Atomic fragments from the nuclear reaction of the ^{6}Li atom with slow neutrons

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Abstract

Approximate probabilities of formation of various atoms and ions in different bound states are determined for the exothermic nuclear $(n, {}^6\mathrm{Li}; t, {}^4\mathrm{He})$-reaction of atomic lithium-6 with slow neutrons. In our calculations of the final state probabilities we have assumed that the incident lithium atom is in its ground (doublet) atomic $1^2S(L = 0)$−state. It is straightforward to generalize our analysis to other bound states of the three-electron Li atom.

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I. INTRODUCTION

The nuclear reaction of ^{6}Li nuclei with slow neutrons is written in the form [1]

$$^6\text{Li} + n = {}^4\text{He} + t + 4.785 \ \ MeV \tag{1}$$

where the notations ^{4}He and t stand for the helium nucleus (often also called the $\alpha-$particle, or α, for short) and tritium (or ^{3}H) nucleus. For thermal neutrons with $E_n \approx 0$ the cross-section σ of this nuclear reaction is very large $\sigma_{max} \approx 960 \cdot 10^{-24} \ cm^2$ or 960 $barn$ [2], for short. The velocities of the two nuclear fragments formed in the reaction, Eq.(1), with slow neutrons are $\approx 6.03986 \ a.u.$ and $\approx 4.52989 \ a.u.$ for the tritium nucleus and $\alpha-$particle, respectively. These velocities are given in atomic units, where $\hbar = 1, m_e = 1, e = 1$. The unit of atomic velocity is $v_e = \alpha c \approx \frac{c}{137} \approx 2.1882661 \cdot 10^8 \ cm \cdot sec^{-1}$, where c is the speed of light and α is the fine structure constant. Formally, the atomic velocity v_e is the velocity of the $1s-$electron in the hydrogen atom with the infinitely heavy nucleus $^\infty$H. It is clear that in atomic units $v_e = 1$.

The nuclear reaction of the ^{6}Li nucleus, Eq.(1), proceeds with neutrons of all energies and the energy released increases almost linearly with the energy of the incident neutron. For fast neutrons with $E_n \geq 1 \ MeV$ the energy released is substantially different from the value quoted in Eq.(1) and the velocities of the atomic fragments increase correspondingly. Note that the cross-section of this reaction has a large resonance (maximum) $\sigma \approx 4.5 \ barn$ at $E_n \approx 240-270 \ keV$, but it is relatively large for neutrons of all energies $E_n \leq 0.8 \ MeV$. This makes the reaction, Eq.(1), extremely important in the thermonuclear ignition and following propagation of the thermonuclear burning wave in highly compressed ($\rho \geq 100 \ g \cdot cm^{-3}$) ^{6}LiD deuteride which is routinely used as a thermonuclear fuel in modern thermonuclear explosive devices (see, e.g., [3], [4]). The analogous $(n, {}^3\text{He})$-reaction [5] also plays a very important role in such processes.

In general, the nuclear (n,t)-reactions of the ^{6}Li and ^{3}He nuclei with neutrons allow one to: (1) reduce drastically the overall bremsstrahlung loss from the combustion zone; and (2) increase the tritium/deuterium ratio which is crucially important to start many new thermonuclear $(d,t)-$reactions. Briefly, by using the ^{6}LiD deuteride in modern thermonuclear explosive devices we can reduce the required compressions to relatively small values. In many cases such compressions are dozens times smaller (usually, in 25 - 40 times smaller [4]) than compressions required for any other (solid) thermonuclear fuel, e.g., ^{7}LiD deuteride.

On the other hand, by using compressions which are provided by a standard 'primary' nuclear charge one can create extremely compact thermonuclear explosive devices based on the ^{6}LiD deuteride. The idea to use the pure ^{6}LiD deuteride in thermonuclear explosive devices was originally proposed by V.L. Ginzburg in 1948-1949 (see discussion and references in [3]).

Our goal in this study is to make accurate numerical predictions of the final state probabilities for the reaction, Eq.(1), with slow neutrons. We want to predict (accurately) the probabilities of formation of various atoms and ions in different (ground and excited) final states. Briefly, we want to determine the probabilities to detect the He and ^{3}H atoms and He$^+$, ^{3}H$^-$ ions in their bound states. Note that all newly created atomic fragments from reaction, Eq.(1), move rapidly even in the case of slow neutrons and that accurate theoretical prediction of the final state probabilities for rapidly moving atomic fragments is not trivial.

On the other hand, the results of our evaluations and methods created for such evaluations are of great interest in many applications related with the nuclear reaction, Eq.(1), and another similar reaction of ^{10}B nuclei with slow neutrons, namely

$$^{10}\text{B} + n = {}^7\text{Li} + {}^4\text{He} + 2.791 \ \ MeV \tag{2}$$

The reaction, Eq.(2), is extensively used in the boron neutron capture therapy (BNCT, for short), or boron neutron-capture synovectomy [6] - [10], to treat different forms of cancer, including brain cancer. The fast $\alpha-$particle produced in the reaction, Eq.(2), kills (or at least 'badly damages') one cancer cell before it finally stops. The modern applications of this reaction to cancer treatment are based on the use of molecules which contain a large number of ^{10}B-atoms, e.g., the Na$_3$[B$_{20}$ H$_{17}$NH$_2$ CH$_2$CH$_2$ NH$_2$] molecule, other similar molecules, and molecular clusters [8], [9] (see also [10] and references therein). In this case the overall energy release from the reaction, Eq.(2), in one cancer cell can be extremely large. Correspondingly, the local temperature in the whole cell suddenly increases to very large values and this kills the incident cancer cell with almost 100 % probability.

Note that the tritium nucleus does not form in the nuclear reaction Eq.(2) which means that it is safe to initiate this reaction inside of a human body. By studying the nuclear reaction, Eq.(1), in few-electron atoms and ions we want to develop a number of reliable theoretical methods and numerical procedures which can be later used in applications to the analogous reaction, Eq.(2).

II. APPROXIMATE VARIATIONAL WAVE FUNCTION OF THE LITHIUM ATOM

For our purposes in this study it is important to construct accurate variational wave function(s) of the ground (doublet) $1^2S(L = 0)-$states of the Li atom which is written in the following general form (see, e.g., [11], [12])

$$\Psi(\text{Li})_{L=0} = \psi_{L=0}(A; \{r_{ij}\})(\alpha\beta\alpha - \beta\alpha\alpha) + \phi_{L=0}(B; \{r_{ij}\})(2\alpha\alpha\beta - \beta\alpha\alpha - \alpha\beta\alpha) \qquad (3)$$

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 norm. The notations α and β in Eq.(3) are the one-electron spin-up and spin-down functions, respectively (see, e.g., [13]). The notations A and B in Eq.(3) mean that the two sets of non-linear parameters associated with radial functions ψ and ϕ can be optimized independently. Note that each of the radial basis functions in Eq.(3) explicitly depends upon all six interparticle (or relative) coordinates $r_{12}, r_{13}, r_{23}, r_{14}, r_{24}, r_{34}$.

In our earlier work [14] we have introduced an advanced set of radial basis functions for bound state computations of three-electron atomic systems. Such a set is called the semi-exponential basis set and it is written in the form

$$\psi_{L=0}(A; \{r_{ij}\}) = \sum_{k=1}^{N} C_k r_{23}^{n_1(k)} r_{13}^{n_2(k)} r_{12}^{n_3(k)} r_{14}^{m_1(k)} r_{24}^{m_2(k)} r_{34}^{m_3(k)} exp(-\alpha_k r_{14} - \beta_k r_{24} - \gamma_k r_{34}) \qquad (4)$$

where $\alpha_k, \beta_k, \gamma_k$ $(k = 1, 2, \ldots, N)$ are the varied non-linear parameters. The use of a large number of non-linear parameters in Eq.(4) allows one to construct compact and very accurate variational wave functions for different three-electron atoms and ions. It was shown in [11] that the semi-exponential basis, Eq.(4), has a large number of other advantages in accurate numerical computations.

In the sudden approximation [15], [16] the numerical determination of the final state probabilities is reduced to the analytical computation of the Fourier transform of the overlap integral between the incident ψ_{in} and final ψ_{fi} wave functions. In the case of the nuclear reaction of ^{6}Li nuclei with slow neutrons under consideration here, the incident wave function represents the ground 1^2S-state of the lithium atom. The final wave function represents the product atom and/or ion. For the helium atom product we need to determine the following

integral (or probability amplitude M_{if})

$$M_{if} = \int \int \int \Psi_{\text{Li}}(r_{14}, r_{24}, r_{34}, r_{12}, r_{13}, r_{23}) \exp(\imath \mathbf{V}_\alpha \cdot \mathbf{r}_{14} + \imath \mathbf{V}_\alpha \cdot \mathbf{r}_{24}) \times \tag{5}$$
$$\Psi_{\text{He}}(r_{14}, r_{24}, r_{12}) d^3 \mathbf{r}_{14} d^3 \mathbf{r}_{24} d^3 \mathbf{r}_{34}$$

where Ψ_{Li} is the wave function of the Li atom, while Ψ_{He} is the wave function of the final (bound) state of the He atom. The velocity $\mathbf{V}_\alpha$ is the final velocity of the $\alpha-$particle after reaction, Eq.(1). For the tritium atom product in one of its bound states the probability amplitude M_{if} is written in a slightly different form

$$M_{if} = \int \int \int \Psi_{\text{Li}}(r_{14}, r_{24}, r_{34}, r_{12}, r_{13}, r_{23}) \exp(\imath \mathbf{V}_t \cdot \mathbf{r}_{14}) \Psi_{\text{H}}(r_{14}) d^3 \mathbf{r}_{14} d^3 \mathbf{r}_{24} d^3 \mathbf{r}_{34} \tag{6}$$

where $\Psi_{\text{H}}(r_{14})$ is the unit-norm wave function of the tritium (or hydrogen) atom and $\mathbf{V}_t$ is its velocity after the reaction, Eq.(1). In our earlier study [17] we have calculated integrals similar to the integrals in Eq.(5) and Eq.(6) for the two-electron atomic systems which are involved in the analogous nuclear reaction of the ^{3}He nuclei with slow neutrons. The integral, Eq.(5), can be considered as a partial Fourier transformation of the overlap of the incident and final wave functions. This integral represents the Galilean transformation between the incident system (which was at rest) and the final system which is rapidly moving with constant speed.

In general, numerical calculations of integrals Eqs.(5) and (6) are difficult to perform due to the presence of the electron-electron coordinates r_{ij} in the wave function. On the other hand, for approximate evaluation of the final state probabilities for the nuclear reaction, Eq.(1), we do not need to use the highly accurate wave functions of the Li and He atoms. In particular, we can use the wave functions of few-electron atomic systems which do not contain any of the electron-electron coordinates. This drastically simplifies analytical/numerical calculation of the integrals, Eq.(5) - Eq.(6). Formally, such approximate wave functions depend on the electron-nucleus coordinates only. Therefore, these wave functions correspond to a system of $A-$electrons which do not interact with each other and can be considered as free-electron wave functions. For the He atom we have $A = 2$, while for the Li atom we have $A = 3$. The explicit construction of the approximate free-electron wave functions for few-electron atomic systems is discussed below.

A. Special form of the trial wave function of the lithium atom

To avoid problems related to the analytical computation of the Fourier transformations given by Eq.(5) one can apply approximate variational expansions of the three-electron wave function. To simplify all following calculations we represent the wave function of the Li atom in the form

$$\psi_{L=0}(r_{14}, r_{24}, r_{34}, 0, 0, 0) = \sum_{i=1}^{N_s} C_k r_{14}^{m_1(k)} r_{24}^{m_2(k)} r_{34}^{m_3(k)} exp(-\alpha_k r_{14} - \beta_k r_{24} - \gamma_k r_{34}) \qquad (7)$$

$$= \sum_{i=1}^{N_s} C_k r_{1}^{m_1(k)} r_{2}^{m_2(k)} r_{3}^{m_3(k)} exp(-\alpha_k r_1 - \beta_k r_2 - \gamma_k r_3)$$

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.(7) has a unit norm. Furthermore, in all calculations performed for this study only one spin function $\chi_1 = \alpha\beta\alpha - \beta\alpha\alpha$ is used. It is clear that the wave function Eq.(7) 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.(7). The wave function, Eq.(7), must be properly symmetrized upon all three electron coordinates. This problem is discussed in the next Subsection.

The principal question for the wave function, Eq.(7), is related to its overall accuracy. If (and only if) such accuracy is relatively high, then such a wave function, Eq.(7), can be used in actual computations of the probability amplitudes, Eqs.(5) and (6). In actual applications the approximate wave function, Eqs.(5) and (6), can be constructed from the highly accurate wave functions already known from earlier works (see, e.g., [11] and references therein). Briefly, we can take our wave function of the ground 1^2S-state of the Li atom from [11] and remove all those terms which contain electron-electron r_{ij} coordinates. Then the non-linear parameters in the trial wave function, Eq.(7), must be re-optimized. The resulting wave function can be considered as an optimal free-electron wave function of the ground state of the $^\infty$Li atom. Using this approach we have determined the 23-term variational wave function shown in Table I. The total energy E of the ground 1^2S-state of the $^\infty$Li atom obtained with this wave function is -7.44859276608 $a.u.$ Note that this value of E is very close to the exact total energy of the ground state of the $^\infty$Li atom. This indicates a very good overall quality for our approximate wave function.

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B. Antisymmetrization of the trial wave function of the lithium atom

The actual many-electron wave function in an atomic system must be completely antisymmetric with respect to all electron variables, i.e. upon all electron spatial and spin variables. This statement is true for all exact and approximate few-electron wave functions, including the optimized free-electron wave functions, Eq.(7). Antisymmetrization of the two-electron wave function is trivial and is not discussed here. For a three-electron atomic wave function this requirement is written in the form $\hat{\mathcal{A}}_{123}\Psi(1,2,3) = -\Psi(1,2,3)$, where Ψ is given by Eq.(3) and $\hat{\mathcal{A}}_e$ is the three-particle (= electron) antisymmetrizer $\hat{\mathcal{A}}_e = \hat{e} - \hat{P}_{12} - \hat{P}_{13} - \hat{P}_{23} + \hat{P}_{123} + \hat{P}_{132}$. 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. In actual computations antisymmetrization of the total wave function is reduced to the proper antisymmetrization of corresponding matrix elements (for more detail, see, e.g., [14]). Each of these matrix elements is written in the form $\langle \Psi \mid \hat{O} \mid \Psi \rangle$, where $\hat{O}$ is an arbitrary spin-independent quantum operator which is symmetric upon all interparticle permutations. The wave function Ψ, Eq.(3), contains the two different radial parts ψ and ϕ. By performing the integration over all spin coordinates one finds the four following spatial projectors $\mathcal{P}_{\psi\psi}, \mathcal{P}_{\psi\phi} = \mathcal{P}_{\phi\psi}$ and $\mathcal{P}_{\phi\phi}$

$$\mathcal{P}_{\psi\psi} = \frac{1}{2\sqrt{3}}\left(2\hat{e} + 2\hat{P}_{12} - \hat{P}_{13} - \hat{P}_{23} - \hat{P}_{123} - \hat{P}_{132}\right) \tag{8}$$

$$\mathcal{P}_{\psi\phi} = \frac{1}{2}\left(\hat{P}_{13} - \hat{P}_{23} + \hat{P}_{123} - \hat{P}_{132}\right) \tag{9}$$

$$\mathcal{P}_{\phi\psi} = \frac{1}{2}\left(\hat{P}_{13} - \hat{P}_{23} + \hat{P}_{123} - \hat{P}_{132}\right) \tag{10}$$

$$\mathcal{P}_{\phi\phi} = \frac{1}{2\sqrt{3}}\left(2\hat{e} - 2\hat{P}_{12} + \hat{P}_{13} + \hat{P}_{23} - \hat{P}_{123} - \hat{P}_{132}\right) \tag{11}$$

Here the indexes ψ and ϕ correspond to the notations used in Eq.(3). For an arbitrary symmetric spin-independent operator $\hat{O}$ each of these four projectors produces matrix elements $\langle \Psi \mid \hat{O} \mid \Psi \rangle$ of the correct permutation symmetry (for doublet states) between all three electrons.

C. Bound state wave functions of the final atomic fragments

The final atomic states arising in the exothermic nuclear $(n, {}^6\text{Li}; t, {}^4\text{He})$-reaction of atomic lithium-6 with slow neutrons contain either one, or two, or zero bound electrons. In this

study our main interest is restricted to one- and two-electron atoms and ions. The explicit form of one-electron atomic wave functions takes the form (see, e.g., [18]) $\Phi_{n\ell m}(r, \Theta, \phi)\alpha = R_{n\ell}(Q,r)Y_{\ell m}(\Theta, \phi)\alpha$, where α is the spin-up wave function, $Y_{\ell m}(\Theta, \phi) = Y_{\ell m}(\mathbf{n})$ is a spherical harmonic and $R_{n\ell}(Q,r)$ is the radial function. The radial function is written in the form

$$R_{n\ell}(Q,r) = \frac{1}{rn}\sqrt{\frac{Q(n-\ell-1)!}{(n+\ell)!}}\left[\frac{2Qr}{n}\right]^{\ell+1}\sum_{k=0}^{n-\ell-1}\frac{(-1)^k}{k!}\left(\begin{array}{c}n+\ell\\2\ell+k+1\end{array}\right)\left[\frac{2Qr}{n}\right]^k\exp\left(-\frac{Qr}{n}\right)\text{(12)}$$

where Q is the nuclear charge, while n and ℓ are the quantum numbers of this bound state. Note that the radial function, Eq.(12), has a unit norm for an arbitrary Q.

The wave function of the two-electron He-atom can be approximated in a variety of different forms. Currently, it is possible to construct approximate wave functions which provide 25 - 50 correct decimal digits for the total energy of the He atom and He-like ions. In this study, however, we shall use an approximate He wave function which does not contain the electron-electron coordinate r_{21}. For the ground 1^1S-state of the $^\infty$He atom the radial part of such a wave function is written in the form

$$\psi_{L=0}(r_1, r_2, r_{12}) = C\exp\left[-(Q - \frac{5}{16})r_1 - (Q - \frac{5}{16})r_2\right] \tag{13}$$

where $Q = 2$ is the nuclear charge for the He nucleus and C is the normalizatrion constant. The corresponding spin part of the total wave function takes the form $\eta = \alpha(1)\beta(2) - \beta(1)\alpha(2) = \alpha\beta - \beta\alpha$. The explicit form of the η spin function is important in the performance of integration over all spin coordinates.

The total energy of the $^\infty$He atom obtained with this wave function, Eq.(13), is -2.85 a.u. which indicates that it provides a relatively good approximation to the actual ground state wave function. The main advantage of the approximate wave function, Eq.(13), is its explicit dependence upon the two electron-nuclear coordinates r_1 and r_2 only. This drastically simplifies the following computation of radial integrals with the Bessel functions (see below). On the other hand, we need to note that the best-to-date one-term radial wave function for the $^\infty$He atom (see, e.g., [5]) corresponds to substantially better numerical accuracy, since it provides the total energy $E =$ -2.899 534 375 443 69 $a.u.$ which is very close to the exact answer (see, e.g., [19]). The corresponding non-linear parameters can be found in [5]. But, in contrast with the wave function, Eq.(13), the wave function from [5] explicitly depends upon the electron-electron coordinate r_{21}.

III. CALCULATIONS

By using the free-electron wave function of the Li atom obtained above we can estimate the probabilities to form various atomic species during the nuclear reaction, Eq.(1). The structure of the trial wave function, Eq.(7), enables one to perform accurate computations of all integrals which include one, two and even three Galilean exponents for electrons. In reality all such integrals are reduced to the products of one-dimensional integrals. In other words, in our approach all electron coordinates are separated and this simplifies drastically the following analytical and numerical computations of all required integrals.

To determine the matrix element of the operator $\exp(\imath \mathbf{V} \cdot \mathbf{r})$ (Galilean exponent) between the wave functions of the initial and final bound, we apply the Rayleigh expansion of a plane wave (with the use of spherical harmonic addition theorem [18], [20]). The explicit formula takes the form (see, e.g., [18], [20], [21])

$$\exp(\imath \mathbf{V} \cdot \mathbf{r}) = 4\pi \sum_{\ell=0} \imath^{\ell} j_{\ell}(Vr) \sum_{m=-\ell}^{\ell} Y_{\ell m}^{*}(\mathbf{n}_V) Y_{\ell m}(\mathbf{n}_r) \tag{14}$$

where $Y_{\ell m}(\mathbf{n})$ are the spherical harmonics, $\mathbf{V}$ is the velocity of the final atomic fragment and $\mathbf{n}_y = \frac{\mathbf{y}}{y}$ is the unit norm vector which corresponds to an arbitrary non-zero vector $\mathbf{y}$. Also in this equation the spherical Bessel functions $j_{\ell}(Vr)$ are defined by the relation (see, e.g., [22], [23])

$$j_{\ell}(Vr) = \sqrt{\frac{\pi}{2Vr}} J_{\ell+\frac{1}{2}}(Vr) \tag{15}$$

where $J_{\ell+\frac{1}{2}}(x)$ are the Bessel functions. These formulas are used in analytical and/or numerical computation of all required matrix elements.

Actual computations of matrix elements with the 'factorized' trial wave functions, Eq.(7) are performed with the use of the following formula

$$\int_{0}^{\infty} t^{\mu} J_{\nu}(bt) exp(-pt) dt = \frac{\Gamma(\mu+\nu+1)}{\Gamma(\nu+1)} \left(\frac{b}{2}\right)^{\nu} \frac{1}{\sqrt{(p^2+b^2)^{\nu+\mu+1}}} \times \tag{16}$$

$$_{2}F_{1}\left(\frac{\nu+\mu+1}{2}, \frac{\nu-\mu}{2}; \nu+1; \frac{b^2}{p^2+b^2}\right)$$

where the notation $_{2}F_{1}(a, b; c; x)$ stands for the hypergeometric function. In many actual cases these hypergeometric functions are related to the elementary/rational functions, since, e.g., $_{2}F_{1}(a, b; b; x) = (1-x)^{-a}$.

The results of our computations of the final state probabilities for various atomic species formed in the reaction, Eq.(1), can be found in Table II. As mentioned above the final states

include various ground and excited states in the helium atom (^{4}He), tritium atom (^{3}H) and He-like one-electron ion (He$^+$). In this study we restrict ourselves to the consideration of the $1s-, 2s-$ and $2p-$states in the final one-electron atoms (protium and tritium) and only one 1^1S-state in the ^{4}He atom.

IV. CONCLUSION

We have considered the nuclear reaction, Eq.(1), involving the ground 1^2S-state of the three-electron Li atom. The probabilities of formation of different atomic species during this reaction have been evaluated numerically. Our newly developed procedure is based on the use of the optimized free-electron wave functions for few-electron atomic systems involved in the process. This allows us to perform all required complete and/or partial Fourier transformations of the wave functions. The computed final state probabilities are very close to the exact values determined with the use of highly accurate (or completely correlated) wave functions which include all electron-electron coordinates.

Our procedure can now be used for the more complicated nuclear reaction, Eq.(2), in the five-electron B-atom. The Li-atom/ion and He-atom/ion which form during this reaction may contain up to three and two electrons, respectively. These atomic fragments move rapidly, with the velocities $v_{Li} \approx 2.40896 \ cm \cdot sec^{-1}$ and $v_\alpha \approx 4.21568 \ cm \cdot sec^{-1}$ in the case of slow neutrons. The sudden approximation can thus certainly be applied to the He-atom and He-like ions. However, this approximation cannot be used for internal electrons (or 1^2s-electrons) of the Li atom/ion, since the velocities of these two electrons are comparable with the final velocity of the ^{7}Li nucleus. If the nuclear reaction, Eq.(1), is produced by the fast neutron with $E_n \geq 1 \ MeV$, then the velocity of the Li atom/ion(s) is larger than the atomic velocities of the 1^2s-electrons in the Li atom and sudden approximation can be applied.

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TABLE I: An example of the trial, three-electron wave function constructed with the use of $N = 23$ semi-exponential radial basis functions, Eq.(7). This wave function produces the total energy $E =$ -7.44859276608 $a.u.$ for the ground $1\,^2S-$state of the $^\infty$Li atom. Only one electron spin-function $\chi_1 = \alpha\beta\alpha - \beta\alpha\alpha$ was used in these calculations.

k	$m_1(k)$	$m_2(k)$	$m_3(k)$	C_k	α_k	β_k	γ_k
1	0	0	1	0.146131429481911E+02	0.416423958308045E+01	0.390330393520923E+01	0.754647967615054E+00
2	1	0	1	0.110681883475133E+03	0.526120133598745E+01	0.699723209902291E+01	0.604874234309236E+00
3	1	1	1	0.234004890152000E+03	0.598950989816454E+01	0.378246213278597E+01	0.590931685390717E+00
4	2	0	1	0.116882861303726E+03	0.413820964104499E+01	0.322650638788059E+01	0.590283203974117E+00
5	0	0	0	-0.112533836667930E+02	0.404234943769060E+01	0.402575246908481E+01	0.136870242306376E+01
6	0	0	2	0.124148253762594E+01	0.772078877480103E+01	0.208089611437233E+01	0.906692873308709E+00
7	0	0	3	0.129950444032051E+01	0.125634586976915E+02	0.167180833975207E+02	0.111484879880926E+01
8	3	0	1	0.121940082563610E+02	0.336154087416427E+01	0.329089537444583E+01	0.569461303170668E+00
9	2	2	1	-0.815264312642982E+01	0.315618697991587E+01	0.293590042487235E+01	0.642752252837086E+00
10	0	0	4	0.231307852206996E-01	0.216119418842614E+01	0.354528921898964E+01	0.848100637437686E+00
11	1	0	0	-0.290323204459308E+02	0.303111504960694E+01	0.340407714984374E+01	0.439831339492880E+00
12	1	0	2	-0.782805087195444E+01	0.319874342329211E+01	0.294880236447181E+01	0.670201325893484E+00
13	4	0	1	0.466451849833029E+05	0.257191421047538E+02	0.198922117452300E+02	0.745721864825035E+00
14	5	0	1	0.102312737866967E+03	0.610735801244370E+01	0.126738573321754E+02	0.583192334409026E+00
15	1	1	0	0.496831723313492E+01	0.214720891197913E+01	0.139151014500059E+02	0.332004403600092E+00
16	1	1	2	0.331570408306929E+01	0.313893628304852E+01	0.288670468153774E+01	0.656255394173358E+00
17	2	0	0	-0.224488896165048E+03	0.111494404746535E+02	0.712253949382151E+01	0.412242317869619E+00
18	2	0	2	-0.200426722868461E+01	0.282336074847368E+01	0.292360100848728E+01	0.638644442755579E+00
19	0	0	5	0.186252350189224E-02	0.103900277658347E+02	0.241603283627644E+01	0.858660133717424E+00
20	2	1	1	0.314011900712871E+01	0.314575640023816E+01	0.238785024725699E+01	0.645792868876097E+00
21	3	0	2	0.164525876141841E+01	0.318702139403640E+01	0.348200049008609E+01	0.663487519449685E+00
22	3	0	0	0.549306690646211E+01	0.313423005590041E+01	0.376361954006700E+01	0.494738425712773E+00
23	3	1	1	0.489167893642778E+01	0.310583281642480E+01	0.299668864388672E+01	0.617551331047668E+00