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# On the Cross Sections for the Excitation of the $2p3p\,^1P$, $2p3d\,^1D$ and $3p3d\,^1D$ Autoionizing States of Helium by Protons

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**Abstract**

In the independent electron approximation, an expression has been obtained for the probability of excitation of parity-unfavored autoionizing states of He atoms bombarded by protons as a function of impact parameter. It is shown that substates with $M_L = 0$ ($M_L$ being the projection of the total orbital angular momentum of the final-state electrons) remain unexcited in proton-induced excitation of parity-unfavored autoionizing states of helium. Calculations have been made of the cross sections for excitation of the $2p3p\,^1P$, $2p3d\,^1D$, and $3p3d\,^1D$ autoionizing states of He atoms for proton energies $E_p$ varying from 0.01 to 2.0 MeV. The results of the calculations show that:

(1) the dipole–dipole transitions resulting in the $2p3p\,^1P$ state are strongly suppressed due to interference;

(2) the main contribution to the cross sections for excitation of the $2p3d\,^1D$ and $3p3d\,^1D$ autoionizing states comes from states with $|M_L| = 1$; this is explained by the predominant role of single-electron transitions $1s \to nlm$ to states with $m = -l, -(l-2), \ldots, +(l-2), +l$.

## 1. Introduction

In the He atom, the simplest two-electron system, all doubly excited states lie above the ionization threshold. Most of doubly excited states decay by Coulomb autoionization with the emission of Auger electrons. Yet, there exist some long-lived states for which autoionization is forbidden and which decay, mainly, as a result of radiative transition. There are the so-called parity-unfavored autoionizing states [1] $n_1l_1n_2l_2\,^{1,3}L$ with odd $l_1 + l_2 - L$ ($n_1$, $n_2$ and $l_1$, $l_2$ are the principal quantum numbers and the orbital angular momenta of excited electrons; $L$ is the total electron orbital angular momentum of a doubly excited state).

In the present study, we have examined cross sections for excitation of the parity-unfavored autoionizing states in collisions between He atoms and protons. To solve the problem, we have used the independent electron approximation within the framework of the impact parameter method. The expediency of the impact parameter method for the present calculations follows, for example, from the results of [2]. It was shown in [2] that the formula

$$\sigma^{\mathrm{mod}}(v_i) = \left(\frac{v_+}{v_i}\right)^2 \sigma_q(v_+) - \left(\frac{v_-}{v_i}\right)^2 \sigma_q(v_-) \qquad (1)$$

in the first-order perturbation theory for the $1s$–$2s$ excitation of H atoms by electrons provides an expression that is identical with the Born quantum-mechanical expression. Here $\sigma_q(v)$ is the scattering cross section in the standard formulation of the impact-parameter method; $v_\pm = (v_i \pm v_f)/2$; $\mathbf{v}_i$ and $\mathbf{v}_f$ are the initial and final velocities of the projectile. It follows from the results of the calculation that at electron energies $E \sim 1.2I_0$ ($I_0$ is the ionization potential of hydrogen) the contribution of the second term (1) is not in excess of 5% of the cross section. As $E$ increases, the contribution tends rapidly to zero and $\sigma^{\mathrm{mod}}(v_i)$ approaches $\sigma_q(v_i)$.

The independent electron approximation permits one to take into account only one of the possible mechanisms of formation of doubly excited states when electron transitions occur as the result of the direct interaction between the incident particle and the atomic electrons. In this approximation, the formation of states $n_1l_1n_2l_2\,^1L$ is due to transitions through two intermediate levels:

$$1s^2\,^1S \to \begin{Bmatrix} 1sn_2l_2\ ^1L_2 \\ n_1l_1 1s\ ^1L_1 \end{Bmatrix} \to n_1l_1n_2l_2\,^1L$$

Here $L_1 = l_1$, $L_2 = l_2$. The formation of doubly excited states due to electron correlations is not described within the above approximation.

It is known [3–5] that the use of the independent electron approximation in collisions between atoms and heavy charged particles leads to a satisfactory description of cross sections for many-electron ionization from inner shells of atoms in the collision energy region corresponding to the maximum cross section value. Moreover, from a comparison of the cross sections for the proton-induced double ionization of helium and for proton-induced ionization of helium with a simultaneous excitation of the atomic residual which have been obtained in the independent electron approximation [6, 7] and in the first Born approximation [8, 9], it follows that, at collision energies from 10 to 300 keV, the contribution of the intermediate-level transitions is dominant. The results of [10] show that in the electron excitation of the autoionizing states of He atoms intermediate-level transitions are essential up to incident electron energies of about 1 keV. It has been shown [11] that in the electron excitation of the lowest-lying $^1S$ and $^1D$ autoionizing states of He atoms at $E_e < 500$ eV the intermediate level transitions play the dominant role.

Thus, one is entirely justified in believing that in the proton excitation of autoionizing states of He atoms intermediate level transitions should also be significant up to high collision energies and for proton energies from several tens of keV to several hundreds of keV they will dominate.

## 2. Amplitudes and probabilities for the single electron excitations

Here we shall obtain expressions for the amplitude and probability of $1s \to nlm$ excitation of a hydrogen-like ion due to scattering from it of a heavy charged particle. We shall need the expression for amplitude when considering the excitation of autoionizing states of He atoms. The probability amplitude for the $1s \to nlm$ excitation is

$$a_{nlm}(\rho) = \langle \phi_{nlm}(Z|\mathbf{r})|S(+\infty,-\infty)|\phi_{1s}(Z|\mathbf{r})\rangle \quad (2)$$

where $Z$ is the nuclear charge of the hydrogen-like ion and $S(+\infty,-\infty)$, the matrix that describes the scattering of the projectile by an ionic electron; $\phi_{1s}(Z|\mathbf{r})$ and $\phi_{nlm}(Z|\mathbf{r})$ are the Coulomb wave functions for an electron in the field of nuclear charge $Z$ in the initial and final states; $\rho$ is the impact vector to be found from the relation $\mathbf{R}(t) = \rho + \mathbf{v}t$; $\mathbf{v}$ the velocity of relative motion of the colliding partners; $n$, $l$ and $m$ are the principal, orbital and magnetic quantum numbers of the final-state electron. In the first-order perturbation theory for $a_{nlm}(\rho)$ we have

$$a^{(1)}_{nlm}(\rho) = -\frac{Z_1 i}{Zv}\int \frac{d^2q_\perp}{\pi q^2} e^{iq_\perp\rho}\langle \phi_{nlm}(Z|\mathbf{r})|e^{iqr}|\phi_{1s}(Z|\mathbf{r})\rangle \quad (3)$$

where $Z_1$ is the charge of the projectile; $\mathbf{q}$ the momentum transfer vector; $q_\parallel$ and $q_\perp$ are the components of the vector $\mathbf{q}$, which are parallel and orthogonal to the vector $\mathbf{v}$. The former of them is found from the electron excitation energy $\Delta E$ and is equal to $\Delta E/v$. All the quantities are expressed in Coulomb units. It will further be convenient to introduce, instead of the coordinate system $OXYZ$ with the $OZ$-axis along $\mathbf{v}$, the coordinate system $O'X'Y'Z'$ with the $OZ'$-axis along the vector $\mathbf{q}$. The change from one system to the other may be brought about by two successive turns (see Fig. 1): one turn through an angle $\beta$ about the $OY$-axis and the other through an angle $\gamma$ about the $OZ$-axis. Let us denote by $\tilde{\phi}_{nlm}(Z|\mathbf{r})$ the electron wave functions in the coordinate system $O'X'Y'Z'$. Using the matrix for three-dimensional rotations $R(\alpha,\beta,\gamma)$ one can write the matrix element $\langle \phi_{nlm}(Z|\mathbf{r})|e^{iqr}|\phi_{1s}(Z|\mathbf{r})\rangle$ in the form [12]

$$\langle \phi_{nlm}(Z|\mathbf{r})|e^{iqr}|\phi_{1s}(Z|\mathbf{r})\rangle = R^l_{0m}(0,\beta,\gamma) \times R^0_{00}(0,\beta,\gamma)\langle \tilde{\phi}_{nl0}(Z|\mathbf{r})|e^{iqr}|\tilde{\phi}_{1s}(Z|\mathbf{r})\rangle \quad (4)$$

The quantization axis in the matrix element $\langle \tilde{\phi}_{nl0}(Z|\mathbf{r})|\times e^{iqr}|\tilde{\phi}_{1s}(Z|\mathbf{r})\rangle$ is directed along the vector $\mathbf{q}$. Let us introduce the symbol

$$M^{1s}_{nl0}(\mathbf{q}) = \langle \tilde{\phi}_{nl0}(Z|\mathbf{r})|e^{iqr}|\tilde{\phi}_{1s}(Z|\mathbf{r})\rangle \quad (5)$$

One can readily demonstrate that $M^{1s}_{nl0}(\mathbf{q}) = M^{1s}_{nl0}(q)$ is a function of the vector $\mathbf{q}$ module. Bearing in mind that [12]

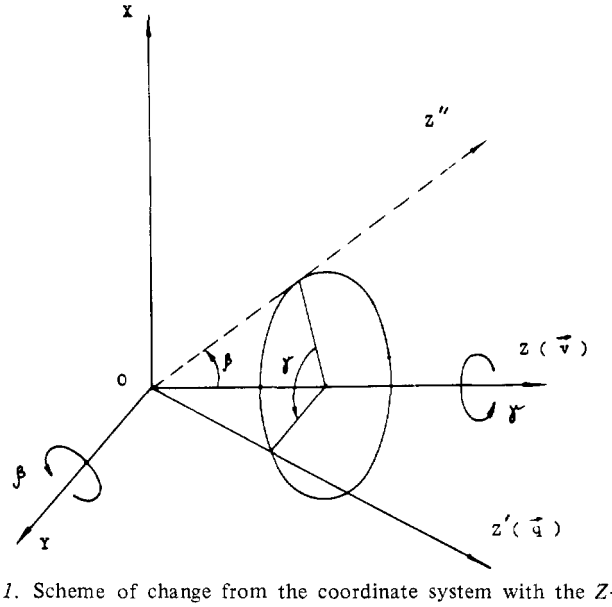


*Fig. 1.* Scheme of change from the coordinate system with the $Z$-axis directed along $\mathbf{v}$ ($OXYZ$) to that with the $Z$-axis along $\mathbf{q}$ ($O'X'Y'Z'$).

$$R^l_{0m}(0,\beta,\gamma) = (-1)^m\sqrt{\frac{4\pi}{2l+1}}\,Y^*_{lm}(\beta,\gamma) \quad (6)$$

for $a^{(1)}_{nlm}(\rho)$ we obtain

$$a^{(1)}_{nlm}(\rho) = \frac{2Z_1(-i)^{m+1}}{Zv}\sqrt{\frac{(l-|m|)!}{(l+|m|)!}}\int\frac{q_\perp dq_\perp}{q^2} \times J_{|m|}(\rho q_\perp)P_l^{|m|}(\cos\beta)M^{1s}_{nl0}(q) \quad (7)$$

Here $Y_{lm}(\beta,\gamma)$ are normalized spherical functions; $J_\mu(\rho q_\perp)$ is the Bessel function of order $\mu$; $P_l^\mu(\cos\beta)$ are the associated Legendre polynomials; $\cos\beta = q_\parallel/\sqrt{q_\parallel^2+q_\perp^2}$. From the expression (7) it can be seen that the amplitude $a^{(1)}_{nlm}(\rho)$ is independent of the azimuthal angle of the vector $\rho$.

From eq. (7), the probability of the $1s\to nlm$ excitation of the hydrogen-like ion by a heavy charged particle, $w_{nlm}(\rho)$ as a function of impact parameter in the first order perturbation theory is given by

$$w^{(1)}_{nlm}(\rho) = |a^{(1)}_{nlm}(\rho)|^2 = \left(\frac{2Z_1}{Zv}\right)^2\frac{(l-|m|)!}{(l+|m|)!}\left|\int\frac{q_\perp dq_\perp}{q^2} \times J_{|m|}(\rho q_\perp)\,P_l^{|m|}(\cos\beta)M^{1s}_{nl0}(q)\right|^2. \quad (8)$$

From formulae (7) and (8) and the general expression for the associated Legendre polynomials [13]

$$P_n^m(x) = (1-x^2)^{m/2}\frac{(2n)!}{2^n n!(n-m)!}\left\{x^{n-m} - \frac{(n-m)(n-m-1)}{2(2n-1)}x^{n-m-2} + \frac{(n-m)(n-m-1)(n-m-2)(n-m-3)}{2.4(2n-1)(2n-3)} \times x^{n-m-4} - \ldots\right\} \quad (9)$$

it follows that at high collision energies when $q_\parallel$ is small, the single-electron states with $m = -l, -(l-2), \ldots, +(l-2), +l$ should be the most excited states. This statement is invalid for odd $l$ at $\rho = 0$, because at $\rho = 0$ the states with $m = 0$ only are excited. From the expression for $w^{(1)}_{nlm}(\rho)$ it follows that at high collision energies $E$ the probabilities of the transitions from $1s$ to $nlm$ states decrease with increasing $E$ identically for all $n$.

## 3. Excitation of parity-unfavored autoionizing states of helium by protons

The electron wave function of the atom in the $LSM_LM_S$ representation, $\Psi_{LSM_LM_S}$ can be recorded as a product of the coordinate $\Phi_{LM_L}$ and spin $Q_{SM_S}$ parts of the wave function [14].

$$\Psi_{LSM_LM_S} = \Phi_{LM_L}Q_{SM_S} \quad (10)$$

where the functions $\Phi_{LM_L}$ and $Q_{SM_S}$ are antisymmetrized and orthonormalized separately. The nuclear interaction potential is independent of spin variables and, hence, the spin parts of the wave function can be disregarded in the calculations of the matrix elements for the two electron transitions, because their product is unit. We shall not record them here. In the independent-electron approximation the coordinate parts of the electron wave function of the $1s^2\,{}^1S$ initial and the $n_1l_1n_2l_2\,{}^1L$ final states appear as

$$\Phi^{\text{int}}_{LM_L}(\mathbf{r}_1, \mathbf{r}_2, t)|_{t\to-\infty} = \phi_{1s}(Z^*|\mathbf{r}_1)\phi_{1s}(Z^*|\mathbf{r}_2) \tag{11}$$

$$\Phi^{\text{int}}_{LM_L}(\mathbf{r}_1, \mathbf{r}_2, t)|_{t\to+\infty} = \frac{1}{\sqrt{2}} \sum_{m_1,m_2} (l_1 m_1 l_2 m_2 | LM_L) \tag{12}$$

$$\{\phi_{n_1 l_1 m_1}(Z^*|\mathbf{r}_1)\phi_{n_2 l_2 m_2}(Z^*|\mathbf{r}_2) + \phi_{n_1 l_1 m_1}(Z^*|\mathbf{r}_2)\phi_{n_2 l_2 m_2}(Z^*|\mathbf{r}_1)\}$$

Here $L$, $S$, $M_L$ and $M_S$ are the total orbital angular and spin momenta of the final-state electrons and their projections upon the direction of the relative motion velocity $\mathbf{v}$; $(l_1 m_1 l_2 m_2 | LM_L)$ are the Clebsch–Gordan coefficients; $\phi_{nlm}(Z^*|\mathbf{r})$ is the Coulomb wave function for the $nlm$ state in the field of a nucleus with effective charge $Z^*$. The symbol int at the wave functions for the initial and final states indicates that the problem is treated in the interaction representation.

From the results of [7] we obtain the probability amplitude $A_{LM_L}(\boldsymbol{\rho})$ of the proton-induced excitation of the $n_1 l_1 n_2 l_2\, {}^1LM_L$ state as a function of impact vector $\boldsymbol{\rho}$

$$A_{LM_L}(\boldsymbol{\rho}) = \sqrt{2} \sum_{m_1,m_2} (l_1 m_1 l_2 m_2 | LM_L) \prod_{j=1}^{2} a_{n_j l_j m_j}(\boldsymbol{\rho}) \tag{13}$$

where $a_{n_j l_j m_j}(\boldsymbol{\rho})$ is the probability amplitude for the $1s \to n_j l_j m_j$ transition of the $j$th electron of a He atom given by the relation (2).

If $a_{nlm}(\boldsymbol{\rho})$ is determined in the first-order perturbation theory, the probability of the proton-induced excitation of the $n_1 l_1 n_2 l_2\, {}^1L$ autoionizing state of helium, as a function of impact parameter $\rho$ will have the form

$$W(\rho) = 2 \sum_{M_L} \left| \sum_{m_1,m_2} (l_1 m_1 l_2 m_2 | LM_L) \prod_{j=1}^{2} \frac{2(-\mathrm{i})^{m_j+1}}{Z^* v} \right.$$
$$\times \sqrt{\frac{(l_j - |m_j|)!}{(l_j + |m_j|)!}} \int \frac{q_\perp \mathrm{d}q_\perp}{q^2}$$
$$\left. \times J_{|m_j|}(\rho q_\perp) P_{l_j}^{|m_j|}(\cos\beta) M^{1s}_{n_j l_j 0}(q) \right|^2 . \tag{14}$$

From the expression (14) and the property of the Clebsch–Gordan coefficients regarding the sign reversal of the projections $m_1$, $m_2$ and $M_L$ it follows that in the excitation of the parity-unfavored autoionizing states $n_1 l_1 n_2 l_2\, {}^1L$ of He atoms by protons the substates with $M_L = 0$ remain unexcited. Moreover, the excitation probabilities of substates with $M_L = \pm K$ are the same, that is, the probability value depends solely on the modulus of the projection of the total electron orbital angular momentum.

## 4. Results and discussion

Using formula (14), we have computed the cross sections for the excitation of the autoionizing states $2p3p\ {}^1P$, $2p3d\ {}^1D$ and $3p3d\ {}^1D$ of He atoms by protons in the collision energy region from 0.01 to 2 MeV. The excitation energy of one electron has been found from the effective charge $Z^*$ of the He atomic nucleus, which, for all single-electron states under consideration, was set equal to 1.69.

Figure 2 presents the results of the calculations of the cross sections for excitation of the autoionizing states $2p3p\ {}^1P$, $2p3d\ {}^1D$ and $3p3d\ {}^1D$ as a function of proton energy. The calculation results show that in the excitation of the autoionizing states the dipole–quadrupole transitions prove to be stronger than the dipole–dipole transitions over the entire collision energies in question. This is accounted for by the fact that the dipole–dipole transitions $1s \to 2p0 - 1s \to 3p(\pm 1)$ and $1s \to 2p(\pm 1) - 1s \to 3p0$ leading to the $2p3p\ {}^1P$ state are strongly suppressed due to interference since the amplitude phases of these transitions differ by $\pi$.

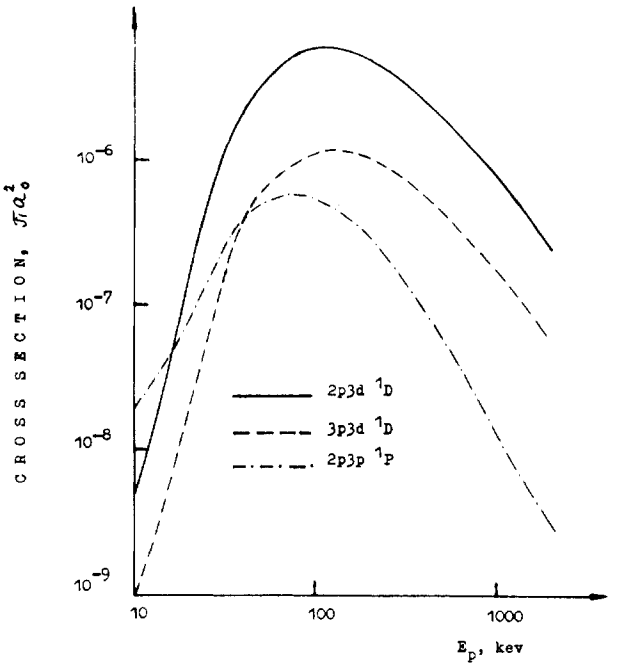


*Fig. 2.* Cross sections for excitation of the $2p3p\ {}^1P$, $2p3d\ {}^1D$, and $3p3d\ {}^1D$ autoionizing states of He atoms as a function of proton energy.

Figure 3 illustrates the energy dependences of the cross sections for formation of substates with various $M_L$ for the autoionizing states $2p3d\ {}^1D$ and $3p3d\ {}^1D$. Since in the excitation of parity-unfavored autoionizing states, substates with $M_L = 0$

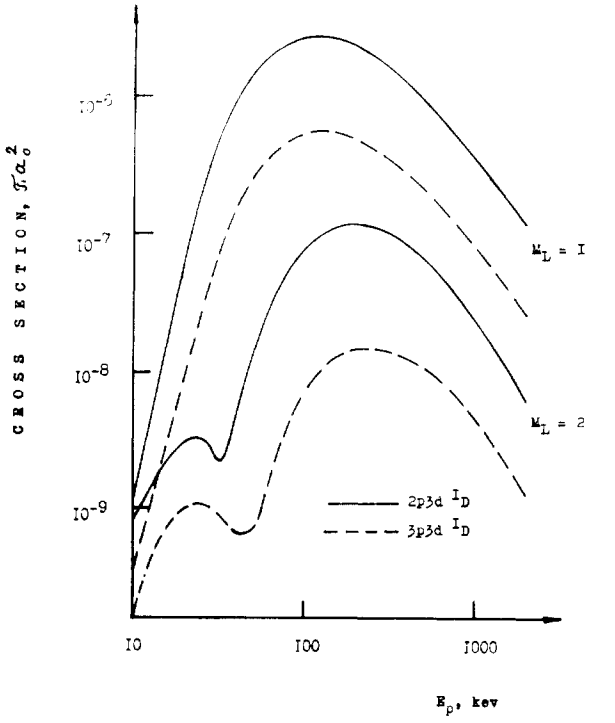


*Fig. 3.* Cross sections for excitation of substates with $M_L = 1$ and 2 for the $2p3d\ {}^1D$ and $3p3d\ {}^1D$ autoionizing states of He atoms as a function of proton energy.

remain unexcited, the substate with $|M_L| = 1$ for the autoionizing state $2p3p\ ^1P$ is the only excited state. As can be seen from Fig. 3, the magnitude of the cross section for excitation of the substate with $M_L = 1$ for the $2p3d\ ^1D$ and $3p3d\ ^1D$ states exceeds that for the substate with $M_L = 2$, at $E > 25$ keV this excess being as high as an order of magnitude and more. This behaviour of the excitation cross sections of the substates with $M_L = 1$ and 2 for the noted terms is accounted for by the predominant role of one-electron transitions to the states with $m = -l, -(l-2), \ldots, +(l-2), +l$. We demonstrate it using the excitation of the $2p3d\ ^1D$ state as an example. The excitation of substates with $M_L = 2$ proceeds via two dipole–quadrupole transitions with the amplitudes whose phases differ by $\pi$. The substates with $M_L = 1$ result from three dipole–quadrupole transitions. The amplitudes of two of them, namely, $1s \to 2p(-1) - 1s \to 3d2$ and $1s \to 2p1 - 1s \to 3d0$, for which the transitions of single electrons occur to the states with $m = -l, -(l-2), \ldots, +(l-2), +l$, are in phase. Therefore, in the case of the excitation of the subshells with $M_L = 2$ the interference leads to a stronger decrease in the cross sections as compared with the excitation of the substates with $M_L = 1$. The interference minima in the excitation cross sections of substates with $M_L = 2$ for the $2p3d\ ^1D$ and $3p3d\ ^1D$ terms are pronounced in Fig. 3.

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