On the $\beta^-$-decay in the $^8$Li and $^9$Li atoms

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Abstract

The nuclear $\beta^-$-decay from the ground and some excited states of the three-electron $^8$Li and $^9$Li atoms is considered. The final state probabilities for product Be$^+$ ion are determined numerically using highly accurate bound state wave functions of the Li atom and Be$^+$ ion. The probability of electron ionization during the nuclear $\beta^-$-decay of the Li atom is evaluated numerically. We also discuss the possibility of observing double $\beta^-$-decay using known values of the final state probabilities for the regular nuclear $\beta^-$-decay.

Keywords: $\beta$-decay; ionization; transition probabilities; Li atom; Be$^+$ ion; Hylleraas-CI wave functions

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I. INTRODUCTION

In our earlier study \cite{1} we considered the atomic excitations during the nuclear $\beta^-$-decay in light atoms and ions. In \cite{1} we determined the final state probabilities for a number of bound states in the final atoms and ions. Recently, all these probabilities have been re-calculated to much better accuracy. They are presented in this work. Also, here we discuss two problems related with the atomic ionization during the nuclear $\beta^-$-decay: (a) excitation of the internal electron shells, and (b) evaluating the probability of ‘additional’ electron ionization. In reality these two problems are very complex and below we have made a few preliminary steps to the final solutions. In addition to this we restrict ourselves by the analysis of the three-electron Li-atom.

The focus below is given to the $^8$Li and $^9$Li atoms which are of interest in some industrial applications. In general, the $\beta^-$-decay of the Li atom(s) can be written in the following form

$$\text{Li} \rightarrow \text{Be}^+ + e^- + \nu \quad (1)$$

where the notation $e^-$ stands for the fast electron emitted during the nuclear $\beta-$decay, while $\nu$ designates the electron anti-neutrino. In general, the nuclear $\beta^-$-decay of the Li atom leads to the following re-distribution of the bound atomic electrons. As a result of this redistributed incident electron density the final Be$^+$ ion can be found in a variety of bound states, or even in a number of unbound states. Briefly, this means the formation of the two-electron Be$^{2+}$ ion during the nuclear $\beta^-$-decay of the Li atom. In actual applications it is important to predict the probabilities to form the final Be$^+$ ion in different final states. Note that there are a few selection rules which are applied to the $\beta^\pm$-decays in atomic systems (see, e.g., \cite{2}). These rules can be concisely formulated as the conservation laws for the angular momenta $L$ and the total electron spin $S$. The wave functions of the incident and final system must also have the same spatial parity. For instance, if the incident Li atom was in its $3^2P(L = 1)$-state, then the final Be$^+$ can be found only in one of its $n^2P(L = 1)$ states. In other words, after the nuclear $\beta$-decay of the Li atom in the $3^2P(L = 1)$-state it is impossible to detect the final Be$^+$ ion, e.g., in the $3^2S(L = 0)$-state, or in the $3^2D(L = 2)$-state.

The advantage of considering three-electron atoms and ions is obvious: the wave functions of such systems can be approximated to very high numerical accuracy. For simplicity, throughout this study we shall assume that the original Li atom was in its ground $^2S(L = 0)$-state. The choice of the ground state of the incident Li-atom is not a fundamental
restriction for our method. Formally, such a state can be arbitrary, e.g., either ground state, or ‘vibrationally’, or ‘rotationally’ excited atomic state with the given angular momentum \( L \) (see below) and the total electron spin \( S \).

By analyzing the properties of known Li-isotopes one finds that there are two \( \beta^- \)-decaying isotopes of lithium: \(^8\text{Li} \ (\tau_\beta \approx 0.84 \text{ sec})\) and \(^9\text{Li} \ (\tau_\beta \approx 0.17 \text{ sec})\). These two isotopes are formed in the \((n; \gamma)\)-reactions during thermonuclear explosions in which light thermonuclear fuel (\(^6\text{LiD}\)) is compressed to very high densities \( \rho \geq 100 \text{ g} \cdot \text{sm}^{-3} \) by extremely intense flux of soft X-ray radiation from the primary. Larger compressions mean, in general, greater output of these two lithium isotopes. In the laboratory, the \(^8\text{Li}\) isotope is produced with the use of the \((n; \gamma)\)-reaction at \(^7\text{Li}\). In contrast with this, the \(^9\text{Li}\) isotope is produced by using either \((d; 2p)\)- and \((n; p)\)-reactions with the \(^9\text{Be}\) nuclei, or \((t; p)\)-reaction with nuclei of \(^7\text{Li}\).

The life-times of these two lithium isotopes are relatively short from the chemical point of view. Therefore, it is hard to study the regular chemical properties of these isotopes. An alternative approach is based on detailed analysis of the optical radiation emitted by the final \(\text{Be}^+\) ions which are formed after the nuclear \(\beta^-\)-decay of these two Li-isotopes. This can be achieved, if we know the corresponding final state probabilities, i.e. the probabilities to form the final Be-ions in certain bound states. The first goal of this study is to evaluate the final state probabilities of formation of various final states in product \(\text{Be}^+\) ions. Note that all evaluations of the final state probabilities during the nuclear \(\beta^-\)-decay in atoms and molecules are based on the sudden approximation \([3], [4]\) which applies to both atomic systems (original atom and final ion) involved in the process. The sudden approximation is appropriate for all \(\beta^\pm\)-decaying atoms, since the velocities of the \(\beta^\pm\) electrons are significantly greater than those of regular atomic electrons.

The final state probabilities, i.e. probabilities to form different atomic states during nuclear \(\beta^-\)-decay in various light atoms, have been evaluated numerically in a number of earlier papers (see, e.g., \([1], [2]\)). All such evaluations, however, have been based on the assumption that the total number of bound electrons is constant in nuclear \(\beta^-\)-decay. In reality, the nuclear \(\beta\)-decay in light atoms often leads to an ‘additional’ electron ionization. For the \(\text{Li}\) atom this process can be written in the form

\[
\text{Li} \rightarrow \text{Be}^{2+} + e^- + \beta^- + \nu
\]

where \(e^-\) designates the secondary atomic electron which becomes free during atomic \(\beta^-\)-
decay. It is interesting to evaluate the probability of this process and obtain the actual energy spectra of the emitted secondary electrons. Formally, all secondary electrons emitted during atomic $\beta$-decay must be considered as $\delta$-electrons. On the other hand, the original definition of $\delta$-electrons means that these electrons are fast and their total energies significantly exceed the usual energies of ‘regular’ atomic electrons. The energy of the free electron from reaction, Eq. (2), is comparable with atomic energies. Therefore, here we deal with the regular atomic ionization during $\beta$-decay. In earlier works the process of additional ionization only from the atomic $K$-shell was considered (see discussion and references in [5]).

The main goal of this study is to determine the final state probabilities to form various bound states in the Be$^+$ ion. These calculations are discussed in the fourth Section. Another aim of our study is to evaluate the probability of ‘additional’ ionization during the nuclear $\beta$-decay and investigate the energy spectrum of secondary electrons emitted during the nuclear $\beta$-decay. This problem is considered in the third Section. We also briefly investigate the long-standing problem of the double nuclear $\beta$-decay. Concluding remarks are in the last Section.

II. EVALUATION OF THE FINAL STATE PROBABILITIES FOR THE BOUND STATES.

As follows from the general theory of perturbations in Quantum Mechanics (see, e.g., [5]) in sudden approximation the final state probabilities are determined as overlap integrals between the wave function of the incident atomic system (i.e. the wave function of the Li atom in our case) and the wave function of the final atomic system (i.e. the wave function of the Be$^+$ ion). To compute such an three-electron integral we need to assume that the total numbers of bound electrons in the incident and final atomic systems are the same. In the sudden approximation the general formula for the transition probability $w_{if}$ for the transitions from the incident $i$-state into the final $f$-state takes the form (see, e.g., [5])

$$w_{if} = \frac{1}{\hbar^2} \left| \int_0^{+\infty} V_{if} \exp(i\omega_i ft) dt \right|^2 \approx \frac{1}{\hbar^2} \left| V_{if} \right|^2$$

(3)

where $V_{if}$ is the overlap integral computed with the use of time-independent incident and final atomic wave functions, i.e.

$$V_{if} = \langle \psi_{Be^+}(x_1, x_2, x_3) | \psi_{Li}(x_1, x_2, x_3) \rangle$$

(4)
where $\Psi_{Li}(\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3)$ and $\psi_{Be^+}(\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3)$ are the wave functions of the Li-atom and Be$^+$ ion, respectively. The derivation of the formula, Eq.(3), is based on the facts that: (1) the velocity of the $\beta$-electron is substantially larger than the velocities of atomic electrons, and (2) the final ion does not move during the nuclear $\beta^\pm$-decay. In atomic units we have $\hbar = 1$, $m_e = 1$ and $e = 1$ and, therefore, $w_{if} = |V_{if}|^2$. The notation $\mathbf{x}_i$ in Eq.(4) designates the spin-spatial coordinates of the $i$-th electron, i.e. $\mathbf{x}_i = (\mathbf{r}_i, \mathbf{s}_i)$. Note that in some papers the integral $V_{fi}$, Eq.(4), (or the ratio $V_{fi}\hbar$) is called the probability amplitude. The two wave functions in Eq.(4) depend only upon spatial and spin coordinates of three electrons and do not depend upon the time $t$. All wave functions used in Eq.(4) are assumed to be properly symmetrized in respect to all spin-spatial permutations of identical particles (electrons).

As follows from Eq.(4) the final state probability for $\beta^-$-decay in the $^8\text{Li}$ and $^9\text{Li}$ atoms can be determined, if the wave functions of the incident and final atomic systems (bound states) are known. The construction of highly accurate variational wave functions for three-electron atoms and ions is considered in the fourth Section. The final state probabilities determined using such wave functions can be found in Tables I and II. Here we assume that the incident Li atom was in its ground $^2S(L = 0)$-state ($^2S$-state). It should be mentioned that in reality the incident Li atoms are formed in the $(n; \gamma)$-, $(n; p)$-, and some other nuclear reactions with neutrons of different energies (see above). In such cases it is hard to expect that all incident Li atoms will always be in the ground $^2S(L = 0)$-state. In fact, these $\beta^-$-decaying Li atoms can be found in a variety of the rotationally and/or vibrationally excited states. After reactions with neutrons the incident Li atom before nuclear $\beta^-$-decay will be likely to have non-zero speed in some direction. Therefore, some other (excited) bound states in the Li atom must also be considered as the incident atomic states before the nuclear $\beta^-$-decay.

Numerical computation of the overlap integrals, Eq.(4), is reduced to calculations of some separated integrals, which include different spin components of the incident and final atomic wave functions.

Discussing e.g. the construction of three-electron variational wave function for the Li atom. Without loss of generality, below we restrict ourselves to the consideration of the ground $^2S(L = 0)$-state of the Li atom. As is well known (see, e.g., [4], [7]) the accurate variational wave function of the ground (doublet) $^2S(L = 0)$-state of the Li atom is written
in the following general form

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

(5)

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. Everywhere below in this study, we shall assume that all mentioned wave functions have unit norms. The notation $\alpha$ and $\beta$ in Eq.(5) denote one-electron spin-up and spin-down functions, respectively (see, e.g., [8]). The notations $A$ and $B$ in Eq.(5) mean that the two sets of non-linear parameters associated with the radial functions $\psi$ and $\phi$ can be optimized independently. In general, each of the radial basis functions in Eq.(5) explicitly depends upon all six inter-particle (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 atomic systems, the wave function must be completely antisymmetric with respect to all electron spin-spatial variables. For three-electron wave function this requirement is written in the form $\hat{A}_e \Psi(1, 2, 3) = \hat{A}_{123} \Psi(1, 2, 3) = -\Psi(1, 2, 3)$, where the wave function $\Psi$ is given by Eq.(5) and $\hat{A}_e$ is the electron antisymmetrizer. In our case $\hat{A}_e$ is the three-electron (or three-particle) antisymmetrizer, i.e. $\hat{A}_e = \hat{e} - \hat{P}_{12} - \hat{P}_{13} - \hat{P}_{23} + \hat{P}_{123} + \hat{P}_{132}$. Here $\hat{e}$ is the identity permutation, while $\hat{P}_{ij}$ is the permutation of the $i$-th and $j$-th particles. Analogously, the operator $\hat{P}_{ijk}$ is the permutation of the $i$-th, $j$-th and $k$-th particles.

Suppose that the incident three-electron wave function of the Li atom has been chosen in the form of Eq.(5). Applying the three-electron antisymmetrizer $\hat{A}_{123}$ to the first part of the total wave function, Eq.(5), one finds

$$\hat{A}_{123}[\psi_{L=0}(A; \{ r_{ij} \})(\alpha \beta \alpha - \beta \alpha \alpha)] = (\hat{e}\psi)(\alpha \beta \alpha - \beta \alpha \alpha) + (\hat{P}_{12}\psi)(\alpha \beta \alpha - \beta \alpha \alpha)$$

$$-(\hat{P}_{13}\psi)(\alpha \beta \alpha - \alpha \alpha \beta) - (\hat{P}_{23}\psi)(\alpha \alpha \beta - \beta \alpha \alpha) + (\hat{P}_{123}\psi)(\alpha \alpha \beta - \alpha \beta \alpha)$$

$$+(\hat{P}_{132}\psi)(\beta \alpha \alpha - \alpha \alpha \beta)$$

(6)

$$\hat{A}_{123}[\phi_{L=0}(B; \{ r_{ij} \})(2\alpha \alpha \beta - \beta \alpha \alpha - \alpha \beta \alpha)] = (\hat{e}\phi)(2\alpha \alpha \beta - \beta \alpha \alpha - \alpha \beta \alpha)$$

$$-(\hat{P}_{12}\phi)(2\alpha \alpha \beta - \beta \alpha \alpha - \alpha \beta \alpha) - (\hat{P}_{13}\phi)(2\beta \alpha \alpha - \alpha \alpha \beta - \alpha \beta \alpha)$$

$$-(\hat{P}_{23}\phi)(2\alpha \beta \alpha - \alpha \alpha \beta - \beta \alpha \alpha) + (\hat{P}_{123}\phi)(2\beta \alpha \alpha - \alpha \beta \alpha - \alpha \alpha \beta)$$

$$+(\hat{P}_{132}\phi)(2\alpha \beta \alpha - \alpha \alpha \beta - \beta \alpha \alpha)$$

(7)
then the final state probabilities are determined using the following formulae

\[ i.e. \text{it is written in the form} \]

three-electron Li atom. For instance, if the final wave function has the same spin-symmetry, i.e. it is written in the form

\[ \psi_{fi} = \psi_{fi}(r_1, r_2, r_3)(\alpha\beta\alpha - \beta\alpha\alpha) + \phi_{fi}(r_1, r_2, r_3)(2\alpha\alpha\beta - \beta\alpha\alpha - \alpha\beta\alpha) \quad (8) \]

then the final state probabilities are determined using the following formulae

\[ P_{\psi\psi} = \langle \psi_{fi}(r_1, r_2, r_3) | \frac{1}{2\sqrt{3}} \left(2\hat{e} + 2(P_{12} - P_{13} - P_{23} - P_{123} - P_{132})\right)\psi_{Li}(A; \{r_{ij}\}) \rangle \quad (9) \]

\[ P_{\phi\phi} = \langle \phi_{fi}(r_1, r_2, r_3) | \frac{1}{2} \left(P_{13} - P_{23} + P_{123} - P_{132}\right)\psi_{Li}(A; \{r_{ij}\}) \rangle \quad (10) \]

\[ P_{\psi\phi} = \langle \psi_{fi}(r_1, r_2, r_3) | \frac{1}{2} \left(P_{13} - P_{23} + P_{123} - P_{132}\right)\phi_{Li}(B; \{r_{ij}\}) \rangle \quad (11) \]

\[ P_{\phi\psi} = \langle \phi_{fi}(r_1, r_2, r_3) | \frac{1}{2\sqrt{3}} \left(2\hat{e} + 2P_{12} - P_{13} - P_{23} - P_{123} - P_{132}\right)\phi_{Li}(B; \{r_{ij}\}) \rangle \quad (12) \]

Note they coincide with the known formulae [9] which correspond to the case when both incident and final atomic states contain three-electrons in the doublet spin configuration (the total electron spin equals \( \frac{1}{2} \)). This is the ‘classical’ \( \beta^\pm \)-decay in few-electron atoms, when the incident and final electron configurations have conserved \( L \) and \( S \) quantum numbers.

In reality, another process is also possible in few-electron atoms during the nuclear \( \beta^\pm \)-decay in few- and many-electron atoms. This process leads to the formation of the final ion/atom in some excited states. For instance, consider the case when the three final electrons form the doublet configuration with the spin function \( \alpha\alpha\beta \). It is clear that such a wave function cannot represent the ground state of the Be\(^+\) ion. However, some excited states (with internal electron shell vacancies) can have this spin function, e.g., 1s2s3p-, 1s2s4d- and 1s3s3p-states of the Be\(^+\) ion. Another example is discussed in the next section. It represents an additional electron ionization during the nuclear \( \beta^-\)—decay in three-electron atoms. If this free electron moves away in the \( \beta^-\)spin state, then the final Be\(^2+\) ion can be only in its triplet spin state (not singlet state). Formally this means formation of the final ion in an excited state (with some vacancies on its internal electron shells). In this case the formulae for the final state probabilities become

\[ P_{tr\psi} = \langle \psi_{fi}(r_1, r_2, r_3) | \frac{1}{2\sqrt{3}} \left(P_{13} - P_{23} + P_{123} - P_{132}\right)\psi_{Li}(A; \{r_{ij}\}) \rangle \quad (13) \]
\[ P_{tr\phi} = \langle \psi_{fi}(r_1, r_2, r_3) \left| \frac{1}{2\sqrt{3}} \left( 2\hat{e} - 2\hat{P}_{12} + \hat{P}_{13} + \hat{P}_{23} - \hat{P}_{123} - \hat{P}_{132} \right) \phi_{Li}(B; \{r_{ij}\}) \rangle \]  

where it is assumed that the incident electron wave function was written in the form of Eq. (15). These formulae indicate clearly that the probability of finding the final Be\(^{2+}\) ion in the excited triplet spin states is non-zero. In all earlier studies the transitions to the final atomic states with different spin states were ignored. Moreover, any possibility to form the final few-electron ion/atom in excited states (with some vacancies on internal electron shells) during nuclear \(\beta^\pm\)-decay was rejected. Demonstrating the very existence of such transitions is a great achievement of this study.

In general, during nuclear \(\beta^-\)-decay of the Li atom the final Be\(^+\) ion can be formed in many different bound and/or unbound states. If such a state is unbound, then we deal with the additional ionization during atomic \(\beta^-\)-decay. It is discussed in the next section. This process is of great interest, since it often leads to the formation of the final ion in an excited state(s) with various vacancies in the internal electron shells. For light atoms and ions this means a possibility to observe emission of the optical quanta after the nuclear \(\beta^\pm\)-decay in many-electron atoms with the total number of electrons \(\geq 3\).

### III. ELECTRON IONIZATION DURING THE NUCLEAR \(\beta^-\)-DECAY.

The probability of ionization (or ‘additional’ ionization) of the final Be\(^+\) ion during the nuclear \(\beta\)-decay can also be evaluated using the sudden approximation. In this case the final wave function is constructed as the product of the bound state wave function of the two-electron Be\(^{2+}\) ion and the wave function of the unbound electron which moves in the central Coulomb field of this two-electron ion. To determine the corresponding final state probability one needs to compute the following overlap integral between the wave functions of the incident and final atomic systems

\[ A_{if} = \langle \psi_{Be^+}(x_1, x_2)\phi(x_3) \left| \Psi_{Li}(x_1, x_2, x_3) \rangle \]  

where \(\phi(x_3)\) is the wave function of the unbound electron which moves in the Coulomb field of the Be\(^{2+}\) ion and \(x_i = (r_i, s_i)\) is the set of the four spin-spatial coordinates of the particle \(i\). This function must include the continuous parameter \(k\) which is the electron’s wave number (see below). It should be mentioned that such an ‘additional’ ionization is
unrelated to the interaction between the emitted $\beta^-$ electron and atomic electron. In fact, the additional ionization is a direct consequence of the non-zero component $\simeq \phi(x_3)$ in the incident atomic wave function.

The probability of additional ionization has been determined for a number of $\beta^-$-decaying atoms in a number of earlier studies (see, e.g., [4] and [5]). This work, however, is restricted to the analysis of electron ionization from the internal $K$-shells only. In this case the original problem was reduced to the solution of the model one-electron problem. Analogous reduction for few-electron atomic systems is much more difficult to perform, since all electron-nucleus and electron-electron coordinates are not truly independent. It complicates accurate computation of integrals which contain electron-electron coordinates explicitly. Nevertheless, numerical computations of the final state probabilities can be conducted even with highly accurate wave functions known for many few-electron atoms. In this section we discuss some details of such calculations.

In atomic units the explicit form of the one-electron wave function is $\phi(r) = \phi_{kl}(r)Y_{lm}(n)$, where $\phi_{kl}(r)$ is the one-electron radial function, while $Y_{lm}(n)$ is the corresponding spherical harmonics and $n = \frac{r}{r}$ is the unit vector associated with $r$. In this Section the parameter $k$ is $k = \sqrt{\frac{2meE}{\hbar^2}} = \sqrt{2E}$ (in atomic units). The explicit formula for the radial function $\phi_{kl}(r)$ (in atomic units) is (see, e.g., [5])

$$\phi_{kl}(r) = \frac{C_{kl}}{(2l + 1)!} (2Qkr)^l \cdot \exp(-\nu Qkr) \cdot {}_1F_1\left(\frac{l}{Qk^2}, + l + 1, 2l + 2, 2\nu Qkr\right)$$

where $1F_1(a, b, x)$ is the confluent hypergeometric function (see, e.g., [11]), while $C_{kl}$ is the following constant

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

In these two equations the parameter $Q$ is the electric charge of the remaining double-charged (positive) ion, i.e. $Q = 2$. In reality, this parameter must 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.

Accurate numerical computations of the final state probabilities during the nuclear $\beta^-$-decay in few-electron atoms with additional electron ionization are very difficult to perform, since all highly accurate wave functions of the bound states explicitly include the electron-electron coordinates (see above). As a rule, the better accuracy of the bound state wave function means more complete and accurate involvement of the terms which describe various
electron-electron correlations. On the other hand, the crucial step of the whole procedure is the numerical and/or analytical computation of the Fourier transforms of the one-electron wave function. This corresponds to the free motion of the final electron. During that step, it is better to consider all electrons as particles independent of each other, i.e. ignore all electron-electron correlations. In the general case, this two-fold problem has no simple solution which is accurate and relatively simple for Fourier transform at the same time.

In this study we have developed an approximate procedure which can be used to perform approximate numerical evaluations for the $\beta^-$-decaying isotopes of three-electron atoms. In this approach the trial wave function is constructed as the sum of many terms and each of these terms contains the products of the electron-nucleus functions. None of the three electron-electron coordinates $r_{32}, r_{31}, r_{21}$ is included in such trial wave functions. For the ground state (the doublet $2S(L = 0)$-state) of the Li atom the radial wave function $\psi_{L=0}(A; \{r_{ij}\})$ is chosen in the following form:

$$\psi_{L=0}(r_{14}, r_{24}, r_{34}, 0, 0, 0) = \sum_{k=1}^{N_s} C_k r_{14}^{m_1(k)} r_{24}^{m_2(k)} r_{34}^{m_3(k)} \exp(-\alpha_k r_{14} - \beta_k r_{24} - \gamma_k r_{34})$$

where $C_k$ are the linear (or variational) coefficients, while $m_1(k), m_2(k)$ and $m_3(k)$ are the three integer (non-negative) parameters, which are, in fact, the powers of the three electron-nucleus coordinates $r_{i4} = r_i \ (i = 1, 2, 3)$. Below, we shall assume that the trial wave function Eq.(18) has a unit norm. Furthermore, in all calculations performed for this study only one spin function $\chi_1(\chi_1 = \alpha \beta \alpha - \beta \alpha \alpha)$ is used. It is clear that the wave function Eq.(18) contains only electron-nuclear coordinates and does not include any of the electron-electron coordinates. The real (and non-negative) parameters $\alpha_k, \beta_k, \gamma_k$ are the $3N_s$ varied parameters of the variational expansion, Eq.(18). The wave function, Eq.(18), must be properly symmetrized upon all three electron coordinates. The main question regarding the wave function, Eq.(18), is related to its overall accuracy. If (and only if) it is relatively accurate, then the trial wave function, Eq.(18), can be used in actual computations of the probability amplitudes. For this study we have constructed the 23-term variational wave function shown in Table I of Ref. [10]. This wave function is represented in the form of Eq.(18) and contains no electron-electron coordinates. All sixty nine ($69 = 3 \times 23$) non-linear parameters in this trial wave function have been optimized carefully in a series of
bound state computations performed for the ground $^2S(L = 0)$-state of the Li atom. Finally, the total energy $E$ of the ground $^2S$-state of the $\infty$Li atom obtained with this independent-electron wave function is $-7.448$ 592 766 1 a.u. Note that this energy value, $E$ is close to the exact total energy for the ground state $\infty$Li atom. It indicates the good overall quality of our approximate wave function with 23 terms with no electron-electron coordinates ($r_{12}, r_{13}, r_{23}$). This wave function is used in computations of the final state probabilities (see below) for the nuclear $\beta^-$-decay with additional electron ionization in the three-electron Li atom.

Note also that in atomic physics based on the Hartree-Fock and even hydrogenic approximations the ground state in the Li atom is designated as the $^2S$-state, while in the classification scheme developed in highly accurate computations the same state is often denoted $1^2S$-state. This classification scheme is very convenient to work with truly correlated few-electron wave functions. It is clear that no hydrogenic quantum numbers are good in such cases, and we have to use the more appropriate (and convenient) classification scheme. To avoid conflicts between these two schemes in this study we follow the system of notation used earlier by Larsson [7] who describe this state in the Li atom as the ‘ground $^2S$-state’.

The wave function of the final two-electron Be$^{2+}$ ion arising during nuclear $\beta^-$-decay with the additional ionization can also be approximated by basis functions depending upon the electron-nuclear coordinates only and do not include the electron-electron coordinate $r_{21}$. For the bound $S(L = 0)$-states of the Be$^{2+}$ ion such an expansion takes the form

$$
\psi_{L=0}(r_1, r_2, 0) = \sum_{k=1}^{N_s} C_k r_1^{m_1(k)} r_2^{m_2(k)} \exp(-\alpha_k r_1 - \beta_k r_2)
$$

(19)

The use of the approximate wave functions Eqs. (18) - (19) with no explicit electron-electron coordinate dependence simplify numerical computations of all integrals required for numerical evaluation of the final state probabilities during the nuclear $\beta^-$-decay in the three-electron atoms and ions. The remaining part of the problem is the analytical computation of the integral between the product of the factor $r^m \exp(-\gamma r)$ and radial function from Eq. (16). Such an integral is computed with the use of the formula (see, e.g., Eq.(7.522.9) from [11]):

$$
\int_0^{+\infty} \exp(-\lambda x)x^\nu \cdot \Gamma_1(a, b; cx)dx = \frac{\Gamma(\nu + 1)}{\chi^{\nu+1}} \cdot \Gamma_2(a, \nu + 1; b; \frac{c}{\chi})
$$

(20)

where $\Gamma(x)$ is the usual $\gamma$-function (see, e.g., Section 8.31 in [11]). Our results for numerical computation of the final states probabilities for the nuclear $\beta^-$-decay with additional electron ionization will be published elsewhere.
IV. BOUND STATE WAVE FUNCTIONS OF THE THREE-ELECTRON ATOMS AND IONS

To determine the final state probabilities during the nuclear $\beta^-$-decay (see above), one needs to know the accurate wave functions of the incident and final atoms and ions. In sudden approximation the angular momentum $L$, electron spin $S$ and spatial parity $\pi$ of the atomic wave function $\Psi$ are conserved during nuclear $\beta^-$-decay. Therefore, all approximate wave functions must be constructed as the eigenfunctions of angular momentum $\hat{L}^2$ and total electron spin $\hat{S}^2$. In this study we use the variational wave functions constructed by Hylleraas-Configuration Interaction (Hy-CI). In general, the wave functions in Hylleraast-type expansions rapidly converge to the exact wave functions. The Hylleraas-Configuration Interaction wave function $[12, 13]$ is a linear combination of symmetry adapted configurations $\Phi_p$:

$$\Psi_{\text{Hy-CI}} = \sum_{p=1}^{N} C_p \Phi_p, \quad \Phi_p = \hat{O}(\hat{L}^2) \hat{A} \psi_p \chi \quad (21)$$

where the spatial part of the basis functions are Hartree products of Slater orbitals containing up to one inter-electronic distance $r_{ij}$ per configuration:

$$\psi_p = r_{ij}^\nu \prod_{k=1}^{n} \phi_k(r_k, \theta_k, \phi_k). \quad (22)$$

If $\nu = 1$, then the wave function, Eq.(21), corresponds to Hy-CI. In the case when $\nu = 0$, it is the usual Configuration Interaction (CI) wave function. The higher powers of the electron-electron distances $r_{ij}^\nu$ can effectively be reduced to the $r_{ij}$ term (or $\nu = 1$). Indeed, all higher terms $\nu > 1$ can be expressed as a product of $r_{ij}$, a polynomial of $r_i, r_j$ and some angular functions. Also, in Eq.(21) $N$ is the number of configurations used in computations. The coefficients $C_p$ are determined variationally. The operator $\hat{O}(\hat{L}^2)$ in Eq.(21) projects over the appropriate space, so that every configuration is an eigenfunction of the square of the angular momentum operator $\hat{L}^2$. $\hat{A}$ is the antisymmetrization operator upon all electron spin-spatial coordinates and $\chi$ is the electron-spin eigenfunction. For the lithium atom and three-electron ions one can choose the total spin function in the one-component form, i.e. $\chi = (\alpha \beta - \beta \alpha) \alpha$.

The basis functions $\phi_k$ in this work are the $s$-, $p$-, $d$-, and $f$-Slater orbitals. Since the convergence of Hy-CI wave functions is usually very fast, there is no need to use orbitals
with higher angular momentum. The un-normalized complex Slater orbitals are defined as:

$$\phi(r) = r^{n-1}e^{-\alpha r}Y_m^m(\theta, \varphi).$$  \hspace{1cm} (23)$$

where the parameter $\alpha$ is the adjustable variable (for each orbital) and $Y_m^m(\theta, \varphi)$ are the complex spherical harmonics. The basis sets employed in this work are $n = 4, 5, 6$ and $7$, where the basis $n = 4$ means the orbital set $[1s2s3s4s2p3p4p3d4d4f]$. With all these orbitals from our basis set we have constructed the most important configurations of the $S(L = 0, M = 0)$-, $P(L = 1, M = 0)$-, and $D(L = 2, M = 0)$-symmetries. All details of construction of the symmetry adapted configurations $\Phi_p$ of Eq.(21) can be found in Ref.[14].

The orbital exponents have been optimized for each atomic state of the Li atom and Be$^+$ ion. A set of two exponents was used, one for the $K$-shell and the other for the odd-electron of the $L$-shell. This is constant for all configurations, to accelerate numerical computations. The results obtained are sufficiently accurate for the purposes of our investigation. It is clear that to obtain highly accurate energies one needs to apply more flexibility in the exponents. It was shown in recent calculations on the lithium atom and beryllium ion [6, 15–20]. The virial factor $\chi = -\langle V \rangle / \langle T \rangle$ is used to check the quality of the wave function and guide the numerical optimization of the exponents in the trial wave functions.

As for a given basis set the number of possible configurations would be too large, we have selected the ‘most important’ configurations according to their contribution to the total energy. In our case the selection criteria is an energy contribution $> 1 \times 10^{-8}$ a.u. with respect to the previous configuration. For that, blocks containing all possible Hy-CI configurations of the same type have been filtered and the configurations with less energetic weight have been thrown out. More details can be found in [14]. Note that the length of the wave functions varies then for every state, and the selected configurations are for every state different. As a result, higher excited states must be approximated with the use of the longer trial functions.

For our calculations in this study we have written a three-electron Hy-CI computer program in the Fortran 90 language. The calculations have been done in quadruple precision. The program has been thoroughly checked by comparing results of our numerical calculations with the analogous results obtained earlier by Sims and Hagstrom [18] and King [19] for the lithium atom. Note that in such calculations we observe complete agreement.

Ground and excited S-state energy calculations of Li both the atom and Be$^+$ ion are
shown in Table I, together with their convergence with the basis set used. For Li atom and Be\textsuperscript{+} ion ground states, an accuracy of $1.4 \cdot 10^{-6}$ a.u. has been achieved with the techniques described in this paper. For the first two excited states of both Li atom and Be\textsuperscript{+} ion the accuracy is of about $(4 - 9) \cdot 10^{-6}$ a.u. In the third and higher excited states within a given symmetry of the S-, P- and D-states the accuracy is of order $\pm 1 \cdot 10^{-4}$ a.u.. For the accurate calculation of these higher excited states it would be necessary to introduce different sets of orbital exponents and to increase the orbital basis. However, numerical calculations on higher excited states are rare in the literature.

For numerical calculations of the amplitudes and transition probabilities during nuclear $\beta^-$-decays in three-electron atomic systems we have developed a new computer program which calculates the overlap integrals, Eq.(4), between the wave functions of Li atom and Be\textsuperscript{+} ion. The previous step is the calculation of the wave functions of the different states of the Li and Be\textsuperscript{+} atoms using the Hy-CI method. The algorithms we have employed for the calculation of the kinetic and potential energy integrals can be found in Refs. [21–23]. The energy values obtained for the ground and S-, P- and D-excited states are given in Ref. [14], as are more details on the calculation and the comparison with the best data of the bibliography. Conversely, in the calculation of the overlaps we need only the overlap-integrals between the configurations, and the coefficients of the Hy-CI wave functions. Therefore in this program only integrals of the types $\langle r_{12}^n \rangle$, $\langle r_{12} r_{13} \rangle$ are needed, while the fully-linked three-electron integral $\langle r_{12} r_{13} r_{23} \rangle$ is not needed, when the overlap between the wave functions containing the $r_{ij}$ terms is calculated.

In this work we have improved our earlier method of calculation of the final state probabilities during the nuclear $\beta^-$-decay [1]. Now, we calculate the overlap between the wave functions of different length. This overlap is the sum of the matrix elements of a rectangular overlap matrix. This method of calculation has an advantage, since there are several possible verifications. First, the permutation symmetry of the overlap matrix $\langle \Psi_1 | \Psi_2 \rangle = \langle \Psi_2 | \Psi_1 \rangle$ and its unit-norm condition, i.e. $\langle \Psi_1 | \Psi_1 \rangle = \langle \Psi_2 | \Psi_2 \rangle = 1$.

The convergence of the probability amplitudes and probabilities increases with the improvement of the total energies of the incident and final atomic systems. The final transition probabilities are calculated with an error $\leq 0.001\%$ (they are summarized in Table II). We have obtained the transition probability from the ground $^2S$-state of the Li atom to the ground state of the Be\textsuperscript{+} ion $\approx 57.712\%$. The transition probability for the transition from
the ground $^2S$-state of the Li atom to the first excited $^2S$-state of Be$^+$ ion is $\approx 26.515\%$ and
to the second excited $^2S$-state such a probability is $\approx 0.544\%$ . The sum of probabilities is
then $\approx 85.09\%$ and the ionization probability calculated as 1.0 minus this sum is $\approx 14.91\%$ .
In addition we have computed the transition probabilities from the lower-lying excited states
of S-, P-, and D- symmetry of the Li atom to the states of the same symmetry states in the
Be$^+$ ion. The probability distributions can be found in Tables III, IV and VI, respectively.
It is clear that the sum of the probabilities of transition from on state of the incident atom
to the states of the final one must always be less (or equal) unity. In this work we have
checked this condition everywhere. In general we have found that the highest transition
probability within a group is between an initial state and its one order higher final state
(i.e. $3^2P \rightarrow 4^2P$). This is consequently fulfilled in all groups of probability distributions. For
low lying states, it converges rapidly to zero. In these groups we calculate the probability
of ionization to be around 15\%. For higher transitions, the probability of ionization is not
calculated here because the transitions to higher excited states like $8^2S$, $8^2P$ and $9^2D$ are
expected to be important and these states are not considered here.

V. ON THE DOUBLE $\beta$ DECAY.

The idea of the double nuclear $\beta^\pm$-decay in some nuclei was proposed in 1935 by Maria
Goepert Mayer [24]. In this study we do not discuss either theoretical significance of
the double $\beta^-$-decay for nuclear physics, or its possible applications. Instead, consider the
difference in the final atomic probabilities which can be obtained in the two following cases:
(a) the double nuclear $\beta$-decay, and (b) two consecutive (single) nuclear $\beta^-$-decays. From
atomic point of view we need to compare the time $\tau_{2\beta}$ for which two $\beta^-$-particles leave the
nucleus with the regular atomic time $\tau_e = \frac{\hbar^2}{m_e e Q^2}$, where $Q$ is the electric charge of
the nucleus expressed in $e$, i.e. $Q = Qe$. The condition $\tau_{2\beta} \ll \tau_e$ means sudden emission of the
two fast $\beta^-$ particles. In this case the probability amplitude is determined as the overlap
integral of the incident and final (atomic) wave functions, Eq.(21). If the equation of the
double $\beta^-$ decay is written in the form $X \rightarrow Z^{2+} + \beta^{-}_1 + \beta^{-}_2 + \nu_1 + \nu_2$, then for the final
state probability one finds (in atomic units)

$$ w_{ii} = | \langle \psi_{Z^{2+}}(x_1, x_2, \ldots, x_n) | \Psi_X(x_1, x_2, \ldots, x_n) \rangle |^2 $$

(24)
In the opposite case, i.e., when $\tau_{2\beta} \gg \tau_e$, we deal with the two consecutive nuclear $\beta^-$ decays. In this case we need to use the sudden approximation twice. The corresponding equations are $X \rightarrow Y^+ + \beta^- + \nu_1$ and $Y^+ \rightarrow Z^{2+} + \beta^- + \nu_2$. The amplitude of the final state probability takes the form

$$A_{if} = \langle \Psi_X(x_1, x_2, \ldots, x_n) \mid \psi_{Y^+}(x_1, x_2, \ldots, x_n) \rangle \langle \Psi_{Y^+}(x_1, x_2, \ldots, x_n) \mid \psi_{Z^{2+}}(x_1, x_2, \ldots, x_n) \rangle$$

and the final state probability is $w_{fi} = |A_{fi}|^2$. The sum over all states of the $Y^+$ ion will lead us back to Eq.\((24)\). However, if $\tau_{2\beta} \gg \tau_e$, then the final state of the $Y^+$ ion is uniformly defined and Eq.\((25)\) can be used in this case only for this unique state of the $Y^+$ ion. The sum over all ‘intermediate’ states of the $Y^+$ ion is reduced to the one term only. From here one easily finds that

$$w_{if}(X \rightarrow Z^{2+}) \geq w_{fi}(X \rightarrow Y^+)w_{if}(Y^+ \rightarrow Z^{2+})$$

(26)

Based on these formulas one can expect to observe substantial differences in the final state (atomic) probabilities of the double $\beta^-$ decay and two consecutive $\beta^-$ decays. Such differences can be found for the ground-ground and ground-excited transition amplitudes in the case of bound state transitions. The corresponding ionization probabilities can also be very different for any atom in which the central nucleus decays with the use of the double $\beta^-$ decay, or by the two consecutive $\beta^-$ decays. In an ideal case, we can observe and measure such differences in ‘traditional’ atoms with the double beta-decaying nuclei, e.g., in the $^{76}$Ge, $^{128}$Te, $^{138}$Xe and $^{238}$U atoms.

In general, the study of the double nuclear $\beta^-$-decay in atoms and molecules can be used as a natural and powerful tool to study electron-nucleus and electron-electron correlations at the femto- and attosecond time-scale. Unfortunately, at this moment no experimental group in the World performs similar research even for atoms and ions.

VI. CONCLUSION

We have considered the nuclear $\beta^-$-decays in the three-electron $^8$Li and $^9$Li atoms. The final state probabilities to form different bound states in the Be$^+$ ion have been determined to very good accuracy which is better than analogous accuracy obtained in our earlier study [1]. The Hylleraas-CI wave functions constructed for atoms/ions involved in the $\beta^-$-decay
are substantially more accurate than wave functions used in earlier studies. They provide a better description of the electron density near of the nucleus. For the first time, the wave functions of the excited states are determined to the same numerical accuracy as the wave functions of the ground states. We can determine the final state probabilities to very high accuracy using them.

We also discuss a possible observation of double nuclear $\beta^-$-decay and nuclear $\beta^-$-decay with the additional electron ionization. It is shown that the Be$^{2+}$ ion formed during the last process can be detected not only in the singlet bound states, but also in the triplet bound states. It was never observed/predicted in earlier studies. It may lead to the fundamental re-structuring of the internal electron shells of the incident atom during $\beta^-$-decay. We also derive some useful formulae which will be used in future studies to determine the probabilities of electron ionization (in different channels) during the nuclear $\beta^-$-decay.

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TABLE I: Convergency of the $\beta^-$-decay transition amplitudes, final-state probabilities and total energies for the ground state of Li atom and different $n^2S$ states of Be$^+$ ion. Energy in a.u., energy differences in $\mu$eV.

| State | Basis | $N^b$ | Amplitude | Probability | Virial | Energy | $N_{\text{Ref}}$ | Ref. Ener. | Ref. Diff. |
|-------|-------|-------|------------|-------------|--------|--------|----------------|------------|------------|
| Li $2^2S$ | n=4 | 308 | 2.000 004 | -7.478 053 222 | 7.1 |
| Li $2^2S$ | n=5 | 517 | 2.000 001 | -7.478 057 825 | 2.5 |
| Li $2^2S$ | n=6 | 620 | 2.000 000 | -7.478 058 892 | 1.4 |
| Be$^+$ $2^2S$ | n=4 | 308 | 0.759 681 281 | 0.577 116 | 2.000 002 | -14.324 757 377 | 15 |
| Be$^+$ $2^2S$ | n=5 | 612 | 0.759 686 424 | 0.577 123 | 2.000 001 | -14.324 760 412 | 14 |
| Be$^+$ $2^2S$ | n=6 | 637 | 0.759 683 487 | 0.577 119 | 2.000 000 | -14.324 761 723 | 14 |
| Be$^+$ $3^2S$ | n=4 | 307 | 0.514 947 878 | 0.265 171 | 2.000 000 | -13.922 759 980 | 16 |
| Be$^+$ $3^2S$ | n=5 | 459 | 0.514 892 996 | 0.265 115 | 2.000 009 | -13.922 781 623 | 14 |
| Be$^+$ $3^2S$ | n=6 | 637 | 0.514 929 058 | 0.265 152 | 2.000 005 | -13.922 784 968 | 14 |
| Be$^+$ $4^2S$ | n=4 | 252 | 0.075 214 427 | 0.005 657 | 2.001 593 | -13.798 520 453 | 14 |
| Be$^+$ $4^2S$ | n=5 | 372 | 0.074 214 825 | 0.005 508 | 2.000 484 | -13.798 704 722 | 14 |
| Be$^+$ $4^2S$ | n=6 | 451 | 0.073 790 160 | 0.005 445 | 2.000 154 | -13.798 706 849 | 14 |
| Be$^+$ $5^2S$ | n=5 | 502 | 0.039 839 395 | 0.001 587 | 2.004 399 | -13.744 513 336 | 14 |
| Be$^+$ $5^2S$ | n=6 | 698 | 0.043 113 179 | 0.001 859 | 2.001 584 | -13.744 589 135 | 14 |
| Be$^+$ $6^2S$ | n=6 | 618 | 0.029 411 301 | 0.000 865 | 2.003 166 | -13.716 286 24 | 14 |

*aBasis set, i.e. $n = 4$ stays for [4s3p2d1f] or [1s2s3s4s2p3p4p3d4d4f].

*bN is the number of Hy-CI symmetry adapted configurations. $N_{\text{Ref}}$ is the number of configurations employed in the calculation of the Ref. Ener.
TABLE II: Transition probabilities for the nuclear $\beta^-$-decay from the ground $2^2S$-state of the Li atom into the ground and various excited $S$–states of the Be$^+$ ion. The probability of ionization from Be$^+$ ion to Be$^{2+}$ ion is calculated as $P_{\text{ion}} = 1 - \sum_{i=1}^{\infty} P_i$.

| State of Be$^+$ | Amplitude        | Probability ($P_i$) | $P_i$ in % |
|-----------------|------------------|---------------------|------------|
| $2^2S$          | 0.759 683 487    | 0.577 119           | 57.71      |
| $3^2S$          | 0.514 929 058    | 0.265 152           | 26.52      |
| $4^2S$          | 0.073 790 160    | 0.005 445           | 0.54       |
| $5^2S$          | 0.043 113 179    | 0.001 859           | 0.19       |
| $6^2S$          | 0.029 411 301    | 0.000 865           | 0.09       |
| $7^2S$          | 0.021 688 396    | 0.000 470           | 0.05       |
| Total           | 0.850 910        | 85.09               |            |
| $P_{\text{ion}}$ |                  | 0.149 090           | 14.91      |
TABLE III: Transition probabilities for the nuclear $\beta^-$ decay from the excited $3^2S$, $4^2S$, $5^2S$, $6^2S$, and $7^2S$-states of the Li atom\(^a\) into the ground and various excited states of the Be\(^+\) ion.

| States Li $\to$ Be\(^+\) | Amplitude | Probability $P_i$ in % |
|---------------------------|-----------|------------------------|
| $3^2S \to 2^2S$           | 0.239 962 786 | 0.057 582 5.76         |
| $3^2S \to 3^2S$           | 0.466 529 800 | 0.217 650 21.76        |
| $3^2S \to 4^2S$           | 0.757 456 066 | 0.573 740 57.37        |
| $3^2S \to 5^2S$           | 0.055 586 071 | 0.003 090 0.31         |
| $3^2S \to 6^2S$           | 0.012 740 357 | 0.000 162 0.02         |
| $3^2S \to 7^2S$           | 0.013 723 711 | 0.000 188 0.02         |
| **Total**                 | 0.852 412    | 85.24                  |
| $P_{\text{ion}}$          | 0.147 588    | 14.76                  |
| $4^2S \to 2^2S$           | 0.132 669 559 | 0.017 601 1.76         |
| $4^2S \to 3^2S$           | 0.236 587 524 | 0.055 974 5.60         |
| $4^2S \to 4^2S$           | 0.122 373 066 | 0.014 975 1.50         |
| $4^2S \to 5^2S$           | 0.828 124 464 | 0.685 790 68.58        |
| $4^2S \to 6^2S$           | 0.277 774 076 | 0.077 158 7.72         |
| $4^2S \to 7^2S$           | 0.007 347 388 | 0.000 054 0.01         |
| **Total**                 | 0.851 552    | 85.16                  |
| $P_{\text{ion}}$          | 0.148 447    | 14.84                  |
| $5^2S \to 2^2S$           | 0.087 318 854 | 0.007 625 0.76         |
| $5^2S \to 3^2S$           | 0.148 984 137 | 0.022 196 2.22         |
| $5^2S \to 4^2S$           | 0.109 684 232 | 0.012 031 1.20         |
| $5^2S \to 5^2S$           | 0.175 864 858 | 0.030 928 3.09         |
| $5^2S \to 6^2S$           | 0.698 154 162 | 0.487 419 48.74        |
| $5^2S \to 7^2S$           | 0.503 067 106 | 0.253 076 25.31        |
| **Total**                 | 0.813 276    | 81.33                  |
| $P_{\text{ion}}$          | 0.186 724    | 18.67                  |
| $6^2S \to 2^2S$           | 0.063 750 613 | 0.004 064 0.41         |
| $6^2S \to 3^2S$           | 0.104 007 178 | 0.010 817 1.08         |
| $6^2S \to 4^2S$           | 0.079 072 301 | 0.006 252 0.63         |
| $6^2S \to 5^2S$           | 0.071 415 619 | 0.005 100 0.51         |
| $6^2S \to 6^2S$           | 0.350 972 033 | 0.123 181 12.32        |
| $6^2S \to 7^2S$           | 0.430 715 551 | 0.185 516 18.55        |

\(^a\)The calculated total energy of the first excited S-state of lithium atom is -7.354 093 706 a.u. (3$^2S$-state), while the total energies of the second and higher excited states are -7.318 517 759 a.u. (4$^2S$-state), -7.303 458 818 a.u. (5$^2S$-state) and -7.295 734 702 a.u. (6$^2S$-state), respectively.

\(^b\)The total energies of the same S−states in the Be\(^+\) can be found in Table I.
TABLE IV: Transition probabilities between states of P-symmetry for the nuclear $\beta^-$-decay of the Li$^a$ atom to the Be$^+$ ion$^b$.

| States Li $\rightarrow$ Be$^+$ | Amplitude | Probability $P_i$ in % |
|-----------------------------|-----------|------------------------|
| $2^2P \rightarrow 2^2P$     | 0.697 549 959 | 0.486 576 48.66       |
| $2^2P \rightarrow 3^2P$     | 0.603 885 572 | 0.364 678 36.47       |
| $2^2P \rightarrow 4^2P$     | 0.003 979 607 | 0.000 016 0.00          |
| $2^2P \rightarrow 5^2P$     | 0.020 232 690 | 0.000 040 0.04          |
| $2^2P \rightarrow 6^2P$     | 0.013 143 263 | 0.000 173 0.02          |
| $2^2P \rightarrow 7^2P$     | 0.013 285 358 | 0.000 176 0.02          |
| Total                       | 0.852 028     | 85.20                   |
| $P_{tot}$                   | 0.147 972     | 14.80                   |
| $3^2P \rightarrow 2^2P$     | 0.307 008 160 | 0.076 125 7.61          |
| $3^2P \rightarrow 3^2P$     | 0.319 479 925 | 0.102 067 10.21         |
| $3^2P \rightarrow 4^2P$     | 0.604 261 129 | 0.642 019 64.20         |
| $3^2P \rightarrow 5^2P$     | 0.166 010 974 | 0.027 560 2.76          |
| $3^2P \rightarrow 6^2P$     | 0.004 047 607 | 0.000 016 0.00          |
| $3^2P \rightarrow 7^2P$     | 0.004 025 567 | 0.000 016 0.00          |
| Total                       | 0.847 804     | 84.78                   |
| $P_{tot}$                   | 0.152 196     | 15.22                   |
| $4^2P \rightarrow 2^2P$     | 0.161 045 822 | 0.025 906 2.59          |
| $4^2P \rightarrow 3^2P$     | 0.195 960 248 | 0.038 400 3.84          |
| $4^2P \rightarrow 4^2P$     | 0.046 100 299 | 0.002 125 0.21          |
| $4^2P \rightarrow 5^2P$     | 0.724 469 360 | 0.524 856 52.49         |
| $4^2P \rightarrow 6^2P$     | 0.425 779 325 | 0.181 288 18.13         |
| $4^2P \rightarrow 7^2P$     | 0.425 325 535 | 0.180 902 18.09         |
| Total                       | 0.953 507     | 95.35                   |
| $P_{tot}$                   | 0.046 493     | 4.65                     |
| $5^2P \rightarrow 2^2P$     | 0.113 441 928 | 0.012 869 1.29          |
| $5^2P \rightarrow 3^2P$     | 0.135 765 197 | 0.018 432 1.84          |
| $5^2P \rightarrow 4^2P$     | 0.017 086 489 | 0.000 292 0.03          |
| $5^2P \rightarrow 5^2P$     | 0.328 135 053 | 0.107 673 10.77         |
| $5^2P \rightarrow 6^2P$     | 0.547 505 865 | 0.299 763 29.98         |
| $5^2P \rightarrow 7^2P$     | 0.550 438 371 | 0.302 982 30.30         |
| Total                       | 0.550 438 371 | 0.302 982 30.30         |
| $6^2P \rightarrow 2^2P$     | 0.081 224 665 | 0.006 597 0.66          |
| $6^2P \rightarrow 3^2P$     | 0.099 158 755 | 0.009 832 0.98          |
| $6^2P \rightarrow 4^2P$     | 0.029 284 955 | 0.000 858 0.09          |
| $6^2P \rightarrow 5^2P$     | 0.177 208 892 | 0.031 403 3.14          |
| $6^2P \rightarrow 6^2P$     | 0.353 201 418 | 0.124 751 12.48         |
| $6^2P \rightarrow 7^2P$     | 0.348 353 090 | 0.121 350 12.13         |

$^a$The total energies of the incident P-states of Li atom are: -7.410 149 067 a.u. (2$^2P$–state), -7.337 050 609 a.u.(3$^2P$–state), -7.311 770 213 a.u.(4$^2P$–state), -7.299 899 542 a.u. (5$^2P$–state) and -7.293 494 640 a.u. (6$^2P$–state), respectively.

$^b$The total energies of the same (final) P–states of the Be$^+$ ion are: -14.179 326 074 a.u., -13.885 034 739 a.u., -13.783 519 845 a.u., -13.733 901 878 a.u., -12.811 935 225 a.u. and -13.711 378 665 a.u., respectively.
TABLE V: Transition probabilities between states of D-symmetry for the nuclear $\beta^{-}$-decay of the Li atom$^a$ to the Be$^+$ ion$^b$.

| States Li → Be$^+$ | Amplitude | Probability $P_i$ in % |
|-------------------|-----------|------------------------|
| $3^2D \rightarrow 3^2D$ | 0.613 879 768 | 0.376 848 37.68 |
| $3^2D \rightarrow 4^2D$ | 0.675 444 736 | 0.456 226 45.62 |
| $3^2D \rightarrow 5^2D$ | 0.124 573 183 | 0.015 518 1.55 |
| $3^2D \rightarrow 6^2D$ | 0.005 331 066 | 0.000 028 0.00 |
| $3^2D \rightarrow 7^2D$ | 0.008 233 705 | 0.000 068 0.01 |
| $3^2D \rightarrow 8^2D$ | 0.004 516 156 | 0.000 020 0.00 |
| **Total** | **0.848 709** | **84.87** |
| $P_{ion}$ | 0.151 291 | 15.13 |
| $4^2D \rightarrow 3^2D$ | 0.297 395 858 | 0.088 444 8.84 |
| $4^2D \rightarrow 4^2D$ | 0.092 613 446 | 0.008 577 0.86 |
| $4^2D \rightarrow 5^2D$ | 0.645 316 813 | 0.416 434 41.64 |
| $4^2D \rightarrow 6^2D$ | 0.314 342 441 | 0.098 811 9.88 |
| $4^2D \rightarrow 7^2D$ | 0.002 237 872 | 0.000 005 0.00 |
| $4^2D \rightarrow 8^2D$ | 0.000 807 365 | 0.000 001 0.00 |
| **Total** | **0.612 272** | **61.23** |
| $P_{ion}$ | 0.387 728 | 38.77 |
| $5^2D \rightarrow 3^2D$ | 0.221 060 550 | 0.048 868 4.89 |
| $5^2D \rightarrow 4^2D$ | 0.131 551 368 | 0.017 306 1.73 |
| $5^2D \rightarrow 5^2D$ | 0.303 521 357 | 0.092 125 9.21 |
| $5^2D \rightarrow 6^2D$ | 0.662 141 399 | 0.438 431 43.84 |
| $5^2D \rightarrow 7^2D$ | 0.408 116 762 | 0.166 559 16.66 |
| $5^2D \rightarrow 8^2D$ | 0.051 512 344 | 0.002 653 0.26 |
| **Total** | **0.765 943** | **76.59** |
| $P_{ion}$ | 0.234 057 | 23.41 |
| $6^2D \rightarrow 3^2D$ | 0.219 012 937 | 0.047 966 4.80 |
| $6^2D \rightarrow 4^2D$ | 0.109 576 684 | 0.012 007 1.20 |
| $6^2D \rightarrow 5^2D$ | 0.275 765 182 | 0.076 046 7.60 |
| $6^2D \rightarrow 6^2D$ | 0.172 623 479 | 0.029 799 2.98 |
| $6^2D \rightarrow 7^2D$ | 0.238 431 045 | 0.056 849 5.68 |
| $6^2D \rightarrow 8^2D$ | 0.469 886 268 | 0.220 793 22.08 |
| **Total** | **1.075 638** | **107.56** |
| $P_{ion}$ | 0.094 570 | 9.45 |
| $7^2D \rightarrow 3^2D$ | 0.250 505 561 | 0.062 753 6.28 |
| $7^2D \rightarrow 4^2D$ | 0.224 414 920 | 0.050 362 5.04 |
| $7^2D \rightarrow 5^2D$ | 0.113 445 739 | 0.012 870 1.29 |
| $7^2D \rightarrow 6^2D$ | 0.227 483 595 | 0.051 749 5.17 |
| $7^2D \rightarrow 7^2D$ | 0.476 006 811 | 0.226 582 22.66 |
| $7^2D \rightarrow 8^2D$ | 0.429 479 022 | 0.184 452 18.45 |

$^a$The total energies of the incident D-states of Li atoms are: -7.335 511 694 a.u. ($3^2D$-state), -7.311 211 047 a.u. ($4^2D$-state), -7.298 835 884 a.u. ($5^2D$-state), -7.288 077 393 a.u. ($6^2D$-state) and -7.268 731 551 a.u. ($7^2D$-state).

$^b$The total energies of the same (final) states of the Be$^+$ ion are: -13.878 004 697 a.u., -13.778 986 828 a.u., -13.733 832 498 a.u., -13.705 903 173 a.u., -13.677 409 085 a.u. and -13.660 271 947 a.u.