Properties of the negatively charged lithium ions and evaluation of the half-life of the $^7$Be atom(s)

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Abstract

Bound state properties of the ground $^1S$−state in the four-electron lithium ion Li$^-$ (or $^7$Li$^-$ ion) are determined from the results of accurate, variational computations. We also determine such properties for the ground $^1S$−state(s) in the $^6$Li$^-$ and $^7$Li$^-$ ions with the finite nuclear masses. Another closely related problem discussed in this study is accurate numerical evaluation of the half-life of the beryllium-7 isotope.

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I. INTRODUCTION

In this communication we consider the bound states properties of the negatively charged Li$^-$ ion in its ground $2^1S(L=0)$–state, or $2^1S$–state, for short. It is well known that such an ion has only one bound state which is the ground $2^1S$–state. The electronic structure of this state in the Li$^-$ ion is $1s^22s^2$. Recently, the negatively charged lithium ion Li$^-$ is of great interest for applications, since, e.g., formation of these ions is an important step for workability of the compact lithium and/or lithium-ion electric batteries. Both lithium and lithium-ion batteries are very compact, relatively cheap and reliable sources of constant electric current which are widely used in our everyday life. However, it appears that the Li$^-$ ion is not a well studied atomic system. Indeed, many bound state properties of this ion were not evaluated et al, or known only approximately. Moreover, almost all known properties have been evaluated for an isolated Li$^-$ ion in vacuum. In reality, it is crucial to evaluate the bound state properties in the presence of different organic acids which are extensively used in lithium-ion batteries.

Our goal in this study is to determine various bound state properties of the four-electron (or five-body) Li$^-$ ion. It should be mentioned that most of these properties have never been evaluated in earlier studies. In the lowest-order approximation upon the fine structure constant \( \alpha (= e^2/\hbar c) \) the negatively charged Li$^-$ ion is described by the non-relativistic Schrödinger equation \( H \Psi = E \Psi \), where \( H \) is the non-relativistic Hamiltonian and \( E (< 0) \) is the eigenvalue. Without loss of generality we shall assume that the bound state wave function \( \Psi \) has the unit norm. The non-relativistic Hamiltonian \( H \) of an arbitrary four-electron atom/ion takes the form (see, e.g., \([1]\))

\[
H = -\frac{\hbar^2}{2m_e} \left[ \nabla_1^2 + \nabla_2^2 + \nabla_3^2 + \nabla_4^2 + \frac{m_e}{M} \nabla_1^2 \right] - Qe^2 \sum_{i=1}^{4} \frac{1}{r_{15}} + e^2 \sum_{i=1}^{3} \sum_{j=2(i>j)}^{4} \frac{1}{r_{ij}},
\]

where \( \hbar = \frac{\hbar}{2\pi} \) is the reduced Planck constant, \( m_e \) is the electron mass and \( e \) is the electric charge of an electron. In this equation and everywhere below in this study the subscripts 1, 2, 3, 4 designate the four atomic electrons \( e^- \), while the subscript 5 (\( = N \)) denotes the heavy atomic nucleus with the mass \( M \) (\( M \gg m_e \)) and positive electric (nuclear) charge \( Qe \) (central particle). The notation \( r_{ij} = |r_i - r_j| = r_{ji} \) in Eq. (1) and everywhere below stand for the interparticle distances between particles \( i \) and \( j \). These distances are also called the relative coordinates to emphasize their differences with three-dimensional coordinates.
$\mathbf{r}_i$, which are the Cartesian coordinates of the particle $i$. In Eq. (1) and everywhere below in this work for four-electron atomic systems we shall assume that $(ij) = (ji) = (12), (13), (14), (15), (23), (24), (25), (34), (35)$ and $(45)$. For three-electron atomic systems we have $(ij) = (ji) = (12), (13), (14), (23), (24)$ and $(34)$. Below only atomic units $\hbar = 1, |e| = 1, m_e = 1$ are employed. In these units the explicit form of the Hamiltonian $H$, Eq. (1), is simplified and takes the form

$$H = -\frac{1}{2}[\nabla_1^2 + \nabla_2^2 + \nabla_3^2 + \nabla_4^2 + \frac{m_e}{M}\nabla_4^2] - Q \sum_{i=1}^{4} \frac{1}{r_{i5}} + \sum_{i=1}^{3} \sum_{j=2 \,(j>i)}^{4} \frac{1}{r_{ij}},$$

where $Q$ is the nuclear charge of the central positively charged nucleus. For the neutral Li-atom and Li$^-$ ion we have $Q = 3$. Note also that in this study the notations Li and Li$^-$ stand for the lithium atom and ion with the infinitely heavy nucleus, while analogous notations with the superscript 6 (and/or 7) mean the $^6$Li ($^7$Li) atom and $^6$Li$^-$ ($^7$Li$^-$) ion, respectively. The nuclear mass of the lithium-6 nucleus used in this study is $M(^6\text{Li}) = 10961.8968 m_e$, while the nuclear mass of the lithium-7 nucleus is $M(^7\text{Li}) = 12786.3927 m_e$.

As mentioned above the bound state spectrum of the negatively charged Li$^-$ ion includes only one bound $2^1S$ state, which is the ground state. The stability of this state means stability against its dissociation (or ionization) Li$^- = \text{Li}(2^2S) + e^-$, where the notation Li$(2^2S)$ means the lithium atom in its ground (doublet) $2^2S$ state. Stability of this state in the Li$^-$ ion is known since the first accurate calculations performed the middle of 1970’s. Note that all methods based on the Hartree-Fock approximation cannot produce any bound state in the Li$^-$ ion. Furthermore, it is clear that to determine this bound state in the Li$^-$ ion such variational expansions must be truly correlated and relatively accurate. Our method discussed in the next Section allows one to construct accurate and highly accurate wave functions for arbitrary few-body systems. This includes few-electron atomic systems, e.g., the Li$^-$ ion, Be atom and Li atom. By using this method we determine a large number of bound state properties of the four-electron Li$^-$ ion(s). The same method is applied to obtain highly accurate wave function(s) of the ground $2^2S$ state in the three-electron Li atom(s).

It is very interesting to compare the bound state properties of the ground $2^1S$ state in the Li$^-$ ion and the ground $2^2S$ state in the neutral Li atom. Another unsolved problem known for four-electron atomic systems is to explain experimental variations of the half-life of the $^7$Be isotope in different chemical backgrounds. This actual problem can be solved by using exactly the same method which we applied for the Li$^-$ ion. This problem is considered in
the third Section. Conclusive remarks can be found in the last Section.

II. VARIATIONAL WAVE FUNCTIONS

To determine accurate solutions of the non-relativistic Schrödinger equation $H \Psi = E \Psi$ in this study we approximate the unknown wave function(s) by the variational expansion in multi-dimensional gaussoids. Each of these gaussoids explicitly depends upon ten relative coordinates $r_{ij}$. For the singlet $^1S(L = 0)$–states in four-electron atomic systems this expansion takes the form $^{1}$, $^{2}$:

$$\psi(L = 0; S = 0) = \sum_{i=1}^{N_A} C_i \exp\left(-\alpha_{ij} r_{ij}^2\right) \chi_{S=0}^{(1)} + \sum_{i=1}^{N_B} G_i \exp\left(-\beta_{ij} r_{ij}^2\right) \chi_{S=0}^{(2)}$$

(3)

where $C_i$ (and $G_i$) are the linear variational coefficients of the trial wave function, while $\alpha_{ij}$ are the ten non-linear parameters and $(ij) = (12), (13), \ldots, (45)$. Analogously, the notation $\beta_{ij}$ stands for other ten non-linear parameters which must also be varied (independently of $\alpha_{ij}$) in calculations. Notations $\chi_{S=0}^{(1)}$ and $\chi_{S=0}^{(2)}$ in Eq.(3) designate the two independent spin functions which can be considered for the singlet $2^1S$–state, or $(2^1S \mid 1s^22s^2)$–electron configuration. The explicit forms of these two spin functions are:

$$\chi_{S=0}^{(1)} = \alpha\beta\alpha\beta + \beta\alpha\beta\alpha - \beta\alpha\beta\alpha - \alpha\beta\beta\alpha$$

(4)

$$\chi_{S=0}^{(2)} = 2\alpha\alpha\beta\beta + 2\beta\beta\alpha\alpha - \beta\alpha\beta\alpha - \alpha\beta\beta\alpha - \beta\alpha\beta\alpha - \alpha\beta\alpha\beta$$

(5)

In numerical calculations of the total energies and other spin-independent properties (i.e. expectation values) one can always use just one spin function, e.g., $\chi_{S=0}^{(1)}$ from Eq.(4). It follows from the fact that the Hamiltonian Eq.(2) does not depend explicitly upon the electron spin and/or any of its components.

The radial basis functions in Eq.(3) are the multi-dimensional gaussoids, or five-dimensional gaussoids (see, Eq.(3) above). These basis functions are not orthogonal to each other. Therefore, the original Schrödinger equation $H \Psi = E \Psi$ is reduced to the solution of the following eigenvalue problem $\hat{H} \hat{C} = E \hat{S} \hat{C}$, where $\hat{H}$ and $\hat{S}$ are the matrixes of the Hamiltonian and overlap, respectively, while $E$ is the unknown eigenvalue and $\hat{C}$ is the vector formed from the linear variational coefficients $C_i$ mentioned in Eq.(3). It is straightforward to derive analogous equations in these cases when the corresponding vector also includes non-zero $G$-components (see Eq.(3)). In fact, the linear coefficients $C_i$ and
$G_i$ from Eq. (3) can be considered as components of the $N_A-$ and $N_B-$dimensional vectors $\mathbf{C}$ and $\mathbf{G}$, respectively. Now, it is clear that we need to obtain the explicit formulas for all matrix elements of the Hamiltonian and overlap matrix. In fact, all these formulas for four- and three-electron atomic systems have been derived and presented in a number of our papers (see, e.g., [6]). Therefore, below we can present only a very brief description of this method.

First, we construct the wave functions of the correct permutation symmetry by applying the complete anti-symmetrizer $A_{1234}$ to the trial wave function represented in the form of Eq. (3). Analytical expression for $A_{1234}\psi(L = 0; S)$ is represented as a finite sum of different spatial and spin terms. The arguments in the spin and spatial functions are interchanged. At the second step of the procedure we need to calculate (analytically) the overlap integrals between all components of the spin functions with the original and interchanged arguments. After computations of these integrals we obtain the final expression for the matrix elements of the Hamiltonian $\hat{H}$ and overlap $\hat{S}$ matrixes. In reality, all matrix elements of $\hat{H}$ and $\hat{S}$ contain finite sums of the radial matrix elements with some numerical (integer) coefficients which are determined by the overlap integrals of the spin functions (for more details, see [6]).

The procedure used to solve three-electron atomic problems (bound states) is completely analogous and here we do not want to repeat its description (see, e.g., [6]). Note also that below we apply three-electron version of our procedure to determine the bound state properties of the ground $2^2S-$state in the neutral Li-atom.

As mentioned above in this paper we consider the ground $2^1S-$state of the Li$^-$ ion (or $\infty$Li$^-$ ion). Our goal is to determine the total energy of this state and expectation values of some of its properties. Such properties include a few powers of interparticle distances $\langle r_{ij}^n \rangle$, where $n = -2, -1, 2, 3, 4$ (for $n = 0$ each of these expectation values equals unity), electron-nucleus and electron-electron delta-functions, single electron kinetic energy $\langle \frac{1}{2}p_e^2 \rangle$, electron-nucleus and electron-electron kinetic correlations $\langle p_e \cdot p_N \rangle$ and $\langle p_e \cdot p_e \rangle$ and a few others (see also discussion in the Appendix). Numerical values of these expectation values can be found in Table I. Table I contains analogous properties for the $^6$Li$^-$ and $^7$Li$^-$ ions which also have only one stable $2^1S-$state. In addition to these ions Table I includes the bound state properties of the ground $2^2S-$state in the neutral Li atom, which is a three-electron atomic system. All these properties are expressed in atomic units. The expectation values of the ground $2^2S-$state of the three-electron Li atom (or $\infty$Li atom) are of interest to
make a direct comparison with the analogous properties of the four-electron Li\(^-\) ion (or \(\infty\)Li ion). It should be mentioned that our method allows one to determine the total energies of the bound states in the four- and three-electron atomic systems to relatively high accuracy. For the Li\(^-\) ion our energy is one of the best total energies ever computed for this ion. In fact, the total energy of the ground state in the Li atom (or \(\infty\)Li atom) is surprisingly accurate and compared with the accuracy known for this atom from Hy-CI calculations with 1000 - 2000 terms in the wave function. The total energies of the \(2^2S\) state in the Li atom determined with \(N = N_A = 700\) and \(N = N_A = 1000\) in Eq.\((3)\) are \(E = 7.4780598540\) a.u. and \(E = 7.4780599631\) a.u., respectively. These values are very close to the ‘exact’ total energy known for this atom, obtained with the use of many thousands of Hylleraas (Hy) and Hylleraas-CI wave functions. Note that our energies for the ground states in both Li\(^-\) ion and Li atom are still converging and we hope to report soon the new total energies which have better overall accuracy.

Let us compare the bound state properties of the Li\(^-\) ion in the ground \(2^1S\) state with the analogous properties of the neutral Li atom in its ground \(2^2S\) state. First, we note a very substantial difference in the electron-nucleus and electron-electron distances \(\langle r_{eN}\rangle\) and \(\langle r_{ee}\rangle\). For the Li\(^-\) ion these distances are substantially larger than for the neutral Li atom. The same statement is correct for all positive powers of these inter-particle distances, i.e. for the \(\langle r_{eN}^k\rangle\) and \(\langle r_{ee}^k\rangle\) (where \(k\) is integer and \(k \geq 2\)) expectation values shown in Table I. This is an indication of the known fact that the Li\(^-\) ion is a weakly-bound, four-electron system atomic system. This fact can be confirmed by calculation of the following dimensionless ratio

\[
\epsilon = \frac{E(\text{Li}^-) - E(\text{Li})}{E(\text{Li}^-)} \approx 0.00301 \tag{6}
\]

where \(E(\text{Li}^-)\) and \(E(\text{Li})\) are the total energies of the negatively charged Li\(^-\) ion in the ground \(2^1S\) state and Li atom in the ground \(2^2S\) state. Very small value of this parameter \(\epsilon\), which is significantly less that 0.01 (or 1 %), is a strong and uniform indication that the Li\(^-\) ion is an extremely weakly-bound atomic system. This allows one to represent the internal structure of the bound state in the Li\(^-\) ion as a motion of one electron in the ‘central’ field created by the infinitely heavy Li atom. In other words, the electronic structure of this ion is \(1s^22s^2\) and one of the two outer-most electrons moves at very large distances from the central nucleus. In reality, this representation is only approximate, since, e.g., there is an exchange symmetry between two electrons form the \(2s^2\) shell. Nevertheless, such a ‘cluster’
structure can be useful to predict and explain a large number of bound state properties of the Li$^-$ ion. For instance, consider the expectation value of the inverse electron-nucleus distance, i.e. $\langle r_{eN}^{-1} \rangle$. From the definition of this expectation value we write the following expression

$$
\langle r_{eN}^{-1} \rangle = \frac{1}{4} \left( \langle r_{1N}^{-1} \rangle + \langle r_{2N}^{-1} \rangle + \langle r_{3N}^{-1} \rangle + \langle r_{4N}^{-1} \rangle \right)
$$

(7)

where all expectation values in the right-hand side are determined without any additional symmetrization between four electrons. As mentioned above the Li$^-$ ion has a sharp cluster structure and fourth electron is located far away from the central nucleus. This means that $\langle r_{4N}^{-1} \rangle \approx 0$. In this case it follows from Eq.(7) that

$$
\langle r_{eN}^{-1} \rangle = \frac{3}{4} \langle r_{1N}^{-1} \rangle = \frac{3}{4} \langle r_{eN}^{-1} \rangle \approx \frac{3}{4} \langle r_{eN}^{-1} \rangle_{\text{Li}}
$$

(8)

where $\langle r_{eN}^{-1} \rangle_{\text{Li}}$ is the corresponding expectation value for the neutral Li-atom. It is clear that this equality is only approximate. Analougous approximate evaluations can be obtained for some other properties, e.g., for the expectation values of all delta-functions and inverse powers of electron-nucleus and electron-electron distances.

Table I contains a large number of bound state properties of the negatively charged Li$^-$ ion. Numerical values of these properties are of interest in various scientific and technical applications, including quite a few applications to electro-chemistry of the lithium and lithium-ion batteries. Our expectation values form a complete basis set of numerical values which can be useful in analysis of different macroscopical systems containing lithium atoms and negatively charged ions.

III. ON THE HALF-LIFE OF THE BERYLLIUM-7 ISOTOPE

Results of our accurate computations of the ground $2^1S$—state in the weakly-bound Li$^-$ ion indicate clearly that our variational expansion Eq.(3) is very effective in applications to four-electron atomic systems. In this Section we apply the same variational expansion, Eq.(3), to investigate another long-standing problem known in atomic physics of the four-electron atomic systems. Briefly, our goal is to explain variations of the half-life of the beryllium-7 isotope in different chemical backgrounds. As follows from the results of numerous experiments half-life of the $^7$Be isotope is ‘chemically dependent’, i.e. it varies by $\approx 0.5 \% - 5 \%$ for different chemical compounds. This fact contradicts an old fundamental statement
(see, e.g., [7]) that actual decay rates of chemical isotopes cannot depend upon any chemical background. This explains a very substantial interest to chemical compounds which contain atoms the beryllium-7 (or atoms of the $^7$Be isotope). It should be mentioned that in modern laboratories different chemical compounds of the $^7$Be atoms are not ‘exotic’ substances. The nuclei of $^7$Be are formed in the $(p; n)$- and $(p; \alpha)$-reactions of the $^7$Li and $^{10}$B nuclei with the accelerated protons. A few other nuclear reactions with the involvement of nuclei of some light and intermediate elements, e.g., C, Al, Cu, Au, etc, also lead to the formation of the $^7$Be nuclei. In general, an isolated $^7$Be nucleus decays by using a few different channels. The most important of these channels is the electron capture (or $e^-\text{—capture}$) of one atomic electron from the internal $1s^2$—shell. The process is described by a simple atomic-nuclear equation $^7$Be $\rightarrow$ $^7$Li, where there is no free electron emitted after the process. During this process the maternal $^7$Be nucleus is transferred into the $^7$Li nucleus which can be found either in the ground, or in the first excited state. The following transition of the excited $^7$Li* nucleus into its ground state $^7$Li proceeds with the emission of $\gamma$—quantum which has the energy $E_\gamma \approx 0.477$ MeV. Such $\gamma$—quanta can easily be registered in modern experiments and this explains numerous applications of chemical compounds of $^7$Be in radio-chemistry.

Let us discuss the process of the electron capture in the $^7$Be-atom in detail. Assuming for a moment that all $^7$Be atoms decay by the electron capture from the ground (atomic) $2^1S$—state. In this case, by using the expectation value of the electron-nucleus delta-function $\langle \delta(r_{eN}) \rangle$ computed for the ground $2^1S$—state of an isolated Be-atom we can write the following expression for the half-life $\tau$ of the $^7$Be atom/isotope

$$\tau = 1 = \frac{1}{\Gamma} = \frac{1}{A \langle \delta(r_{eN}) \rangle}$$  \hspace{1cm} (9)

where $\Gamma$ is the corresponding width and $A$ is an additional factor for a given compound of beryllium. The half-life $\tau_{\frac{1}{2}}$ determines the moment when 50 % of the incident $^7$Be will decay by the electron capture. Analytical formula for $\tau$, Eq.(9), follows from the fact that the corresponding width $\Gamma = \tau^{-1}$ must be proportional to the product of expectation value of the electron-nucleus delta-function and one additional factor $A$. The expectation value of the electron-nucleus delta-function computed with the non-relativistic wavefunction determines the electron density at the surface of a sphere with the spatial radius $R \approx \Lambda_e = \frac{\hbar^2}{m_e c^2} = \alpha a_0$, where $a_0$ is the Bohr radius $a_0 \approx \frac{\hbar^2}{m_e c^2} (\approx 5.292 \cdot 10^{-9} \text{ cm})$, $c$ is the speed of light and $\Lambda_e$ is the Compton wave length. The ‘constant’ $A$ in Eq.(9) determines an ‘additional’ probability for
an electron (point particle) to penetrate from the distances \( R \approx \Lambda_e \) to the nuclear surface \( R_N \approx 1 \cdot 10^{-13} \text{ cm} \).

Numerical value of \( A \) can be evaluated by assuming that the mean half-life of the \(^7\)Be-atom in its ground \( 2^1S \)-state equals 53.60 days and by using our best expectation value obtained for the expectation value of the electron-nucleus delta-function \( \langle \delta(r_eN) \rangle \approx 8.82515 \) a.u., one finds that \( \Gamma \approx 2.1593422 \cdot 10^{-7} \) sec\(^{-1}\). From here we find that the factor \( A \) in Eq.(9) equals

\[
A \approx \frac{2.1593422 \cdot 10^{-7}}{\langle \delta(r_eN) \rangle} \tag{10}
\]

where the expectation value \( \langle \delta(r_eN) \rangle \) must be taken in atomic units. To move further we have to assume that the additional factor \( A \) does not depend neither upon the conserving quantum numbers of the Be-atom, nor upon the actual chemical background of this atom. In this case we can write the following formula for the ratio of half-life of the two different molecules \( X(\text{Be}) \) and \( Y(\text{Be}) \) which contain \(^7\)Be atoms

\[
\frac{\tau(X(\text{Be}))}{\tau(Y(\text{Be}))} = \frac{\langle \delta(r_eN); Y(\text{Be}) \rangle}{\langle \delta(r_eN); X(\text{Be}) \rangle} \tag{11}
\]

Let us apply this formula to the case when one of the \(^7\)Be-atoms is in the ground \( 2^1S \)-state, while another such an atom is in the triplet \( 2^3S \)-state. The expectation value of the \( \delta_eN \)-function for the ground state in the Be-atom is given above, while for the triplet state we have \( \langle \delta(r_eN) \rangle \approx 8.739558 \) a.u. Both these expectation values were determined in our highly accurate computations of the ground \( 2^1S \)- and \( 2^3S \)-state in the four-electron Be atom. With these numerical values one finds from Eq.(11) that the half-life of the \(^7\)Be atom in its triplet \( 2^3S \)-state is 1.009794 times (or by 1 \%) longer than the corresponding half-life of the \(^7\)Be atom in its ground singlet \( 2^1S \)-state. This simple example includes two different bound states in an isolated \(^7\)Be-atom. In general, by using the formula Eq.(11) we can approximately evaluate the half-life of the \(^7\)Be atoms in different molecules and compounds. The formula Eq.(11) can be applied, e.g., to BeO, BeC\(_2\), BeH\(_2\) and many other beryllium compounds, including Be-polymers, e.g., Be\(_n\)H\(_{2n}\) for \( n \approx 100 - 1000 \) (see, e.g., [11] - [14] and references therein).

As is well known from atomic physics, the electronic structure of the bound states of the Be-atom(s) is \( 1s^22s^22\ell \) (or \( 1s^22s^12\ell^1 \)), where \( \ell \geq 0 \). This state arises after excitation of a single electron from the \( 1s^22s^2 \) electron configuration, which correspond to the ground state, or ‘core’, for short. It is clear that the final \( 1s^22s^12\ell^1 \) configuration is the result of
a single electron excitation $2s \rightarrow 2\ell$. All other states with excitation(s) of two and more electrons from the core are unbound. In general, the contribution to the expectation value of the electron-nucleus delta-function comes from the two internal electrons (or $1s^2$—electrons) and electrons from outer shells (or $2s2\ell$—electrons). It can be shown that a very significant contribution ($\geq 97\%$) into this expectation value comes from the two internal $1s^2$-electrons. The two outer-most electrons do not contribute substantially into the expectation value of the electron-nucleus delta-function $\langle \delta(r_{eN}) \rangle$. As follows from computational results the overall contribution from two outer-most electrons is only $3\% - 5\%$ of the total numerical value. This means that variations in the chemical background of one $^7$Be atom can change the half-life of this atom in $1.03 - 1.05$ times (maximum). The life-time changes correspondingly. In reality, such changes are significantly smaller, but they can be noticed in modern experiments.

It is interesting to note that analogous result ($3\% - 6\%$ differences as maximum) can be predicted for other nuclear processes which are influenced by variations in the chemical background, e.g., for the excitation of the $^{235}$U nucleus which also depend upon chemical background $[15], [16], [17], [18]$. It is well known (see, e.g., $[17]$) that the $^{235}$U nucleus has an excited state with the energy $\approx 75 - 77\, eV$. There is no such a level in the $^{234}$U, $^{236}$U and $^{238}$U nuclei. Nuclear properties of the ground and first excited states in the $^{235}$U nucleus differ substantially. Moreover, by changing the actual chemical background of the $^{235}$U atom we can change the probabilities of excitation of the central nucleus. From here we arrive to the idea to vary chemical background of the $^{235}$U atoms, e.g., by using different alloys of uranium, in order to change and even control nuclear properties. For instance, it can be used to achieve and even exceed critical conditions with respect to the neutron fission. Theoretical evaluations and preliminary experiments show that possible changes in nuclear properties of different compounds of uranium-235 do not exceed $3 - 7\%$. Very likely, these $3 - 7\%$ are the upper limit of influence of atomic (and molecular) properties on the nuclear properties of different isotopes. On the other hand, possible changes in atomic and molecular properties produced by the processes, reactions and decays in atomic nuclei are always fundamental.

Thus, if we know the expectation value of the electron-nucleus delta-function for the beryllium-7 atom included in some molecule with other chemical elements, then we can evaluate the corresponding half-life of such an atom in respect to the electron capture.
Currently, however, this problem can be solved only approximately, since there are quite a few problems in accurate computations of complex molecules as well as in actual experiments, since, e.g., the exact value of the constant $A$ in Eq. (9) is not known. In other words, we cannot be sure that the experimental half-life mentioned above (53.60 days) corresponds to the electron capture from in ground $2^1S$–state of an isolated $^7\text{Be}$ atom. In fact, it is not clear what chemical compounds were used (and at what conditions) to obtain this half-life. Very likely, we are dealing with some ‘averaged’ value determined for a mixture of different molecules. It is clear that the overall experimental accuracy and purity of future experiments must be improved drastically. The accuracy of theoretical computations is also needed to be improved drastically. All similar calculations must oriented for obtaining very accurate expectation value of the electron-nucleus delta-function $\langle \delta(r_{eN}) \rangle$, rather than for production of ‘another’ very accurate value of abstract total energy. Right now, we can only hope that in the future these problems can be solved and sorted out. Then the formula, Eq. (11), can be used to determine the actual life-times of the $^7\text{Be}$ atoms, which are included into different chemical compounds.

IV. CONCLUSION

We have considered the bound state properties of the negatively charged Li$^-\,$ion in the ground $2^1S$–state. The same bound state properties are also determined for the $^6\text{Li}^-$ and $^7\text{Li}^-$ ions with the finite nuclear masses and they are compared with the analogous properties of the neutral Li atom. Our analysis of the bound state properties of the Li$^-\,$ion is of interest, since the constant formation of the negatively charged Li ions plays an important role in the modern, compact lithium and lithium-ion batteries. Such an extensive analysis of the bound state properties of the negatively charged Li$^-\,$ion(s) has been performed for the first time. Expectation values of different properties determined in this study are sufficient for all current and future experimental needs. On the other hand, it is clear that overall accuracy achieved for some of the properties is not sufficient and must be improved in future studies. It follows from our calculations that the Li$^-\,$ion is a weakly-bound atomic system which has only one bound $2^2S$–state. The internal structure of this state is represented as a motion of one ‘almost free’ electron in the field of a heavy atomic cluster which is the neutral Li atom in its ground $2^2S$–state. The computed expectation values of the bound state properties of
the Li$^-$ ion in the $2^1S$–state and neutral Li atom in the $2^2S$–state do not contradict such a picture. Moreover, the whole internal structure of the Li$^-$ ion can be reconstructed to very good accuracy, if we know the model potential between an electron and neutral Li atom (two-body approximation). An accurate reconstruction of such a model $e^-$-Li interaction potential must be a goal of future research. The same model potential can be used to obtain the cross-section of the elastic scattering (at relatively small energies) for the electron-lithium scattering.

The negatively charged $^6$Li$^-$ ion is of interest for possible creation and observation of an unstable (three-electron) $^4$He$^-$ ion which is formed in one of the channels of the reaction of the $^6$Li$^-$ ion with slow neutrons, e.g.,

$$^6\text{Li}^- + n = ^4\text{He}^- + ^3\text{H}^+ + e^- + 4.785 \text{ MeV} ,$$

Preliminary evaluations indicate that the probability of formation of the $^4$He$^-$ ion in this reaction is $\approx 0.02 \%- 0.04 \%$. Nevertheless, this nuclear reaction of the $^6$Li$^-$ ion with slow neutrons has a very large cross-section and it can be used to produce the negatively charged He$^-$ ion which is unstable and decays into the neutral He atom with the emission of one electron. Other approaches to create and observe creations and decays of the $^4$He$^-$ ions have failed.

We also investigated the problem of experimental variations of the half-life of the beryllium-7 isotope placed in different chemical backgrounds. Since the middle of 1930’s this interesting problem has attracted a significant experimental and theoretical attention. It is shown that the half-life of the beryllium-7 isotope in different chemical backgrounds may vary by $3\,-\,5\%$ (maximum). A central computational part of this problem is to determine to high accuracy the electron-nucleus delta-function of the Be-atom placed into different molecules, ‘quasi-metalic’ alloys and other chemical compounds. Currently, such an accuracy is not sufficient to make accurate predictions of the half-life of the beryllium-7 atom in many molecules. Another part of the problem is to improve the overall purity and accuracy of current experiments performed with different molecules which include atoms of the beryllium-7.
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Appendix

The expectation values \( \langle \mathbf{p}_e \cdot \mathbf{p}_N \rangle \) and \( \langle \mathbf{p}_e \cdot \mathbf{p}_e \rangle \) are not presented in Table I, since they are not truly independent from the \( \langle \frac{1}{2}p_e^2 \rangle \) and \( \langle \frac{1}{2}p_N^2 \rangle \) expectation values given in this Table. Indeed, I have found that in an arbitrary \( K \)-electron atom/ion the expectation values of the scalar products of the vectors of electron’s momenta \( \mathbf{p}_i \ (i = 1, \ldots, K) \) with each other and momentum of the nucleus \( \mathbf{p}_N \) are simply related with the expectation values of the single-electron kinetic energy and kinetic energy of the nucleus:

\[
\langle \mathbf{p}_i \cdot \mathbf{p}_j \rangle = \langle \mathbf{p}_1 \cdot \mathbf{p}_2 \rangle = \frac{2}{K(K-1)} \left[ \langle \frac{1}{2}p_N^2 \rangle - 2 \langle \frac{1}{2}p_e^2 \rangle \right],
\]

\[
\langle \mathbf{p}_i \cdot \mathbf{p}_N \rangle = \langle \mathbf{p}_1 \cdot \mathbf{p}_N \rangle = -\frac{2}{K} \langle \frac{1}{2}p_N^2 \rangle,
\]

where \( K \) is total number of electrons, \( \langle \mathbf{p}_i \cdot \mathbf{p}_j \rangle \) is the scalar product of the electron momenta of two atomic electrons (with indexes \( i \) and \( j \)), while \( \langle \mathbf{p}_i \cdot \mathbf{p}_N \rangle \) is the scalar product of the atomic nucleus and electron (with index \( i \)). Since the electron’s indexes are arbitrary we can replace these scalar products by the \( \langle \mathbf{p}_1 \cdot \mathbf{p}_2 \rangle \) and \( \langle \mathbf{p}_1 \cdot \mathbf{p}_N \rangle \) values, respectively. These expectation values determine the kinematic correlations, or kinematic interparticle correlations. In Eqs. (13) and (14) the notations \( \langle \frac{1}{2}p_e^2 \rangle \) and \( \langle \frac{1}{2}p_N^2 \rangle \) designate the single-electron kinetic energy and nucleus kinetic energy, respectively. It is interesting to note that the nuclear charge \( Q \) is not included in these expressions. These equalities are obeyed for an arbitrary \( K \)-electron atom/ion, where \( K \leq Q \) (or, in general, \( K \leq Q + 1 \)). Therefore, there is no need to include the \( \langle \mathbf{p}_1 \cdot \mathbf{p}_2 \rangle \) and \( \langle \mathbf{p}_1 \cdot \mathbf{p}_N \rangle \) expectation values in Table I. For two-electron atomic systems \( K = 2 \) and equalities mentioned above take the well known form:

\[
\langle \mathbf{p}_1 \cdot \mathbf{p}_2 \rangle = \langle \frac{1}{2}p_N^2 \rangle - 2 \langle \frac{1}{2}p_e^2 \rangle, \quad \langle \mathbf{p}_e \cdot \mathbf{p}_N \rangle = \langle \mathbf{p}_1 \cdot \mathbf{p}_N \rangle = -\frac{1}{2} \langle p_N^2 \rangle,
\]

where \( K \) is total number of electrons, \( \langle \mathbf{p}_i \cdot \mathbf{p}_j \rangle \) is the scalar product of the electron momenta of two atomic electrons (with indexes \( i \) and \( j \)), while \( \langle \mathbf{p}_i \cdot \mathbf{p}_N \rangle \) is the scalar product of the atomic nucleus and electron (with index \( i \)). Since the electron’s indexes are arbitrary we can replace these scalar products by the \( \langle \mathbf{p}_1 \cdot \mathbf{p}_2 \rangle \) and \( \langle \mathbf{p}_1 \cdot \mathbf{p}_N \rangle \) values, respectively. These expectation values determine the kinematic correlations, or kinematic interparticle correlations. In Eqs. (13) and (14) the notations \( \langle \frac{1}{2}p_e^2 \rangle \) and \( \langle \frac{1}{2}p_N^2 \rangle \) designate the single-electron kinetic energy and nucleus kinetic energy, respectively. It is interesting to note that the nuclear charge \( Q \) is not included in these expressions. These equalities are obeyed for an arbitrary \( K \)-electron atom/ion, where \( K \leq Q \) (or, in general, \( K \leq Q + 1 \)). Therefore, there is no need to include the \( \langle \mathbf{p}_1 \cdot \mathbf{p}_2 \rangle \) and \( \langle \mathbf{p}_1 \cdot \mathbf{p}_N \rangle \) expectation values in Table I. For two-electron atomic systems \( K = 2 \) and equalities mentioned above take the well known form:

\[
\langle \mathbf{p}_1 \cdot \mathbf{p}_2 \rangle = \langle \frac{1}{2}p_N^2 \rangle - 2 \langle \frac{1}{2}p_e^2 \rangle, \quad \langle \mathbf{p}_e \cdot \mathbf{p}_N \rangle = \langle \mathbf{p}_1 \cdot \mathbf{p}_N \rangle = -\frac{1}{2} \langle p_N^2 \rangle.
\]
These identities are often used as a test in highly accurate, bound state computations of various two-electron atom/ions and arbitrary three-body systems.

[1] L.D. Landau and E.M. Lifshitz, *Quantum Mechanics. Non-Relativistic Theory*, (3rd. ed., Oxford, England, Pergamon Press (1977)).

[2] S. Larsson, Phys. Rev. 169, 49 (1968).

[3] A.M. Frolov, Phys. Rev. A 59, 4270 (1999).

[4] N.N. Kolesnikov and V.I. Tarasov, Yad. Fiz. 35, 609 (1982), [Sov. J. Nucl. Phys. 35, 354 (1982)].

[5] A.M. Frolov and D.M. Wardlaw, Phys. Rev. A Phys. Rev. A 78, 042506 (2008).

[6] A.M. Frolov and D.M. Wardlaw, JETP 138, 5 (2010).

[7] H. Remy, *Treatise on Inorganic Chemistry*, vol. 2 (Elsevier Science Ltd., Netherlands (1965)).

[8] R.F. Leininger, E. Segre and C. Wiegard, Phys. Rev. 76, 897 (1949).

[9] J.J. Kraushaar, E.D. Wilson and K.T. Bainbridge, Phys. Rev. 90, 610 (1953).

[10] G.F. Thomas, Foundation of Chemistry 14, 109 (2012).

[11] A. Ray, P. Das, S.K. Sahab and S.K. Das, Phys. Lett. B 531 187 (2002).

[12] M. Jaeger, S. Wilmes, V. Kölle, and G. Staudt Phys. Rev. C 54, 423 (1996).

[13] E.V. Tkalya, A.V. Avdeenkov, A.V. Bibikov, I.V. Bodrenko and A.V. Nikolaev, Phys. Rev. C 86, 014608 (2012).

[14] T. Ohtsuki, K. Ohno, T. Morisato, T. Mitsugashira, K. Hirose, H. Yuki and J. Kasagi, Phys. Rev. Lett. 98, 252501 (2007).

[15] F. Asaro and I. Perlman, Phys. Rev. 107, 318 (1957).

[16] T. Almeida, T. Von Egidy, P.H.M. Van Assche et al, Nucl. Phys. A 315, 71 (1979).

[17] V.I. Zhudov, A.G. Zelenkov, A.G., V.M. Kulakov, V.I. Mostovoi and B.V. Odinov, Pisma Zh. Eksp. Teor. Fiz. 30, 549 [JETP Lett. 30, 516 (1979)].

[18] A.M. Frolov, Radiation Physics and Chemistry 72, 541 (2005).

[19] A.M. Frolov, J. Chem. Phys. 126, 104302 (2007).
TABLE I: The expectation values of a number of electron-nuclear (en) and electron-electron (ee) properties in a.u. of the ground $2S^1$− and $2S^2$−states of the of the Li$^-$ ($\infty$Li$^-$) ion and neutral Li ($\infty$Li) atom, respectively. The bound states of the negatively charged $^6$Li$^-$ and $^7$Li$^-$ ions are also presented (in a.u.)

| atom/ion state | state | $\langle r_{en}^{-2}\rangle$ | $\langle r_{en}^{-1}\rangle$ | $\langle r_{en}\rangle$ | $\langle r_{en}^2\rangle$ | $\langle r_{en}^3\rangle$ | $\langle r_{en}^4\rangle$ |
|----------------|-------|-----------------------------|-----------------------------|-----------------------------|-----------------------------|-----------------------------|-----------------------------|
| Li$^-$         | $2^1 S$ | 7.5686995                   | 1.474975                    | 2.893593                    | 17.31428                    | 136.6435                    | 1285.5                      |
| Li             | $2^2 S$ | 10.0803019                  | 1.9060380                   | 1.6631516                   | 6.1178185                   | 30.86145                    | 183.264                     |
| $^6$Li$^-$     | $2^1 S$ | 7.5672973                   | 1.474838                    | 2.893823                    | 17.31677                    | 136.6698                    | 1285.8                      |
| $^7$Li$^-$     | $2^1 S$ | 7.5674973                   | 1.474858                    | 2.893789                    | 17.31641                    | 136.6659                    | 1285.8                      |

| atom/ion state | state | $\langle r_{ee}^{-2}\rangle$ | $\langle r_{ee}^{-1}\rangle$ | $\langle r_{ee}\rangle$ | $\langle r_{ee}^2\rangle$ | $\langle r_{ee}^3\rangle$ | $\langle r_{ee}^4\rangle$ |
|----------------|-------|-----------------------------|-----------------------------|-----------------------------|-----------------------------|-----------------------------|-----------------------------|
| Li$^-$         | $2^1 S$ | 0.747893                    | 0.449288                    | 5.099841                    | 37.60226                    | 343.467                     | 3666.8                      |
| Li             | $2^2 S$ | 1.4603972                   | 0.732739                    | 2.8894200                   | 12.2818335                  | 64.01690                    | 385.063                     |
| $^6$Li$^-$     | $2^1 S$ | 0.747770                    | 0.449251                    | 5.100233                    | 37.60758                    | 343.533                     | 3667.7                      |
| $^7$Li$^-$     | $2^1 S$ | 0.747787                    | 0.449256                    | 5.100175                    | 37.60679                    | 343.524                     | 3667.5                      |

| atom/ion state | state | $E$ | $\langle \frac{1}{2}p_e^2\rangle$ | $\langle \frac{1}{2}p_N^2\rangle$ | $\langle \delta_{en}\rangle$ | $\langle \delta_{ee}\rangle$ | $\langle \delta_{eee}\rangle$ |
|----------------|-------|-----|--------------------------------|--------------------------------|-----------------------------|-----------------------------|-----------------------------|
| Li$^-$         | $2^1 S$ | -7.50059653 | 1.87514912 | 7.81120535 | 3.428488 | 0.0918344 | 0.0 |
| Li             | $2^2 S$ | -7.478059854 | 2.492686620 | 7.79904922 | 4.6071191 | 0.18166027 | 0.0 |
| $^6$Li$^-$     | $2^1 S$ | -7.49976425 | 1.87551850 | 7.80946261 | 3.427545 | 0.0918105 | 0.0 |
| $^7$Li$^-$     | $2^1 S$ | -7.49986590 | 1.87556901 | 7.80971246 | 3.427679 | 0.0918139 | 0.0 |