

## Final-state probability distribution for atomic fragments arising in the ( ${}^3\text{He}, n; p, t$ ) reaction with slow neutrons

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Final-state probabilities are determined for different atomic fragments arising in the ( ${}^3\text{He}, n; p, t$ ) reactions with slow neutrons. We consider the ( ${}^3\text{He}, n; p, t$ ) reactions in the one-electron  ${}^3\text{He}^+$  ion and in the two-electron  ${}^3\text{He}$  atom. It is shown that highly exothermic nuclear reactions in light nuclei can be used as a very effective tool to study the electron-density distribution in light atoms and its redistribution during such reactions. The idea of bremsstrahlung amplifiers based on the ( $n, Q; q_1, q_2$ ) reactions in accelerated many-electron ions is proposed.

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### I. INTRODUCTION

In this study we consider the problem of atomic (=electron) excitations in few-electron atoms and ions during the nuclear ( ${}^3\text{He}, n; p, t$ ) reaction of the  ${}^3\text{He}$  nucleus with slow neutrons. This nuclear reaction



of slow neutrons with the  ${}^3\text{He}$  nuclei is extremely important for simplifying thermonuclear burning wave propagation in highly compressed ( $\rho \geq 100 \text{ g cm}^{-3}$ ) deuterium containing thermonuclear fuel. Indeed, this reaction allows one to convert slow neutrons into the tritium nuclei and, therefore, increases the tritium-deuterium ratio [1–3]. In this work, however, we shall consider the ( ${}^3\text{He}, n; p, t$ ) reaction involving an isolated  ${}^3\text{He}$  atom. Such an atom has two electrons. Without loss of generality, we shall assume that originally the  ${}^3\text{He}$  atom was in its ground  $1^1S$  state. We also consider the nuclear ( ${}^3\text{He}, n; p, t$ ) reaction involving the  ${}^3\text{He}^+$  ion. Our main goal below is to determine the final-state probabilities for different states in the final protium and tritium atoms.

It should be mentioned that the general theory of excitations of atomic fragments arising in the exothermic nuclear ( $n, Q; q_1, q_2$ ) reactions of light atoms with slow neutrons was considered in our earlier study [4]. Here we choose not to repeat formulas and conclusions from that work and focus on consideration of reaction [Eq. (1)] only. Some other similar nuclear reactions are mentioned only as examples. The approach used in this study relies on the use of the sudden approximation (see, e.g., [5] and references therein). Moreover, we assume that the incident (slow) neutron does not affect (by its magnetic moment) noticeably any of the electron shells in the incident  ${}^3\text{He}$  atom or ion. The validity of these approximations was discussed, e.g., in [4]. The notation  $p$  and  $t$  stand below in some cases for the  ${}^1\text{H}$  and  ${}^3\text{H}$  nuclei arising in Eq. (1).

Let us evaluate the velocities of the  $p$ (= ${}^1\text{H}$ ) and  $t$ (= ${}^3\text{H}$ ) nuclei arising in the reaction [Eq. (1)] with slow neutrons. In general, the kinetic energies  $T_i$ (MeV) ( $i=1, 2$ ) and corresponding velocities  $v_i$  ( $\text{cm s}^{-1}$ ) of the two nuclear fragments formed in an arbitrary nuclear ( $n, Q; q_1, q_2$ ) reaction of the incident nucleus  $Q$  with slow (or thermal) neutrons ( $v_n \approx 0$  and  $T_n \approx 0$ ) can be evaluated as follows:

$$T_i \approx \frac{M_j}{M_1 + M_2} \mathcal{E} \text{ MeV},$$

$$v_i \approx 0.138 \, 411 \, 2 \times 10^{10} \sqrt{\frac{T_i}{M_i}} \text{ cm s}^{-1}, \quad (2)$$

where  $i \neq j = (1, 2)$  and  $\mathcal{E}$  is the energy released during the ( $n, Q; q_1, q_2$ ) reaction (in MeV). In the last formula for  $v_i$ , we assume that the nuclear mass  $M_i$  is expressed in the units of the neutron mass  $m_n$ . As follows from Eq. (2), the velocities of the tritium  $t$  and protium  $p$  nuclei produced in the reaction [Eq. (1)] are  $v_t \approx 3.493 \, 17 \times 10^8 \text{ cm s}^{-1}$  and  $v_p \approx 1.047 \, 73 \times 10^9 \text{ cm s}^{-1}$ , respectively, for  $E = 0.764 \text{ MeV}$ . The numerical value of the atomic velocity, i.e., the velocity of electron in the ground state of hydrogen atom, is  $v_e = \alpha \cdot c \approx 2.188 \, 266 \, 1 \times 10^8 \text{ cm s}^{-1}$ , where  $\alpha$  is the fine-structure constant and  $c$  is the speed of light in vacuum. Therefore, in atomic units (in which  $v_e = 1$ ), the velocities of the protium and tritium nuclei emitted in the reaction [Eq. (1)] are  $v_p \approx 4.787 \, 97 \text{ a.u.}$  and  $v_t \approx 1.596 \, 32 \text{ a.u.}$

Note that the velocities  $v_t$  and  $v_p$  are approximately 1.6–4.8 times larger than the velocities of the  $1s$  electron in the hydrogen atom. This means that we can apply the sudden approximation for describing electron transitions during the ( ${}^3\text{He}, n; p, t$ ) reaction. On the other hand, the  $v_p$  and  $v_t$  velocities are 30–45 times smaller than the speed of light  $c$ . This means that we can restrict ourselves to the nonrelativistic wave functions of the incident and final fragments.

### II. ONE-ELECTRON HELIUM ION

First, consider the reaction [Eq. (1)] in the one-electron  ${}^3\text{He}^+$  ion which originally was in a hydrogenic ( $n_1 \ell_1 m_1$ ) state. The corresponding wave function takes the form  $\Psi_{n_1, \ell_1}(\mathbf{r}) = R_{n_1, \ell_1}(r) Y_{\ell_1 m_1}(\mathbf{n})$ , where  $\mathbf{n} = \frac{\mathbf{r}}{r}$  is the unit norm vector. After the nuclear reaction [Eq. (1)], one can find either the neutral  ${}^3\text{H}$  atom (tritium atom), or neutral  ${}^1\text{H}$  atom, or two bare nuclei  ${}^3\text{H}^+$  and  ${}^1\text{H}^+$  which do not contain bound electrons. In this work our main interest is related to the bound one-electron atoms or ions at the final stage. Therefore, the wave function of the final state is also written in the hydrogenic form  $\Psi_{n_2, \ell_2}(\mathbf{r}) = R_{n_2, \ell_2}(r) Y_{\ell_2 m_2}(\mathbf{n})$ , but the final

fragment is also moving with the velocity  $v$ , where  $v$  represents the velocity of the tritium nucleus  $v_t$  or the velocity of the protium nucleus  $v_p$ .

Thus to determine the final-state probability, we need to compute the matrix element of the operator  $\exp(i\mathbf{v}\cdot\mathbf{r})$  between the wave functions of the initial and final states in the two atomic systems (original and final). For one-electron atoms or ions, the corresponding wave functions are hydrogenic bound-state wave functions. In such a case, the computation of the final-state probability is performed in the following way.

First, we write the Rayleigh expansion of a plane wave (with the use of spherical harmonic addition theorem). The explicit formula takes the form (see, e.g., [6])

$$\exp(i\mathbf{v}\cdot\mathbf{r}) = 4\pi \sum_{\ell=0}^{\infty} i^{\ell} j_{\ell}(vr) \sum_{m=-\ell}^{\ell} Y_{\ell m}^*(\mathbf{n}_v) Y_{\ell m}(\mathbf{n}_r), \quad (3)$$

where  $Y_{\ell m}(\mathbf{n})$  are the spherical harmonics,  $\mathbf{v}$  is the velocity of the final atomic fragment, and  $\mathbf{n}_v = \frac{\mathbf{v}}{v}$  is the unit norm vector which corresponds to an arbitrary nonzero vector  $\mathbf{v}$ . Also in this equation the spherical Bessel functions  $j_{\ell}(vr)$  are defined by the relation (see, e.g., [7]),

$$j_{\ell}(vr) = \sqrt{\frac{\pi}{2vr}} J_{\ell+1/2}(vr), \quad (4)$$

where  $J_{\ell+1/2}(x)$  are the Bessel functions. Now, by applying the sudden approximation mentioned above (for more detail, see [4] and references therein) and with the use of Eq. (3), one finds the following explicit expression for the transition-probability amplitude  $A_{in:fi}$ :

$$\begin{aligned} A_{in:fi} &= A_{n_1, \ell_1, m_1; n_2, \ell_2, m_2} \\ &= \langle \Psi_{n_2, \ell_2, m_2}(\mathbf{r}) | \exp(i\mathbf{v}_N \cdot \mathbf{r}) | \Psi_{n_1, \ell_1, m_1}(\mathbf{r}) \rangle \\ &= \sum_{LM} (-1)^{m_1 L} \sqrt{4\pi(2\ell_1+1)(2\ell_2+1)(2L+1)} \\ &\quad \times \begin{pmatrix} \ell_1 & \ell_2 & L \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} \ell_1 & \ell_2 & L \\ -m_1 & m_2 & -M \end{pmatrix} Y_{LM}(\mathbf{n}_v) \\ &\quad \times \langle R_{n_2, \ell_2}(r) | j_L(vr) | R_{n_1, \ell_1}(r) \rangle, \end{aligned} \quad (5)$$

where  $R_{n_i, \ell_i}(r)$  ( $i=1, 2$ ) are the radial functions of the initial and final states in the hydrogenlike system. In this formula, we also use the standard notation for the Wigner  $3j$  coefficients (see, e.g., [6,8]). This expression for the transition-probability amplitude  $A_{in:fi}$  ( $=A_{n_1, \ell_1, m_1; n_2, \ell_2, m_2}$ ) contains all partial spherical waves  $Y_{LM}(\mathbf{n}_v)$ , where  $L=|\ell_1-\ell_2|, \dots, \ell_1+\ell_2$ .

In the usual situation, the magnetic quantum numbers of the initial and final states are unknown. Therefore, the formula for the final-state probability  $P_{in:fi} = |A_{\ell_1, m_1; \ell_2, m_2}|^2$  must be averaged over the initial-state magnetic and summed over all final-state quantum numbers. After a few simple transformations, one finds for the final-state probability,

$$\begin{aligned} \bar{P}_{n_1, \ell_1; n_2, \ell_2}(v) &= (2\ell_2+1) \sum_L (2L+1) \\ &\quad \times \begin{pmatrix} \ell_1 & \ell_2 & L \\ 0 & 0 & 0 \end{pmatrix}^2 |\langle R_{n_2, \ell_2}(r) | j_L(vr) | R_{n_1, \ell_1}(r) \rangle|^2. \end{aligned} \quad (6)$$

In fact, this formula corresponds to the transitions between two bound states in one-electron systems, but the nuclei in these systems have different electric charges and one of the one-electron systems moves with the relatively large velocity  $v$ . It follows from the last formula that, e.g., if the incident one-electron atom or ion is in its ground  $s$  state then the excited  $L$  state of the final atom can be observed if (and only if) the experiment allows one to detect the  $L$  wave. In other words, if in some experiment one can observe only  $S$ ,  $P$ , and  $D$  waves then it is impossible to detect in this experiment the  $F$  state of the final atomic system.

Thus, for hydrogenlike (or one-electron) systems, the computation of the final-state probability  $P_{in:fi}$  is reduced to the analytical/numerical computation of the corresponding radial integrals. Let us consider this problem in detail. The unit norm radial functions of the hydrogenlike wave functions for atom or ion (bound state) with the infinitely heavy nucleus with nuclear charge  $Q$  are written in the form (see, e.g., [8]),

$$\begin{aligned} R_{n, \ell}(Q, r) &= \frac{1}{rn} \sqrt{\frac{Q(n-\ell-1)!}{(n+\ell)!}} \left[ \frac{2Qr}{n} \right]^{\ell+1} \sum_{k=0}^{n-\ell-1} \frac{(-1)^k}{k!} \\ &\quad \times \binom{n+\ell}{2\ell+k+1} \left[ \frac{2Qr}{n} \right]^k \exp\left(-\frac{Qr}{n}\right). \end{aligned} \quad (7)$$

If the final state in the moving hydrogenlike system with the new nuclear charge  $q(\leq Q)$  is also bound then the computation of radial integral in Eq. (6) is reduced to the calculation of the following matrix element:

$$\begin{aligned} &\langle R_{n_2, \ell_2}(r) | j_L(vr) | R_{n_1, \ell_1}(r) \rangle \\ &= \int_0^{\infty} R_{n_2, \ell_2}(Q, r) j_L(vr) R_{n_1, \ell_1}(q, r) r^2 dr. \end{aligned} \quad (8)$$

The radial functions  $R_{n_2, \ell_2}(r)$  and  $R_{n_1, \ell_1}(r)$  can be represented as finite sums of the products of powers of  $r$  and exponents  $\exp(-Xr)$ , where  $X>0$ . This matrix element can be computed with the use of Eq. (4) for radial Bessel functions. Finally, the integral [Eq. (8)] is computed as the finite sum of the following integrals:

$$\begin{aligned} &\sqrt{\frac{\pi}{2v}} \int_0^{\infty} t^{\mu-1} J_{\nu}(vt) \exp(-Xt) dt \\ &= \sqrt{\frac{\pi}{2v}} \frac{\Gamma(\mu+\nu)}{\Gamma(\nu+1)} \frac{v^{\nu}}{2^{\nu}(X^2+v^2)^{\mu+\nu/2}} \\ &\quad \times {}_2F_1\left(\frac{\mu+\nu}{2}, \frac{\nu-\mu+1}{2}; \nu+1; \frac{v^2}{X^2+v^2}\right), \end{aligned} \quad (9)$$

where  ${}_2F_1(a, b; c; x)$  is the hypergeometric function (see e.g., [7]). To obtain the final expression, one can use

TABLE I. The velocities  $v$  of reaction fragments (in a.u.) and probabilities (in %) of the final states for four exothermic nuclear reactions ( $a-c$ ) of some light one-electron atoms or ions with slow neutrons. The notation  $a(b)$  stands for  $a \times 10^{-b}$ .

State	[a] $t$	[a] $p$	[b] $\alpha$	[b] $t$	[c] ${}^7\text{Li}$	[c] $\alpha$
$V$	1.59632	4.78897	4.52989	6.03986	2.40896	4.21568
$1s$	25.90880	0.443082	8.049481	0.364496	58.22843	15.77608
$2s$	4.617567	0.832412(1)	1.752660	0.612056(1)	9.037463	2.710316
$2p$	0.292997	0.197967(2)	0.127544	0.961119(3)	0.645213	0.112925
$3s$	0.440895(4)	0.514240(3)	0.395100(4)	0.543558(3)	0.533448(4)	0.335469(3)
$3p$	0.125430(1)	0.390495(2)	0.170681(1)	0.291928(2)	0.500858(2)	0.996830(2)
$3d$	0.798786(2)	0.284628(5)	0.645351(3)	0.498505(6)	0.734082(2)	0.285480(3)

various formulas known for the hypergeometric functions, e.g.,  ${}_2F_1(a, 0; c, x) = {}_2F_1(0, a; c, x) = 1$ ,  ${}_2F_1(a, b; a, x) = {}_2F_1(b, a; a, x) = (1-x)^{-b}$  and many others. The explicit formula for the final-state probabilities for the  $1s \rightarrow (n\ell)$  transition in one-electron atom or ion is derived in Appendix A.

Let us present the explicit formulas for the transition probabilities to the ground and excited states of the tritium and protium atoms which are formed in nuclear reaction [Eq. (1)] from the ground state of the  $\text{He}^+$  ion. Let  $Q$  be the nuclear charge of the incident nucleus ( ${}^3\text{He}$ ), while  $q$  designates the nuclear charge of the final nuclei ( ${}^3\text{H}$  and/or  ${}^1\text{H}$ ), which move with the speeds  $v_t$  and  $v_p$ , respectively. The probability of formation of the tritium ( ${}^3\text{H}$ ) atom in its ground state is

$$P_{g,g} = P_{1s,1s} = \frac{64(Qq)^3}{(Q+q)^6} \frac{1}{\left[1 + \left(\frac{v}{Q+q}\right)^2\right]^4}. \quad (10)$$

From this formula one finds for the  ${}^3\text{H}$  atom from the reaction [Eq. (1)], ( $Q=2, q=1, v=v_t$ )  $P_{g,g} \approx 0.259\,088$ , i.e., approximately 25.9% of all  ${}^3\text{H}$  atoms formed in the reaction [Eq. (1)] will be in their ground states. The analogous probability for the  ${}^1\text{H}$  atom will be  $\approx 0.004\,430\,8$ , i.e., approximately 0.44% of all protium atoms will be in their ground states. In fact, Eq. (10) shows a very sharp dependence of the total probability on the velocity and nuclear charge of the final fragment.

The probability of formation of the tritium atom in its  $2p$  state is

$$P_{1s,2p} = \frac{32(Qq)^3 q^2 v^2}{3 \left(Q + \frac{q}{2}\right)^{10}} \frac{1}{\left[1 + \left(\frac{v}{Q + \frac{q}{2}}\right)^2\right]^6}. \quad (11)$$

For the  ${}^3\text{H}$  atom from the reaction [Eq. (1)], one finds  $P_{1s,2p} \approx 0.293\,0\%$ , while for the protium atom  $P_{1s,2p} \approx 0.019\,80\%$ . In the case  $Q=q=1$ , our formula [Eq. (11)] coincides with Eq. (24) from [9]. The analogous probability for the  $3d$  final state is

$$P_{1s,3d} = \frac{2}{15} \left(\frac{4}{3}\right)^8 \frac{(3Q+q)^2 (Qq)^3 q^4 v^2}{\left[\left(Q + \frac{q}{3}\right)^2 + v^2\right]^8}. \quad (12)$$

Again for  $Q=q=1$ , this formula coincides with Eq. (25) from [9]. The probability amplitude for the  $g \rightarrow 2s$  transition takes the form

$$M_{1s,2s} = \frac{\sqrt{2}(qQ)^{3/2}}{\left[\left(Q + \frac{q}{2}\right)^2 + v^2\right]^2} \left\{ 2Q - q + \frac{4qv^2}{\left[\left(Q + \frac{q}{2}\right)^2 + v^2\right]} \right\}. \quad (13)$$

The corresponding transition probability  $P_{g,2s} = |M_{1s,2s}|^2$  thus contains in this case a number of terms.

The explicit analytical formulas for the amplitudes of the final-state probabilities in the case of  $3p$  and  $3d$  final states are

$$M_{1s,3p} = \frac{64v^2}{27\sqrt{6}(X^2 + v^2)^3} (Qq)^{3/2} \times \left[ \frac{2X}{5} {}_2F_1\left(1, 3; \frac{7}{2}; \frac{v^2}{X^2 + v^2}\right) - \frac{q}{3} \right], \quad (14)$$

where  $X = Q + \frac{q}{3}$ , and

$$M_{1s,3s} = \frac{32v^2}{27(X^2 + v^2)^3} (Qq)^{3/2} \times \left[ \frac{X}{5} {}_2F_1\left(1, 3; \frac{7}{2}; \frac{v^2}{X^2 + v^2}\right) - \frac{2q}{3} + \frac{4q^2}{9} \frac{X}{X^2 + v^2} \right], \quad (15)$$

respectively. The numerical value of the hypergeometric function used in these both formulas can easily be determined.

The computed numerical values of the probabilities to form the six lowest electronic states in the tritium and hydrogen atoms can be found in Table I. This case corresponds to the  $({}^3\text{He}, n; p, t)$  nuclear reaction and it is designated with the letter [a]. Table I also contains the final-state probabilities determined for two other exothermic nuclear reactions

with slow neutrons:  $[b]$  ( ${}^6\text{Li}, n; \alpha, t$ ) ( $E \approx 4.785$  MeV) and  $[c]$  ( ${}^{10}\text{B}, n; {}^7\text{Li}, \alpha$ ) ( $E \approx 2.791$  MeV). All three nuclear reactions are considered in the corresponding one-electron ions, i.e., in the  ${}^3\text{H}^+$ ,  ${}^6\text{Li}^{2+}$ , and  ${}^{10}\text{B}^{4+}$  ions.

The final-state probabilities determined for all atomic fragments arising during these nuclear reactions (i.e., in the  $[a]$ ,  $[b]$ , and  $[c]$  cases) with slow neutrons show similar dependencies upon the velocity of reaction fragment, its electric charge, and quantum number(s) of the final state. An obvious exception is the  ${}^7\text{Li}$  nucleus from the ( ${}^{10}\text{B}, n; {}^7\text{Li}, \alpha$ ) reaction. But in this case, we cannot apply the sudden approximation, since the velocity of this nucleus is only  $\approx 2.40896$  a.u. This is smaller than the velocity of  $1s$  electron (or  $K$  electron) in the final lithium atom. Nevertheless, the sudden approximation can still be applied to the  ${}^4\text{He}^+$  ion arising in the ( ${}^{10}\text{B}, n; {}^7\text{Li}, \alpha$ ) reaction. The velocity of  $\alpha$  particle from this reaction is  $\approx 4.21568$  a.u. is approximately twice as large as the velocity of  $1s$  electron in the He atom. Therefore, the results from Table I make sense (and close to our expectations) for all atomic fragments, but not for the  ${}^7\text{Li}^{2+}$  ion. In general, this explains the reason why one can apply the sudden approximation to determine the final electronic state probabilities in the hydrogen atom arising in many exothermic ( $n, p$ ) reactions, e.g., in the ( ${}^{14}\text{N}, n; {}^{14}\text{C}, p$ ) reaction ( $E \approx 0.625$  MeV).

### III. TWO-ELECTRON HELIUM ATOM

Let us consider a different situation when the incident atomic system in Eq. (1) is the two-electron helium atom  ${}^3\text{He}$ . In this case, we also need to consider various bound states in this two-electron atom. In principle, each of these states can be chosen as an incident atomic state for the reaction (1). In this study, however, we shall restrict ourselves to the cases when the two-electron helium atom  ${}^3\text{He}$  is in its ground  $1^1S$  state. The total wave function of the ground  $1^1S$  state is represented as the product of the radial and spin components, i.e.,  $\Psi_{L=0}(\mathbf{x}_1, \mathbf{x}_2) = \Psi(\mathbf{r}_1, \mathbf{r}_2) \frac{1}{\sqrt{2}}(\alpha\beta - \beta\alpha)$ , where  $\phi(\mathbf{r}_1, \mathbf{r}_2) = \phi(r_1, r_2, r_{12})$  is the radial part (component) of the total wave function, while  $\frac{1}{\sqrt{2}}(\alpha\beta - \beta\alpha)$  is the corresponding spin (singlet) part of the total wave function.

In the general case, we can write for the probability to find the tritium atom in its  $n$ th state, if the incident He atom was in the ground  $1^1S$  state,

$$P_{\text{He}, {}^3\text{H}} = |\langle \Psi_n(q=1; \mathbf{x}_1) | \exp(i\mathbf{v}_t \cdot \mathbf{r}_1) | \Psi_g(Q=2, \mathbf{x}_1, \mathbf{x}_2) \rangle|^2, \quad (16)$$

where  $\mathbf{v}_t$  is the final velocity of the tritium atom and  $\mathbf{x}_i$  are the compact notations used to designate the spatial ( $\mathbf{r}_i$ ) and spin ( $\sigma_i$ ) coordinates of the  $i$ th electron. Also, in this equation  $\Psi_n(q=1; \mathbf{x}_1)$  is the one-electron wave function of the final hydrogenlike atom ( ${}^3\text{H}$  or  ${}^1\text{H}$ ), while  $\Psi_g(Q=2, \mathbf{x}_1, \mathbf{x}_2)$  is the two-electron wave function of the incident  ${}^3\text{He}$  atom. The generalization of this formula to the  $N$  electron systems in an arbitrary state can be found in [4]. In this work, we are not interested in the spin variables. For the one- and two-electron systems, the spin variables can be always separated from the electron parts of the total wave functions. There-

fore, by integrating over all spin variables, one finds the formula

$$P_{\text{He}, {}^3\text{H}} = |\langle \Psi_n(q=1; \mathbf{r}_1) | \exp(i\mathbf{v}_t \cdot \mathbf{r}_1) | \Psi_g(Q=2, \mathbf{r}_1, \mathbf{r}_2) \rangle|^2, \quad (17)$$

which contains only spatial variables. This integral can be computed in a number of ways, e.g., directly with the use of three-body perimetric coordinates. This approach is discussed in Appendix B. It has extensively been used in calculations for this study. An alternative approach includes the operations with the density matrices. This approach is considered below.

#### One-electron-density matrix

By introducing the one-electron-density matrix  $\rho_g(\mathbf{r}_1, \mathbf{r}'_1)$  [10] for the ground  $1^1S$  state of the two-electron He atom

$$\rho_g(\mathbf{r}_1, \mathbf{r}'_1) = \int |\Psi_g(\mathbf{r}_1, \mathbf{r}_2) \rangle \langle \Psi_g(\mathbf{r}'_1, \mathbf{r}_2) | d^3\mathbf{r}_2, \quad (18)$$

one can rewrite the formula [Eq. (17)] for the final-state probability in the form

$$P_{\text{He}, {}^3\text{H}} = \left| \int \rho_g(\mathbf{r}_1, \mathbf{r}'_1) \exp[i\mathbf{v}_t \cdot (\mathbf{r}_1 - \mathbf{r}'_1)] \times \psi_n(\mathbf{r}_1) \psi_n(\mathbf{r}'_1) d^3\mathbf{r}_1 d^3\mathbf{r}'_1 \right|^2, \quad (19)$$

where  $\psi_n$  is the hydrogenic (one-electron) wave function of the final state of the  ${}^3\text{H}$  atom. In the general case, when we have  $N$  electrons in the incident state and  $K$  electrons in the final state, one has to introduce various many-electron-density matrices and transition matrices [4]. Note also that the one-electron-density matrix has “unit norm,” i.e.,

$$\int \rho_g(\mathbf{r}_1, \mathbf{r}_1) d^3\mathbf{r}_1 = 1. \quad (20)$$

To illustrate the formulas derived above, let us apply them to the computation of the final-state probabilities of atomic fragments arising during the nuclear ( ${}^3\text{He}, n; p, t$ ) reaction. Let us assume that the incident helium atom was in its ground  $1^1S(L=0)$  state with the approximate wave function

$$\Psi(\mathbf{r}_1, \mathbf{r}_2) = \frac{Q^3}{\pi} \exp[-Q(r_1 + r_2)], \quad (21)$$

where  $r_i = |\mathbf{r}_i|$  ( $i=1, 2$ ), while the parameter  $Q = Z - \frac{5}{16}$  (so-called optimal nuclear charge, see, e.g., [8, 11]) and  $Z=2$  for the helium atom. From here, one finds the explicit expression for the one-electron spinless density matrix in the helium atom

$$\rho(\mathbf{r}_1, \mathbf{r}'_1) = \frac{Q^3}{\pi} \exp[-Q(r_1 + r'_1)]. \quad (22)$$

Now, for the ground  $1s$  state in the tritium atom, the final-state probability is given by the expression given in Eq. (19),

$$\begin{aligned}
P(G(\text{He}) \rightarrow G(T, \mathbf{V}_t)) &= \langle \rho_{\text{He}}^{(1)}(G(\text{He}); \mathbf{r}_1; \mathbf{r}'_1) | \exp(i\mathbf{V}_t \cdot (\mathbf{r}_1 - \mathbf{r}'_1)) \\
&\quad \times |\psi_T(G(T); \mathbf{r}_1) \psi_T(G(T); \mathbf{r}'_1)\rangle \\
&= \frac{4(q \cdot Q)^3}{\pi} \\
&\quad \times \left\{ \int_0^\infty dr r^2 \exp[-(Q+q)r + i\mathbf{V}_t \cdot \mathbf{r}] \right\} \\
&\quad \times \left\{ \int_0^\infty dr r^2 \exp[-(Q+q)r - i\mathbf{V}_t \cdot \mathbf{r}] \right\}, \tag{23}
\end{aligned}$$

where  $G$  designates the ground state of the corresponding system, i.e.,  $1^1S$  state in the He atom and  $1s$  state in the  $^3\text{H}$  and/or  $^1\text{H}$  atom.

It is clear that the result [Eq. (23)] does not depend upon the direction of the final tritium nucleus, i.e., it does not change upon the substitution  $\mathbf{V}_t \rightarrow -\mathbf{V}_t$ . By computing both integrals in Eq. (23), one finds

$$P(G(\text{He}) \rightarrow G(T, \mathbf{V}_t)) = \frac{64Q^3q^3}{(Q+q)^6} \frac{1}{\left[1 + \frac{V_t^2}{(Q+q)^2}\right]^4}. \tag{24}$$

Note that this formula coincides exactly with Eq. (10). By using the values  $Q = \frac{27}{16}$  [8],  $q = 1$ , and  $V_t = 1.59632$ , one finds that  $P(G(\text{He}) \rightarrow G(T, \mathbf{V}_t)) \approx 24.37\%$ . Analogously, the probability to form the  $2s$  state in the tritium atom is  $\approx 0.418\%$  [this follows from Eq. (11) with  $Q = \frac{27}{16}$ ]. For the protium atom  $^1\text{H}$  (or  $p$ ) which is formed in the nuclear ( $^3\text{He}, n; p, t$ ) reaction of two-electron helium atom, one finds  $P(G(\text{He}) \rightarrow 1s(^1\text{H}, \mathbf{V}_p)) \approx 0.269\%$  and  $P(G(\text{He}) \rightarrow 2s(^1\text{H}, \mathbf{V}_p)) \approx 3.62 \times 10^{-3}\%$ . The actual probabilities computed with the use of highly accurate wave functions for the helium atom are slightly different from these values (see below).

The simplicity of the one-electron spinless density matrix used above [see Eq. (22)] can force one to search for some special functions which reduce the  $\rho(\mathbf{r}_1, \mathbf{r}'_1)$  matrix to a diagonal form. It appears that the one-electron spinless density matrix  $\rho(\mathbf{r}_1, \mathbf{r}'_1)$  can always be so reduced, i.e.,

$$\rho(\mathbf{r}; \mathbf{r}') = \sum_{j=1}^{\infty} n_j \chi_j(\mathbf{r}) \chi_j(\mathbf{r}'), \tag{25}$$

where the  $\chi_j(\mathbf{r})$  are spin-free functions of one variable. These functions are called the natural orbitals, while the corresponding numbers  $n_j$  are the occupation numbers [12] (see also [13,14] and references therein). The natural orbitals  $\chi_j(\mathbf{r})$  are pairwise orthogonal and have unit norm, i.e.,  $\langle \chi_i(\mathbf{r}) | \chi_j(\mathbf{r}) \rangle = \delta_{ij}$ . The occupation numbers  $n_j$  in this equation are always non-negative and for an arbitrary  $j$ ,  $0 \leq n_j \leq 1$ . The number of nonzero occupation numbers is called the rank  $r$  of the  $\rho(\mathbf{r}_1, \mathbf{r}'_1)$  matrix. The advantage of using the natural orbital expansion [Eq. (25)] for the one-electron spin-

less density matrix of the He atom is obvious, since in such cases the computation of corresponding probabilities is reduced to a trivial problem. However, an overall accuracy can be lost during this procedure and below we shall not use it. Instead, we want to construct the one-electron (spinless) density matrix  $\rho(\mathbf{r}_1, \mathbf{r}'_1)$  from highly accurate three-body wave functions.

Note that all final-state probabilities for the ( $^3\text{He}, n; p, t$ ) reaction in atoms can be obtained from Eq. (19). However, for two-electron atomic systems which take part (or arise) in the ( $^3\text{He}, n; p, t$ ) reaction, we have developed a procedure which can be used to construct the one-electron-density matrices from the explicitly correlated two-electron wave function. Additional complexity of the problem follows from the fact that three relative coordinates  $r_{32}$ ,  $r_{31}$ , and  $r_{21}$  used in the explicitly correlated wave functions cannot be separated from each other. Here and below in this study, the relative coordinate is  $r_{ij} = |\mathbf{r}_i - \mathbf{r}_j| = r_{ji}$ , where  $\mathbf{r}_i$  and  $\mathbf{r}_j$  are Cartesian coordinates of the particles with indexes  $i$  and  $j$ , respectively. The subscripts 1 and 2 designate the two electrons, while subscript 3 always means the positively charged nucleus. In fact, for atomic two-electron systems and for our present purposes, the following system of interparticle notation  $r_2 (= r_{32})$ ,  $r_1 (= r_{31})$ , and  $r_{21}$  is more convenient.

The advantage of relative coordinates follows from the fact that highly accurate wave functions of arbitrary two-electron atomic systems can easily be determined numerically with the use of the following variational expansions for the wave function  $\Phi_A(r_1, r_2, r_{12})$ :

$$\Phi_A(r_1, r_2, r_{12}) = \sum_{i=1}^{N_1} \sum_{j=1}^{N_2} \sum_{k=1}^{N_3} C_{ijk} \phi_i(r_1) \phi_j(r_2) \phi_k(r_{12}), \tag{26}$$

where  $C_{ijk}$  are the known variational coefficients and  $\phi_i$ ,  $\phi_j$ , and  $\phi_k$  are the single-argument basis functions. Below, for simplicity we restrict ourselves to the consideration of the  $S(L=0)$  states in two-electron atomic systems only. The generalization of our present method to the states with  $L \geq 1$  is straightforward, but it requires numerous additional notations and explanations.

The formula [Eq. (26)] is applied to the bound  $S(L=0)$  state in an arbitrary three-body system. For two-electron systems, the actual permutation symmetry between two electrons must also be taken into account. As we mentioned above, all states of the two-electron atoms and ions are separated into two series: singlet and triplet states. For singlet states, all radial parts of the total wave functions must be symmetrized in the following way:

$$\begin{aligned}
\Phi_A(r_1, r_2, r_{12}) &= \frac{1}{2} (1 + \hat{P}_{12}) \sum_{i=1}^{N_1} \sum_{j=1}^{N_2} \sum_{k=1}^{N_3} C_{ijk} \phi_i(r_1) \phi_j(r_2) \phi_k(r_{12}) \\
&= \frac{1}{2} \sum_{i=1}^{N_1} \sum_{j=1}^{N_2} \sum_{k=1}^{N_3} C_{ijk} [\phi_i(r_1) \phi_j(r_2) \phi_k(r_{12}) \\
&\quad + \phi_j(r_1) \phi_i(r_2) \phi_k(r_{12})], \tag{27}
\end{aligned}$$

where  $\hat{P}_{12}$  is the electron-electron permutation ( $\hat{P}_{12}^2 = 1$ ).

First, consider a three-particle system which contains three nonidentical particles. In this case, the one-particle density matrix for the bound  $S(L=0)$  state can be written in the form

$$\begin{aligned} \rho_g(r_1, r'_1) &= \sum_{i=1}^{N_1} \sum_{j=1}^{N_2} \sum_{k=1}^{N_3} \sum_{l=1}^{N_1} \sum_{J=1}^{N_2} \sum_{K=1}^{N_3} C_{ijk} C_{lJK} \\ &\times \left[ \phi_i(r_1) \phi_l(r'_1) \int_{A_1}^{A_2} \phi_j(r_2) \phi_J(r_2) r_2 dr_2 \right. \\ &\left. \times \int_{B_1}^{B_2} \phi_k(r_{12}) \phi_K(r_{12}) r_{12} dr_{12} \right], \end{aligned} \quad (28)$$

where the limits  $A_1$  and  $A_2$  are the functions of  $r_1$  and  $r'_1$ , while the internal limits  $B_1$  and  $B_2$  depend upon the  $r_1, r_2, r'_1$ , and  $r'_2$  variables. Finally, the explicit expression for the internal product of integrals

$$G = \int_{A_1}^{A_2} \phi_j(r_2) \phi_J(r_2) r_2 dr_2 \int_{B_1}^{B_2} \phi_k(r_{12}) \phi_K(r_{12}) r_{12} dr_{12} \quad (29)$$

contains 16 different terms which represent all possible locations of the four points  $(r_1, r'_1, r_2, r'_2)$  on the real axes. From Eq. (28), one also finds that

$$\begin{aligned} \int_0^\infty \rho_g(r_1, r_1) r_1 dr_1 &= \sum_{i=1}^{N_1} \sum_{j=1}^{N_2} \sum_{k=1}^{N_3} \sum_{l=1}^{N_1} \sum_{J=1}^{N_2} \sum_{K=1}^{N_3} C_{ijk} C_{lJK} \left[ \int_0^\infty \phi_i(r_1) \phi_l(r_1) r_1 dr_1 \int_{A_1}^{A_2} \phi_j(r_2) \phi_J(r_2) r_2 dr_2 \int_{|r_1-r_2|}^{r_1+r_2} \phi_k(r_{12}) \phi_K(r_{12}) r_{12} dr_{12} \right] \\ &= 1, \end{aligned} \quad (30)$$

where  $A_1$  can be 0 or  $r_1$ , while  $A_2$  can be  $r_1$  or  $\infty$ . Formally, in this case Eq. (29) is equivalent to the condition that the wave function  $\Phi_A(r_1, r_2, r_{12})$  [Eq. (26)] has a unit norm.

For two-electron atomic systems, the one-particle density matrix for the bound  $S(L=0)$  state can be written in the form,

$$\begin{aligned} \rho_g(r_1, r'_1) &= \sum_{i=1}^{N_1} \sum_{j=1}^{N_2} \sum_{k=1}^{N_3} \sum_{l=1}^{N_1} \sum_{J=1}^{N_2} \sum_{K=1}^{N_3} C_{ijk} C_{lJK} \left[ \phi_i(r_1) \phi_l(r'_1) \int_{A_1}^{A_2} \phi_j(r_2) \phi_J(r_2) r_2 dr_2 \int_{B_1}^{B_2} \phi_k(r_{12}) \phi_K(r_{12}) r_{12} dr_{12} \right. \\ &\left. + \phi_i(r_1) \phi_j(r'_1) \int_{A_1}^{A_2} \phi_j(r_2) \phi_l(r_2) r_2 dr_2 \int_{B_1}^{B_2} \phi_k(r_{12}) \phi_K(r_{12}) r_{12} dr_{12} \right]. \end{aligned} \quad (31)$$

By using the analytical formulas derived above, we have evaluated the final-state probabilities to detect one-electron tritium/protium atoms in those cases in which the incident He atom is in its ground state. In particular, we have found for the ground state of the tritium ( $^3\text{H}$ ) atom  $P_{g,g}(^3\text{H}) \approx 27.3\%$ , while for the corresponding protium ( $^1\text{H}$ ) atom  $P_{g,g}(^1\text{H}) \approx 0.51\%$ . The corresponding probabilities to find the final tritium and protium atoms in the excited  $2s$  states are  $P_{g,2s}(^3\text{H}) \approx 4.75\%$  and  $P_{g,g}(^1\text{H}) \approx 0.93\%$ , respectively. In general, these results are quite close to the corresponding probabilities obtained in Sec. II for the one-electron  $\text{He}^+$  ion. It should be mentioned that if the nuclear ( $^3\text{He}, n; p, t$ ) reaction proceeds in the two-electron He atom then one can also detect the formation of two-electron tritium ion ( $^3\text{H}^-$ ) in the final state. The probability of such a process is evaluated below.

#### IV. FORMATION OF THE TWO-ELECTRON FRAGMENTS

If the nuclear  $(n, Q; q_1, q_2)$  reaction involves many-electron atoms or ions then it is possible to detect atomic fragments of this reaction which contain two and even more electrons. For the ( $^3\text{He}, n; p, t$ ) and ( $^6\text{Li}, n; \alpha, t$ ) reactions, the observation of the final atomic fragments with two elec-

trons is of some interest in applications. From a theoretical point of view, it is interesting to evaluate the total probability of tritium  $^3\text{H}^-$  ion formation from the ( $^3\text{He}, n; p, t$ ) reaction, if it proceeds in a two-electron  $^3\text{He}$  atom. It is clear *a priori* that such probabilities are small. For instance, by using data from Table I, one can evaluate that the total probability to form the  $^3\text{H}^-$  ion (negatively charged tritium ion) in the ( $^3\text{He}, n; p, t$ ) reaction is  $\approx 0.625\%$ . Here we want to develop a rigorous procedure for evaluating the final-state probabilities in those cases when two-electron atomic fragments are formed during exothermic nuclear reactions of light nuclei with slow neutrons.

To obtain the complete solution of this problem, consider first the approximate wave function for both two-electron systems, i.e., for the helium atom (ground state) and tritium ion  $^3\text{H}^-$ . The two-electron tritium ion  $^3\text{H}^-$  has only one bound state ( $1^1S$ -ground state). The approximate ground-state wave functions of these ions at rest are represented in the following one-term form:

$$\Psi_g(r_1, r_2, r_{12}) = \mathcal{C} \frac{1}{2} (1 + P_{12}) \exp(-\alpha_1 r_1 - \alpha_2 r_2 - \alpha_3 r_{12}), \quad (32)$$

where  $r_1$  and  $r_2$  are the two scalar electron-nuclear coordinates,  $r_{12}$  is the scalar electron-electron coordinate. The op-

TABLE II. Optimal values of the nonlinear parameters  $\alpha_1$ ,  $\alpha_2$ , and  $\alpha_3$  and normalization constants  $C$  (the value of  $C^{-2}$  is presented) used in the one-term wave function [Eq. (18)].

System	$\alpha_1$	$\alpha_2$	$\alpha_3$	$C^{-2}$
${}^\infty\text{H}^-$	1.07502156952042 <sup>a</sup>	0.483749895649205	-0.146567513488393	1.08729676507270
${}^\infty\text{He}$	2.20655916007215 <sup>b</sup>	1.44058525334471	-0.207334197404063	$3.16685234182372 \times 10^{-3}$

<sup>a</sup>The total energy of this system is -0.523 865 929 763 678 a.u.

<sup>b</sup>The total energy of this system is -2.899 534 375 443 69 a.u.

erator  $\hat{P}_{12}$  designates the electron-electron permutation. The optimal values of nonlinear parameters  $\alpha_1$ ,  $\alpha_2$ , and  $\alpha_3$  for this one-term trial wave functions can be found in Table II (in atomic units). Table II also contains the numerical values of normalization constant  $C$  and variational energy  $E$  for each one-term wave function. Note that our ‘‘one-term’’ wave functions for both systems with carefully optimized nonlinear parameters are the best functions in their class.

As follows from Table II, the nonlinear parameter  $\alpha_3$  is relatively small for both systems. So, in the first approximation, we can assume that  $\alpha_3=0$ . Note that this parameter is responsible for describing the electron-electron correlations. In the systems with  $\alpha_3=0$ , there is no correlation at all and the two electrons are considered to be independent. For atomic systems with two independent electrons, the corresponding amplitude  $M$  of the final-state probability is the symmetrized sum of the two following terms:

$$\begin{aligned}
 M = & \frac{1}{2}C_{\text{He}}C_{\text{H}^-} \left[ \int_0^{+\infty} \exp[-(\alpha_1 + \beta_1)r_1]j_0(vr_1)r_1^2 dr_1 \right. \\
 & \times \int_0^{+\infty} \exp[-(\alpha_2 + \beta_2)r_2]j_0(vr_2)r_2^2 dr_2 \\
 & + \int_0^{+\infty} \exp[-(\alpha_1 + \beta_2)r_1]j_0(vr_1)r_1^2 dr_1 \\
 & \left. \times \int_0^{+\infty} \exp[-(\alpha_2 + \beta_1)r_2]j_0(vr_2)r_2^2 dr_2 \right], \quad (33)
 \end{aligned}$$

where  $\alpha_i$  and  $\beta_i$  ( $i=1,2$ ) are the ‘‘optimal’’ exponents determined for the He atom and  ${}^3\text{H}^-$  ion, respectively. Note that each of these terms is the product of two one-electron integrals which can be computed independently. By applying this approximate formula to the ( ${}^3\text{He}, n; p, t$ ) reaction in two-electron He atom, one finds that the probability of formation of the  ${}^3\text{H}^-$  ion is  $\approx 2.94\%$ , while the probability of  ${}^1\text{H}^-$  ion formation is  $\approx 5.23 \times 10^{-5}\%$ .

Now, if the one-term wave functions also contain interelectron exponents, i.e.,  $\exp(-\gamma_1 r_{12})$  and  $\exp(-\gamma_2 r_{12})$ , respectively, then the last formula is modified to the form,

$$\begin{aligned}
 M = & \frac{1}{2}C_{\text{He}}C_{\text{H}^-} \left[ \int_0^{+\infty} \exp[-(\alpha_1 + \beta_1)r_1]j_0(vr_1)r_1 dr_1 \right. \\
 & \times \int_0^{+\infty} \exp[-(\alpha_2 + \beta_2)r_2]j_0(vr_2)r_2 dr_2 \\
 & \left. \times \int_{|r_1-r_2|}^{r_1+r_2} \exp[-(\gamma_1 + \gamma_2)r_{12}]r_{12} dr_{12} \right]
 \end{aligned}$$

$$\begin{aligned}
 & + \int_0^{+\infty} \exp[-(\alpha_1 + \beta_2)r_1]j_0(vr_1)r_1 dr_1 \\
 & \times \int_0^{+\infty} \exp[-(\alpha_2 + \beta_1)r_2]j_0(vr_2)r_2 dr_2 \\
 & \left. \times \int_{|r_1-r_2|}^{r_1+r_2} \exp[-(\gamma_1 + \gamma_2)r_{12}]r_{12} dr_{12} \right]. \quad (34)
 \end{aligned}$$

Note that despite some similarities between this formula and previous formula [Eq. (33)], these formulas have completely different meaning. In Eq. (33) the variables  $r_1$  and  $r_2$  can be considered as independent variables. This drastically simplifies all the following computations (i.e., integration over all variables). In Eq. (34), we have to integrate first over the interelectron variable  $r_{12}$ . But such an integration will change the explicit form of functions upon  $r_1$  and  $r_2$  variables. Finally, the analytical computation of the integrals over the  $r_1$  and  $r_2$  variables is not an easy task even in simple cases.

Based on the last formula, it is easy to obtain the closed expression for the probability amplitude  $M$  to form the negatively charged  $\text{H}^-$  ion, during the nuclear ( ${}^3\text{He}, n; p, t$ ) reaction in two-electron  ${}^3\text{He}$  atom. Let  $\Psi$  and  $\Phi$  be the three-body wave functions of the helium atom and  $\text{H}^-$  ion, respectively. Below we shall consider the case when these two systems are in their ground states only. As per Eq. (26), we represent these wave functions in the form

$$\Psi(r_1, r_2, r_{12}) = \frac{1}{2}(1 + \hat{P}_{12}) \sum_{i=1}^{N_1} \sum_{j=1}^{N_2} \sum_{k=1}^{N_3} A_{ijk} \psi_i(r_1) \psi_j(r_2) \psi_k(r_{12}), \quad (35)$$

$$\Phi(r_1, r_2, r_{12}) = \frac{1}{2}(1 + \hat{P}_{12}) \sum_{i=1}^{N_1} \sum_{j=1}^{N_2} \sum_{k=1}^{N_3} B_{ijk} \phi_i(r_1) \phi_j(r_2) \phi_k(r_{12}), \quad (36)$$

where  $A_{ijk}$  and  $B_{ijk}$  are the corresponding variational coefficients determined from the results of highly accurate computations of these systems and  $\hat{P}_{12}$  is the electron-electron permutation. In this notation, one can write the closed expression for the probability amplitude,

$$\begin{aligned}
M = & \frac{1}{2} C_{\text{He}} C_{\text{H}^-} \sum_{i=1}^{N_1} \sum_{j=1}^{N_2} \sum_{k=1}^{N_3} \sum_{l=1}^{K_1} \sum_{J=1}^{K_2} \sum_{K=1}^{K_3} A_{ijk} B_{IJK} \\
& \times \left[ \int_0^{+\infty} \psi_i(r_1) \phi_l(r_1) j_0(vr_1) r_1 dr_1 \int_0^{+\infty} \psi_j(r_2) \phi_J(r_2) j_0(vr_2) r_2 dr_2 \int_{|r_1-r_2|}^{r_1+r_2} \psi_k(r_{12}) \phi_K(r_{12}) r_{12} dr_{12} \right. \\
& \left. + \int_0^{+\infty} \psi_i(r_1) \phi_j(r_1) j_0(vr_1) r_1 dr_1 \int_0^{+\infty} \psi_j(r_2) \phi_l(r_2) j_0(vr_2) r_2 dr_2 \int_{|r_1-r_2|}^{r_1+r_2} \psi_k(r_{12}) \phi_K(r_{12}) r_{12} dr_{12} \right]. \quad (37)
\end{aligned}$$

By using this formula, we can evaluate the amplitude of the final-state probability to form the  ${}^3\text{H}^-$  ion from the two-electron He atom during the  $(n, {}^3\text{He}, t, p)$  nuclear reaction. Indeed, each of the integrals in this formula can be computed (in many cases analytically, in some cases numerically), while the coefficients  $A_{ijk}$  and  $B_{IJK}$  are assumed to be known from the corresponding variational expansions. To illustrate this formula, we determined the probability amplitude to detect the  ${}^3\text{H}^-$  ion in its ground state in the nuclear reaction [Eq. (1)], in which the original He atom was also in its ground state. The result is  $M \approx 0.095$  and the total probability  $P = |M|^2 \approx 0.00925 = 0.925\%$ . Note that the computed probability is quite close to the expected value, i.e., it is relatively small.

## V. TRANSITIONS IN THE MOVING ATOMIC FRAGMENTS

In all the calculations above, we have ignored the transitions between different excited and ground states in the moving atomic fragments. It is clear, however, that such transitions can be important in some cases because their overall contribution may change the final-state probabilities predicted in our calculations. For instance, let us assume that during the nuclear reaction [Eq. (1)], the tritium atom  ${}^3\text{H}$  was formed in the excited  $2p$  state. At the same time the positively charged  ${}^1\text{H}^+$  ion was formed in the same reaction. The atom and ion are rapidly moving from each other in the two opposite directions (in the case of slow neutrons). The original (=minimal) distance  $D$  between these two ions is larger (or equal to)  $a_0 = 1$  a.u., where  $a_0$  is the Bohr radius. At shorter distances (i.e.,  $D < 1$  a.u.), the formation of the tritium atom is not completed and an atomic wave function cannot be associated with the nascent atom. Therefore, we cannot use such distances in our analysis.

In the tritium atom rest frame, the outgoing  ${}^1\text{H}^+$  ion moves with the velocity  $V \approx v_p + v_t \approx 6.5$  a.u. This value is  $\approx 20$  times smaller than the speed of light  $c$ . The electromagnetic interaction between the  ${}^3\text{H}$  atom and rapidly moving  ${}^1\text{H}^+$  ion (i.e., proton) can stimulate the transition from  $2p$  state (and other excited states) of the tritium atom into its ground  $1s$  state. In the case of the  $({}^6\text{Li}, n; \alpha, t)$  reaction, the electromagnetic interaction between fast reaction fragments is even larger.

In this section, we want to consider the interaction between the proton and tritium atoms. This problem was dis-

cussed in [4]. Here we develop a different approach which is significantly simpler and has a number of advantages in applications. The main idea of this approach is very transparent. It was shown [15] that already at very short internuclear distances  $R \geq 0.1$  a.u., the motion of the two reaction fragments proceeds with constant velocities. Therefore, our original problem is reduced to the well-known problem of atomic excitations by a rapidly moving charged particle (proton). The probability of transition from the state  $i$  into the state  $f$  is given by the formula (see, e.g., [8,16])

$$P_{fi} = \frac{1}{\hbar^2} \left| \int_0^T \langle f | \hat{W}(t) | i \rangle \exp(i\omega_{fi}t) dt \right|^2, \quad (38)$$

where  $\hat{W}(t)$  is the perturbation,  $T$  is the time when this perturbation acts, and  $\omega_{fi}$  is the transition frequency. In this section we shall use regular (i.e., nonatomic) units. Let  $\mathbf{r} = (x, y, z)$  be the vector which defines the position of the electron in the tritium atom. The origin of our coordinate system is placed at the tritium nucleus which is assumed to be at rest. The proton moves along the  $x$  direction. The proton position at the moment  $t$  is defined by the initial vector  $\mathbf{R} = (Vt + D, 0, 0)$ .

In this notation, the interaction between the electron and moving proton [i.e., the perturbation  $\hat{W}(t)$  in Eq. (38)] is written in the form

$$\hat{W}(t) = -\frac{Qe^2}{|\mathbf{R} - \mathbf{r}|} = -\frac{Qe^2}{R} - \frac{Qe^2(Vt + D)x}{R^3} - \dots, \quad (39)$$

where  $R = \sqrt{(Vt)^2 + D^2}$ . Since  $x \leq D$  and  $V$  is large then we have  $x \leq R$  and for  $t > 1$  one also finds that  $x \ll R$ . Here and below we restrict ourselves to the two lowest-order terms in the expansion for  $\hat{W}(t)$ . Terms which contain  $y^2$ ,  $z^2$ , and  $x^2$  contribute in higher orders. Note that the first term does not depend upon the electron coordinates. Using Eq. (39) the matrix element in Eq. (38) becomes

$$\langle f | \hat{W}(t) | i \rangle = -\frac{Qe^2}{R} \delta_{fi} - \frac{Qe^2}{R^3} (Vt + D) x_{fi}, \quad (40)$$

where  $x_{fi} = \int \phi_f^* x \phi_i d^3\mathbf{r}$ , while  $\phi_f$  and  $\phi_i$  are the wave functions of the stationary states in the tritium atom and integration is performed over the electron coordinates  $d^3\mathbf{r} = dx dy dz$ . Now, the transition probability  $i \rightarrow f$  takes the form



$$\begin{aligned}
P_{fi} &= \frac{Q^2 e^4 |x_{fi}|^2}{\hbar^2} \left| \int_0^\infty \frac{Vt + D}{[(Vt)^2 + D^2]^{3/2}} \exp(i\omega_{fi}t) dt \right|^2 \\
&= \frac{Q^2 e^4 |x_{fi}|^2}{\hbar^2 V^2} \left| \frac{D}{V} F\left(\omega_{fi}, \frac{D}{V}\right) - i \frac{\partial}{\partial \omega_{fi}} F\left(\omega_{fi}, \frac{D}{V}\right) \right|^2,
\end{aligned} \quad (41)$$

where  $i \neq f$  and the function  $F$  is

$$F\left(\omega_{fi}, \frac{D}{V}\right) = \int_0^\infty \frac{\cos(\omega_{fi}t) dt}{t^2 + \frac{D^2}{V^2}} = \frac{V\omega_{fi}}{D} K_1\left(\frac{D\omega_{fi}}{V}\right). \quad (42)$$

Here and below, the notation  $K_i(x)$  stands for the modified Bessel functions [17] (also called MacDonald or Schläfli functions).

To finish these computations, one needs to use the following formula:

$$\frac{\partial}{\partial \omega} K_1(\omega z) = -z K_0(\omega z) - \frac{1}{\omega} K_1(\omega z), \quad (43)$$

where  $z$  is a parameter. From here one finds

$$\frac{\partial}{\partial \omega} \left[ \frac{\omega}{z} K_1(\omega z) \right] = -\omega K_0(\omega z). \quad (44)$$

Now, the final formula takes the form

$$\begin{aligned}
P_{fi} &= \frac{Q^2 e^4 |x_{fi}|^2 \omega_{fi}^2}{\hbar^2 V^2} \left[ K_1^2\left(\frac{D\omega_{fi}}{V}\right) + K_0^2\left(\frac{D\omega_{fi}}{V}\right) \right] \\
&= \frac{Q^2 e^4 |x_{fi}|^2}{\hbar^2 D^2} \Phi\left(\frac{D\omega_{fi}}{V}\right),
\end{aligned} \quad (45)$$

where

$$\Phi(x) = x^2 [K_1^2(x) + K_0^2(x)] \quad (46)$$

is the internal bremsstrahlung function.

Note that the internal bremsstrahlung function depends only upon the ratio  $\frac{D\omega_{fi}}{V}$ . The maximal (additional) excitation is reached when  $D\omega_{fi} = V$ . In atomic units the formula for probability [Eq. (45)] takes the form

$$P_{fi} = \frac{Q^2 |x_{fi}|^2}{D^2} \Phi\left(\frac{D\omega_{fi}}{V}\right), \quad (47)$$

where for protons  $Q=1$ . From this formula, one finds the limits for the variation of  $x_{fi}$  values. Indeed, since  $P_{fi} \leq 1$  then it follows from Eq. (47) that  $|x_{fi}| \leq \frac{D}{Q}$ .

The formulas derived in this section allow one to evaluate the probabilities of “additional” transitions between different excited states and between excited and ground states. In general, such transitions may change the probabilities predicted in our calculations performed in Secs. I–IV.

## VI. BREMSSTRAHLUNG AMPLIFIERS

The exothermic nuclear ( $n, Q; q_1, q_2$ ) reactions in few-electron ions can be used to create special devices which can be called the bremsstrahlung amplifiers. Such devices can be used to generate very intense pulses of x-ray radiation. Here we briefly discuss the basic physics of such amplifiers for internal bremsstrahlung. In general, if  $N_f$  electrons from some ion suddenly become free due to some nuclear reaction in an atom then they emit radiation, which is called the internal bremsstrahlung (see, e.g., [18,19] and references therein). The intensity distribution in frequency  $\omega$  of such a radiation takes the form [20]

$$\begin{aligned}
\frac{dI(\omega)}{d\omega} &= \frac{e^2 N_f^2}{\pi c} \left[ \frac{1}{\beta} \ln\left(\frac{1+\beta}{1-\beta}\right) - 2 \right] \\
&+ \frac{2e^2 \omega^2}{15\pi c^3} \left\{ 2\beta^2 \sum_{i>j=1}^{N_f} R_{ij}^2(0) - \sum_{i>j=1}^{N_f} [\vec{\beta} \cdot \mathbf{R}_{ij}(0)]^2 \right\} \\
&+ \dots,
\end{aligned} \quad (48)$$

where  $\vec{\beta} = \frac{\mathbf{v}}{c}$ ,  $\beta = \frac{v}{c}$ , and  $\mathbf{v}$  is the velocity of the ion before nuclear reaction,  $c$  is the speed of light,  $\omega$  is the frequency of radiation, and  $e$  is the electron charge. The first term in this expansion ( $\sim \frac{e^2 N_f^2}{\pi c}$ ) represents the spectrum known for internal bremsstrahlung (see, e.g., Eq. (15.66) in [19]). The second term  $\sim \frac{2e^2 \omega^2}{15\pi c^3}$  is the small correction to such a spectrum. This term is proportional to the sudden electron-electron distance  $\mathbf{R}_{ij}(0) = \mathbf{r}_i(0) - \mathbf{r}_j(0)$  which represents the lowest-order correction on the spatial electron-electron correlation in the maternal atom. In this formula, we have neglected by all higher-order terms upon the small parameter  $\tau = \frac{\omega a}{c}$ , where  $a$  is atomic radius. In general, by measuring the appropriate corrections experimentally, one can study the spatial electron-electron correlations (and the electron distribution) in outer electronic shells of the maternal atom.

Let us briefly discuss the idea which may allow one to amplify the emitted radiation (i.e., bremsstrahlung) by accelerating the incident positively charged ions to very large energies. Suppose the two-electron  ${}^6\text{Li}^+$  ion has been accelerated to a very large energy, e.g., its Lorentz  $\gamma$  factor is  $\gamma = \frac{1}{\sqrt{1-\beta^2}} \approx 1 \times 10^6$ . Now, if the ( ${}^6\text{Li}, n; \alpha, t$ ) reaction occurs in this ion then the two electrons suddenly become free. A sudden appearance of two very fast electrons will produce a very intense pulse of radiation (bremsstrahlung). It looks like the two-electron  $\beta$  decay, but the energy of the emitted electrons is  $\approx 100\,000$  times larger than the energy of very fast  $\beta$  electrons. In fact, the emitted radiation (bremsstrahlung) can be amplified even further if the ( ${}^6\text{Li}, n; \alpha, t$ ) reaction proceeds in a very strong magnetic field  $\mathbf{H}$ . An additional (synchrotron) amplification of electron bremsstrahlung in this case will be defined by the factor  $\gamma^2 H^2$ . For very large  $H$ , the intensity of such a radiation can be extremely large. In general, by using very intense magnetic fields and accelerating the incident  ${}^6\text{Li}^+$  (or  ${}^{10}\text{B}^+$ ) ions to very large energies, one

can amplify the original nonrelativistic bremsstrahlung in  $10^{12}$ – $10^{14}$  times. Further amplification can be related with the use of reactions of fast neutrons with nuclei in many-electron atoms. If during such a reaction  $N_f$  electrons from the incident atom become free then we have an additional amplification factor  $N_f^2$ , which represents the coherent bremsstrahlung from  $N_f$  electrons. It should be noted that the described mechanism of bremsstrahlung amplification is of interest in some astrophysical applications.

## VII. CONCLUSION

We have considered the nuclear ( ${}^3\text{He}, n; p, t$ ) reaction of the  ${}^3\text{He}$  nucleus with slow neutrons in the one-electron helium ion ( ${}^3\text{He}^+$ ) and the two-electron helium atom ( ${}^3\text{He}$ ). The final-state probabilities are determined for a number of excited states in the final tritium and protium atoms arising in the reaction (1). Analogous final-state probabilities are also evaluated for some other highly exothermic nuclear reactions involving light one-electron ions: ( ${}^6\text{Li}, n; \alpha, t$ ) and ( ${}^{10}\text{B}, n; {}^7\text{Li}, \alpha$ ). All these reactions are of great interest in various applications. The probability of formation of the two-electron tritium  ${}^3\text{H}^-$  and protium  ${}^1\text{H}^-$  ions in the nuclear reaction ( ${}^3\text{He}, n; p, t$ ) reaction in the two-electron He atom is also evaluated. The total probability to form any of these negatively charged hydrogen ions is relatively small.

It is shown that highly exothermic nuclear reactions in atoms and ions can be used to study the electron-density distribution in the incident atomic systems and its redistribution during such reactions. In fact, the same nuclear reactions can be used for the same purposes in many complex molecules which contain Li, B, N, and some other atoms. In most cases, the rapidly moving atomic fragment contains either one electron or no electrons at all. In some cases, however, such a fragment may contain two and even three atomic electrons. In fact, the total probability to form two- and three-electron atomic fragments in exothermic nuclear reactions with slow neutrons is less than 1% for light atoms. We also discuss the redistribution of the final-state probabilities due to additional transitions in the nascent final atomic fragments. A number of exothermic nuclear ( $n, Q; q_1, q_2$ ) reactions in a few-electron atoms or ions with neutrons can also be used to create some special devices which can be called the (internal) bremsstrahlung amplifiers. Such devices can be used to generate very intense pulses of x-ray radiation.

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## APPENDIX A

Let us present the closed formula for the final-state probability amplitude for a one-electron atom or ion in the ( $n, Q; q_1, q_2$ ) reaction. The incident state of the one-electron system is the ground  $1s$  state, while the final ( $n\ell$ ) hydrogenic state can be arbitrary. All nuclear masses are assumed to be

infinite. In this case, the expression for the final-state probability amplitude is

$$\begin{aligned} M(1s \rightarrow n\ell)(Q, q, v) &= \frac{\sqrt{\pi}Q}{n} \sqrt{\frac{q(n-\ell-1)!}{(n+\ell)!}} \\ &\times \left[ \frac{2q}{n} \right]^{\ell+1} \sum_{k=0}^{n-\ell-1} \frac{(-1)^k}{k!} \binom{n+\ell}{2\ell+k+1} \\ &\times \left[ \frac{2q}{n} \right]^k \frac{(k+2\ell+2)!}{\Gamma\left(\ell+\frac{3}{2}\right)} \frac{v^\ell}{2^\ell (X^2+v^2)^{k+3/2+\ell}} \\ &\times {}_2F_1\left(\frac{k+3}{2} + \ell, -\frac{k+1}{2}; \ell + \frac{3}{2}; \frac{v^2}{X^2+v^2}\right), \quad (\text{A1}) \end{aligned}$$

where  $X=Q+\frac{q}{n}$ . In this case, in Eq. (6) we have  $\ell_1=0$  and  $\ell_2=\ell=L$ . Finally, one finds that additional angular factor in Eq. (6) equals unity, and therefore, one finds that the total probability is  $P=|M(1s \rightarrow n\ell)(Q, q, v)|^2$ .

## APPENDIX B

In this appendix, we derive analytical formulas for some three-body radial integrals which play a great role in this study. First, let us present the explicit formula for the  $\Gamma_{l,m,n}(\alpha, \beta, \gamma)$  integral, where

$$\begin{aligned} \Gamma_{n,k,l}(\alpha, \beta, \gamma) &= \int_0^\infty \int_0^\infty \int_{|r_{32}-r_{31}|}^{r_{32}+r_{31}} \exp(-\alpha r_{32} - \beta r_{31} - \gamma r_{21}) \\ &\times r_{32}^l r_{31}^m r_{21}^n dr_{32} dr_{31} dr_{21}, \quad (\text{B1}) \end{aligned}$$

where  $\alpha, \beta$ , and  $\gamma$  are the three real parameters, while  $l, m$ , and  $n$  are the integer numbers. If integer parameters  $l, m$ , and  $n$  are “substantially negative” then this integral [Eq. (B1)] is singular. This case was considered in [23]. Here we want to consider only regular three-body integrals, i.e., the cases when all  $l, m$ , and  $n$  are non-negative. The analytical formula for the  $\Gamma_{n,k,l}(\alpha, \beta, \gamma)$  integral is easily obtained in perimetric coordinates  $u_1, u_2$ , and  $u_3$ , where  $u_i = \frac{1}{2}(r_{ij} + r_{ik} - r_{jk})$  and  $r_{ij} = u_i + u_j$  [21, 22]. Here and everywhere below in this section,  $(i, j, k) = (1, 2, 3)$  and  $r_{ij} = r_{ji}$ . In perimetric coordinates the integral [Eq. (B1)] takes the form

$$\begin{aligned} \Gamma_{n,k,l}(\alpha, \beta, \gamma) &= 2 \int_0^\infty \int_0^\infty \int_0^\infty \\ &\times \exp[-(\alpha + \beta)u_1 - (\alpha + \gamma)u_2 - (\beta + \gamma)u_3] \\ &\times (u_1 + u_2)^n (u_1 + u_3)^m (u_2 + u_3)^l du_1 du_2 du_3. \quad (\text{B2}) \end{aligned}$$

The integration over three independent perimetric coordinates  $u_i$  ( $0 \leq u_i < \infty$ ) is trivial and the explicit formula for the  $\Gamma_{n,k,l}(\alpha, \beta, \gamma)$  integral is written in the form

$$\Gamma_{n,k,l}(\alpha, \beta, \gamma) = 2l! m! n! \sum_{l_1=0}^l \sum_{m_1=0}^m \sum_{n_1=0}^n \frac{C_{m-m_1+l_1}^{l_1} C_{l-l_1+n_1}^{n_1} C_{n-n_1+m_1}^{m_1}}{(\alpha + \beta)^{m-m_1+l_1+1} (\alpha + \gamma)^{l-l_1+n_1+1} (\beta + \gamma)^{n-n_1+m_1+1}}, \quad (\text{B3})$$

where  $C_k^m$  are the binomial coefficients (=number of combinations from  $k$  by  $m$ ).

Now, consider different three-body integrals which can be written in the following form:

$$\Lambda_{1,1,1}^{(0)}(\alpha, \beta, \gamma; V) = \int_0^\infty \int_0^\infty \int_{|r_{32}-r_{31}|}^{r_{32}+r_{31}} \exp(-\alpha r_{32} - \beta r_{31} - \gamma r_{21}) \times j_0(Vr_{32}) r_{32} r_{31} r_{21} dr_{32} dr_{31} dr_{21}, \quad (\text{B4})$$

which also depend upon the parameter  $V$  and contain one Bessel function  $j_0(Vr_{32})$ . This integral can easily be computed analytically in perimetric coordinates. First, note that  $j_0(Vr_{32})r_{32} = \sin(Vr_{32}) = \sin(Vu_2)\cos(Vu_3) + \cos(Vu_2)\sin(Vu_3)$ . From here one finds

$$\begin{aligned} \Lambda_{1,1,1}^{(0)}(\alpha, \beta, \gamma; V) &= 2 \int_0^\infty \int_0^\infty \int_0^\infty \exp[-(\alpha + \beta)u_1 - (\alpha + \gamma)u_2 - (\beta + \gamma)u_3] \\ &\quad \times (u_1^2 + u_1u_2 + u_1u_3 + u_2u_3) \sin(Vu_2) \\ &\quad \times \cos(Vu_3) du_1 du_2 du_3 \\ &\quad + 2 \int_0^\infty \int_0^\infty \int_0^\infty (u_1^2 + u_1u_2 + u_1u_3 + u_2u_3) \\ &\quad \times \cos(Vu_2) \sin(Vu_3) \\ &\quad \times \exp[-(\alpha + \beta)u_1 - (\alpha + \gamma)u_2 - (\beta + \gamma)u_3] du_1 du_2 du_3. \end{aligned} \quad (\text{B5})$$

Analytical computation of each of these eight integrals is performed with the use of formula (3.944) from [7] [see Eqs. (5) and (6)]. For instance, consider the first integral in the last formula

$$\begin{aligned} &2 \int_0^\infty \exp[-(\alpha + \beta)u_1] u_1^2 du_1 \int_0^\infty \exp[-(\alpha + \gamma)u_2] \\ &\quad \times \sin(Vu_2) du_2 \int_0^\infty \exp[-(\beta + \gamma)u_3] \cos(Vu_3) du_3 \\ &= \frac{4 \sin\left(\arctan \frac{V}{\alpha + \gamma}\right) \cos\left(\arctan \frac{V}{\beta + \gamma}\right)}{(\alpha + \beta)^3 [(\alpha + \gamma)^2 + V^2]^{1/2} [(\beta + \gamma)^2 + V^2]^{1/2}} \\ &= \frac{4V(\beta + \gamma)}{(\alpha + \beta)^3 [(\alpha + \gamma)^2 + V^2][(\beta + \gamma)^2 + V^2]}. \end{aligned} \quad (\text{B6})$$

To obtain the final expression, we have used formulas (7) and (8) from Eq. (1.624) [7]. Note that here we have  $V > 0$  (always) and  $\beta + \gamma > 0$  (this condition follows from the convergence of corresponding integrals in perimetric coordinates). The computation of all remaining integrals is also straightforward. The analytical expression for the  $\Lambda_{1,1,1}^{(0)}(\alpha, \beta, \gamma; V)$  is used in Sec. III above. The approach developed in this appendix allows one to derive the analytical formulas for three-body integrals which contain two Bessel functions  $j_0(Vr_{32})$  and  $j_0(Vr_{31})$ . These formulas are needed in Sec. IV above. In fact, our method can be used to calculate (analytically) the whole different class of three-body integrals.

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