin, J. Komasa, M. Stanke, and L. Adamowicz, J. Chem. Phys. **132**, 114109 (2010).
[34] M. Hoffmann-Ostenhof and T. Hoffmann-Ostenhof, Phys. Rev. A **16**, 1782 (1977).
[35] A. I. Akhiezer and V. B. Beresteskii, *Quantum Electrodynamics*, 4th ed. (Nauka Science, Moscow, 1981), Chaps. 4 and 5 [in Russian].
[36] W. Greiner and J. Reinhardt, *Quantum Electrodynamics*, 2nd ed. (Springer-Verlag, New York, 1994).
[37] A. M. Frolov and D. M. Wardlaw, Phys. Rev. A **79**, 032703 (2009).
[38] T. A. Carlson, Phys. Rev. **130**, 2361 (1963).
[39] T. A. Carlson, Phys. Rev. **131**, 676 (1963).
[40] N. D. Scielzo, S. J. Freedman, B. K. Fujikawa, and P. A. Vetter, Phys. Rev. A **68**, 022716 (2003). this work also contains an extensive review of experimental literature related to various atomic phenomena observed during the nuclear $\beta^{\pm}$ decays in atoms.