ORBITAL QUANTUM NUMBER DISTRIBUTION OF HIGHLY EXCITED ATOMS PRODUCED IN COLLISIONS BETWEEN HEAVY PARTICLES

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Submitted January 25, 1971

Zh. Eksp. Teor. Fiz. **60**, 2060–2065 (June, 1971)

Collisions between fast protons or atoms and various atomic targets involving formation of highly excited hydrogen atoms H(nl), $n \gg 1$, are considered. The dependence of the charge exchange and excitation cross sections on the orbital momentum l is derived. As expected, hydrogen atoms are produced with greatest probability in states with $l = 0$ and 1. Numerical calculations carried out for collisions with argon atoms show that the formulas derived in the present paper are valid for principal quantum number values as low as $n \gtrsim 3$.

THE formation of highly-excited atoms as the result of atomic collisions is of interest for a number of problems of astrophysics and plasma physics. Since the energy spectrum of a highly-excited atom is close to hydrogen-like, it is particularly important to investigate the processes that lead to the formation of excited hydrogen atoms. The main method of obtaining excited hydrogen atoms in a laboratory plasma is charge exchange and excitation of H atoms in collisions with different atomic targets. For these processes, the total cross sections for the formation of hydrogen atoms in a state with definite principal quantum number n have been investigated in sufficient detail experimentally[1] and theoretically.[2–6] At the same time, in many problems it is necessary to have information on the distribution of the excited H atoms with respect to the orbital quantum numbers l. There are practically no direct experimental data on the dependence of the processes in question on l. Theoretical calculations encounter considerable difficulties connected with the cumbersome character of the numerical calculations of the matrix elements at large values of n. Such calculations were performed in [3] for the charge-exchange cross sections at only a few values of n and l and of the collision energy E. For the case of charge exchange of protons on hydrogen atoms, the distribution with respect to l at large values of n was obtained in [7].

We derive in this paper analytic expressions for the cross sections for the production of fast H atoms in the reactions $H^+ + A \rightarrow H(nl) + A^+$ and $H(1s) + A \rightarrow H(nl) + A$ (A is an arbitrary atom); these expressions are valid if $n \gg 1$. Comparison with the exact calculations performed with an argon target as an example has shown that these formulas can be used already at $n \gtrsim 3$.

1. CHARGE EXCHANGE: $H^+ + A(n_0l_0) \rightarrow H(nl) + A^+$

In the Brinkman-Kramers approximation, the cross section for the capture of an electron from a shell containing N equivalent electrons can be represented in the form (see [4])[1)]

$$\sigma(n_0l_0 \rightarrow nl) = \pi\frac{8N}{v^2}\int_{\varkappa_{min}}^{\infty} P^2(\varkappa)Q^2(\sqrt{\varkappa^2-\omega})\varkappa d\varkappa,$$
$$\varkappa_{min} = |\omega/2v + v/2|, \tag{1}$$

where $\omega = I - 1/n^2$ is the resonance defect, I the ionization potential of the target-atom shell, and v the relative velocity. The quantities P and Q are defined by the relations

$$P(\varkappa) = \sqrt{2l+1}\int_0^\infty R_{nl}(r)j_l(\varkappa r)r^2dr, \tag{2}$$

$$Q(\sqrt{\varkappa^2-\omega}) = \int_0^\infty R_{n_0l_0}(r)j_{l_0}(r\sqrt{\varkappa^2-\omega})\zeta(r)r\,dr, \tag{3}$$

where R_{nl} and $R_{n_0l_0}$ are the radial wave functions of the atoms H and A, respectively, $\zeta(r)$ is the effective charge of the atomic remainder, $j_l(\kappa r) = \sqrt{\pi/2\pi r}\,J_{l+1/2} \times (\kappa, r)$, and $J_{l+1/2}(\kappa r)$ is a Bessel function.

The integral in (2) is expressed in terms of the hypergeometric function $F(n + l + 1, -n + l + 1, l + 3/2; 1/n^2\kappa^2)$. Using the limiting relation for F at large n

$$F\left(n+l+1,\ -n+l+1,\ l+\frac{3}{2},\ \frac{1}{n^2\varkappa^2}\right) \rightarrow \Gamma\left(l+\frac{3}{2}\right)\varkappa^{l+1/2}J_{l+1/2}\left(\frac{2}{\varkappa}\right)$$
$$n\varkappa \gg 1, \quad n \gg l, \tag{4}$$

it is easy to transform the expression for $P^2(\kappa)$ into

$$P^2(\varkappa) = \frac{4\pi(2l+1)}{n^3\varkappa^7}J^2_{l+1/2}\left(\frac{2}{\varkappa}\right). \tag{5}$$

Substituting (5) in (1), we obtain ultimately

$$n^3\sigma_l \equiv n^3\sigma(n_0l_0 \rightarrow nl)|_{n\rightarrow\infty}$$

$$= \pi^2\frac{32N(2l+1)}{v^2}\int_{\varkappa_{min}}^{\infty} J^2_{l+1/2}\left(\frac{2}{\varkappa}\right)Q^2(\sqrt{\varkappa^2-\omega})\frac{d\varkappa}{\varkappa^6}. \tag{6}$$

Using the properties of the sums of Bessel functions, we can obtain from (6) the known expression for the cross section, summed over l, for capture in a state with given n:[2]

$$n^3\sum_l \sigma_l = \pi\frac{2^7N}{v^2}\int_{\varkappa_{min}} \frac{d\varkappa}{\varkappa^7}Q^2(\sqrt{\varkappa^2-\omega}). \tag{7}$$

[1)] We use the atomic system of units, with the Rydberg unit for the energy.

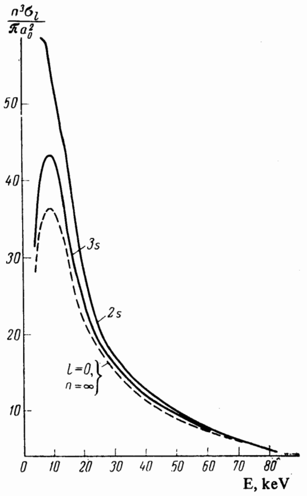

FIG. 1

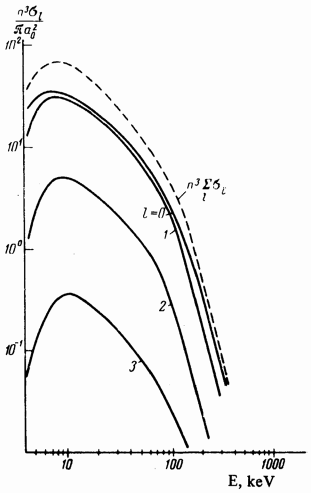

FIG. 2

FIG. 1. Cross section for the charge exchange $H^+ + Ar \to H(ns) + Ar^+$ vs. the principal quantum number n (at $l = 0$); solid curves—exact calculations with formulas (1)–(3); dashed curve—calculation with formula (6).

FIG. 2. Dependence of the cross sections for the charge exchange $H^+ + Ar \to H(nl) + Ar^+$, $n \to \infty$ on the orbital angular momentum l: solid curves—calculation with formula (6), dashed—calculation with formula (7).

Unlike in (1)–(3), the dependence of the scattering amplitude on n and l in (6) is factored out. This greatly simplifies practical calculations and makes it possible to investigate analytically the dependence of the cross sections on the orbital angular momentum l.

At $l > 2/\kappa_{\min}$ (which is certainly satisfied if $l > 2/\sqrt{I}$), we confine ourselves in (6) to the first term of the series expansion of the Bessel function

$$J_{l+\frac{1}{2}}^2\left(\frac{2}{\varkappa}\right) \approx \varkappa^{-2l-1}\Gamma^{-2}\left(l+\frac{3}{2}\right) \tag{8}$$

and we calculate the integral in (6) by the Laplace method. Omitting the intermediate manipulations, we present the final result:

$$n^3\sigma_l \approx \pi^2 \frac{32N(2l+1)}{\Gamma^2(l+{}^3/_2)(2l-1)} \frac{1}{v^2} \left(\frac{I}{2v}+\frac{v}{2}\right)^{-2l-6} Q^2\left(\left|\frac{I}{2v}-\frac{v}{2}\right|\right). \tag{9}$$

We see therefore that the charge-exchange section decreases rapidly with increasing l.

Formula (9) does not hold when $l < 2/\kappa_{\min}$, and it is necessary to use (6). Figure 1 compares the results of the calculations of the cross sections for charge exchange on Ar atoms with the approximate formula (6), which is valid when $n \gg 1$, with the exact calculations with formulas (1)–(3). As seen from the figure, the error of formula (6) does not exceed 20% already at n = 3. The dependence of the cross sections on l is shown in Fig. 2. The main contribution to the total cross section is made by charge exchange with $l = 0$ and 1.

The curves of Figs. 1 and 2 were plotted without allowance for the possible capture of electrons by the inner shells of the target atom. Actually this process can make an appreciable contribution to the total charge-exchange cross section. For inert-gas atoms at collision energies $E < 300$ keV, however, the inner shells play no role.[6]

2. EXCITATION: $H(1s) + A \to H(nl) + A$

To calculate the cross section for the excitation of a fast hydrogen atom, we use the Born approximation:[8]

$$\sigma(1s \to nl) = \frac{8\pi}{v^2}\int_{\varkappa_{min}}^{\infty} F_H^2(\varkappa)F_A^2(\varkappa)\frac{d\varkappa}{\varkappa^3},$$

$$\varkappa_{min} = (1 - 1/n^2)/2v. \tag{10}$$

The form factors F_H and F_A are determined by the expressions

$$F_H^2(\varkappa) = (2l+1)\left[\int_0^\infty R_{1s}(r)R_{nl}(r)j_l(\varkappa r)r^2dr\right]^2 \tag{11}$$

$$F_A^2(\varkappa) = \varkappa^2\left[\int_0^\infty \zeta_A(r)\sin(\varkappa r)\,dr\right]^2, \tag{12}$$

where ζ_A is the effective charge of the target atom (see [9]).

Expressing $j_l(\kappa r)$ in terms of the confluent hypergeometric function and using formula (f:10) of [10], we represent $F_H^2(\kappa)$ in the form:

$$F_H^2(\varkappa) = (2l+1)\left\{\frac{2\sqrt{\pi}\,\varkappa^l}{(2l+1)!\,\Gamma(l+{}^3/_2)n^{l+2}}\sqrt{\frac{(n+l)!}{(n-l-1)!}}\left[\frac{dI_\lambda}{d\lambda}\right]_{\lambda=1}\right\}^2$$

$$I_\lambda = \Gamma(2l+2)\left[\left(\lambda+\frac{1}{n}\right)^2+\varkappa^2\right]^{-n}\left(\frac{nz}{4i\varkappa}\right)^{-n+l+1} \tag{13}$$

$$\times F(l+1,\ -n+l+1,\ 2l+4;\ z), \tag{14}$$

$$z = \frac{4i\varkappa}{n(\lambda^2+\varkappa^2-1/n^2+2i\varkappa/n)}. \tag{15}$$

In the case of large n ($n \gg l$) formulas (13)–(15) simplify greatly. Substituting the limiting expression for $F_H^2(\kappa)$ in (10), we obtain

$$n^3\sigma_l \equiv n^3\sigma(1s \to nl)\,|_{n\to\infty} = \frac{8\pi}{v^2}\int_{\varkappa_{min}}^{\infty} F_l^2(\varkappa)F_A^2(\varkappa)\frac{d\varkappa}{\varkappa^3}, \tag{16}$$

$$F_l^2(\varkappa) \equiv n^3F_H^2(\varkappa)\,|_{n\to\infty} = (2l+1)\frac{4\pi e^{-4/(1+\varkappa^2)}}{\varkappa(1+\varkappa^2)^5}$$
$$\times\left[4\varkappa J'_{l+\frac{1}{2}}\left(\frac{2\varkappa}{1+\varkappa^2}\right)-(1-3\varkappa^2)J_{l+\frac{1}{2}}\left(\frac{2\varkappa}{1+\varkappa^2}\right)\right]^2. \tag{17}$$

We note that the expression for $F_H^2(\kappa)$ is exactly the same as for the excitation amplitude of the $1s \to nl$ transition of the H atom by electron impact. Therefore expression (17) can be used to find the distribution of the highly-excited hydrogen atoms with respect to l in collisions with electrons.

With the aid of the formulas given in [11] it is easy to obtain from (17) the square of the amplitude of excitation of the n-th discrete level, summed over l:

$$\sum_l F_l^2(\varkappa) = 2^8\varkappa^2\frac{{}^1/_3+\varkappa^2}{(1+\varkappa^2)^6}e^{-4/(1+\varkappa^2)} \tag{18}$$

Formula (18) coincides with the asymptotic expression given in [10] for the amplitude of the inelastic collision of an electron with an H atom.

The dependence of the cross section in l, just as in the case of charge exchange, can be investigated by ap-

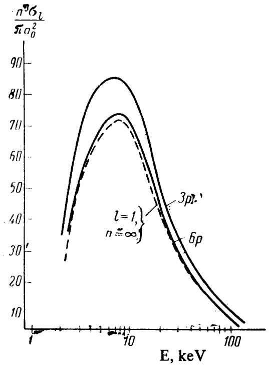

FIG. 3

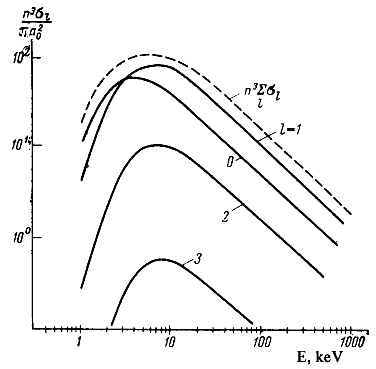

FIG. 4

FIG. 3. Dependence of the cross sections for the excitation of the hydrogen atom H(1s) + Ar → H(np) + Ar on the principal quantum number n of the final state (at $l = 1$): solid curves—exact calculation with formulas (10)–(12), dashed curve—calculation with (16) and (17).

FIG. 4. Dependence of the cross sections for excitation H(1s) + Ar → H(nl) + Ar, n → ∞, on the orbital angular momentum l of the final state: solid curves—calculation with (16) and (17), dashed—summary cross section calculated with (16) and (18).

proximately calculating the integral of (16) by the Laplace method:

$$n^3\sigma_l \approx 2^5 \frac{\pi^{3/2}\sqrt{l}}{v^2e^2}\left(\frac{e}{2l}\right)^{2l} F_A^2(1). \tag{19}$$

This expression is valid for $\kappa_{\min} < 1$, i.e., $v > 1/2$. As seen from (19), at $l > 2$ the excitation cross section decreases sharply with increasing l.

Figures 3 and 4 show the results of numerical calculations of the excitation cross section of hydrogen atoms colliding with Ar atoms. As in the case of charge exchange, formulas (16) and (17), obtained under the assumption that $n \gg l$, are applicable already at small values of n. The distribution of the excited hydrogen atoms with respect to l is shown in Fig. 4. As expected, the main contribution to the total cross section is made by the optically allowed 1s–np transition.

Excitation of the 1s–nl transition of the hydrogen atom is accompanied, generally speaking, by excitation of the target atom. In the presence of strong coupling of the initial and final states, the indicated process can make an appreciable contribution to the total excitation cross section.[9] With increasing n, however, the role of the strong coupling decreases, the Born approximation becomes applicable, and the total excitation cross section is determined by collisions that do not change the state of the target.

The authors are grateful to L. A. Vaĭnshteĭn, R. N. Il'in, V. A. Oparin, and I. I. Sobel'man for a discussion of a number of problems touched upon in the paper.

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Translated by J. G. Adashko
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