

*CALCULATION OF THE EFFECTIVE CROSS SECTIONS FOR PROTON CHARGE EXCHANGE  
IN COLLISIONS WITH MULTI-ELECTRON ATOMS*

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The charge exchange effective cross sections for fast protons in hydrogen, helium, lithium, nitrogen, neon, argon, and krypton are calculated in the one-electron variant of the Brinkman-Kramers approximation, using hydrogen-like wave functions. A simple generalization of the Brinkman-Kramers formula is obtained for arbitrary values of the external and internal screening parameters. The ratio of experimental to calculated cross sections can be represented, accurate to 20-25%, by a single-parameter function that is valid for all media. This function is used to determine the proton charge exchange cross section in the indicated media at energies between 20 keV and 13 MeV. The procedure is proposed as a semi-empirical method for calculating the charge exchange cross sections of protons colliding with atoms or simple molecules. The latest experimental data on cross sections for electron capture by highly excited hydrogen atom states are discussed.

## 1. INTRODUCTION

A CONSISTENT theoretical calculation of the effective cross sections of charge exchange of fast ions in rapid atomic collisions entails considerable difficulties even in the simplest case when the electron is captured by protons in collisions with hydrogen and helium atoms.<sup>[1-5]</sup> In this connection, appreciable interest attaches to attempts to determine, from the empirical laws, the parameters that exert the strongest influence on the values of the cross section, to attempts at an approximate theoretical description of the charge exchange by using a minimum number of the most important parameters, and to the development on this basis of semi-empirical methods of cross-section calculation.

From the presently available experimental data it is seen that in the region of relative colliding-particle velocities  $v > v_0 = e^2/\hbar$ , there exist definite approximate relations, which depend little on the medium,<sup>[6]</sup> between the cross sections for proton charge exchange and the cross sections for the capture of electrons by other nuclei (and ions having sufficiently large charges). Using these relations, we can estimate, from the known proton charge-exchange cross sections, the cross sections for the capture of the electron by other nuclei and large-charge ions in the same medium, so that the problem of finding the cross sections for the capture of the electron by different ions

reduces to a considerable degree to the problem of finding the cross sections for charge exchange of protons in different media.

At a proton energy  $E \gtrsim 25$  keV, corresponding to  $v \gtrsim v_0 = 2.19 \times 10^8$  cm/sec, theoretical values close to those given by experiment are obtained for the cross sections of charge exchange of protons in hydrogen and helium in the first Born<sup>1)</sup> and other approximations of the same order (or higher), and these call for cumbersome calculations.<sup>[1-5]</sup> However, the most important regularities in the cross sections for electron capture are fairly well described also by the simplest Brinkman-Kramers approximation,<sup>[11]</sup> which is characterized by the fact that in the expression for the matrix element of the transition, taken in the usual first Born approximation, one omits the term corresponding to the interaction of the proton by the atomic nucleus, and one retains only one term, corresponding to the interaction of the proton with the captured electron. Although the cross sections obtained in this approximation turns out to be exaggerated by a factor of several times, the Brinkman-Kramers approximation, as shown by theory and experiment,<sup>[1-6, 12, 15]</sup> gives a qualitatively correct dependence of the differential cross sec-

<sup>1)</sup>We use here the most widely accepted terminology, adopted in particular in the reviews of Bates and McCarroll<sup>[1]</sup> and Gerjuoy<sup>[2]</sup>. In the papers of Butler and May and co-workers<sup>[7-10]</sup>, the Brinkman-Kramers approximation<sup>[11]</sup> is called the Born approximation.

tions on the impact parameter, a dependence of the cross sections on the proton velocity  $v$  which is close to reality, and a qualitatively correct dependence of the cross sections for the capture of the electron in the state with a given value of the principal quantum number  $n$  on  $n$ . Because of this, the Brinkman-Kramers approximation can be used in estimates of the relative role of the capture of the electron in different excited states and the relations between the cross sections for the charge exchange of protons at different velocities  $v$ .<sup>[7-10, 16, 17]</sup>

The cross section for the capture of electrons by atoms containing more than two electrons was calculated only in the Brinkman-Kramers approximation.<sup>[18, 19]</sup> Mapleton<sup>[18]</sup> calculated in this approximation the cross section for the capture of 2p-electrons from oxygen and nitrogen atoms by a proton, and then, using the relations between the cross sections in the Born and the Brinkman-Kramers approximations for the cases of charge exchange of protons in collisions with hydrogen and helium atoms, he estimated the same cross sections in the Born approximation. Florance et al.<sup>[19]</sup> used the Brinkman-Kramers approximation in the calculation of the cross sections for the capture of an electron by singly charged ions of aluminum in collisions with argon atoms.

In this paper we calculate the cross sections for charge exchange of protons in different media at velocity  $v$  ranging from  $2 \times 10^8$  to  $5 \times 10^9$  cm/sec, corresponding to a proton energy  $E$  from 0.02 to 13 MeV, in the simplest single-electron variant of the Brinkman-Kramers approximation. By introducing the parameters of the external screening we obtain a generalization of the well known Brinkman-Kramers formula for the cross sections of capture of electrons by atomic nuclei in collisions with hydrogen-like particles to the case of capture of an electron from completely filled atomic shells<sup>2)</sup> and configurations  $2s$ ,  $3s^2 3p^6$ , and  $4s^2 4p^6$  of arbitrary atoms. The ratio of the experimental cross sections for the charge exchange of protons in different media to those calculated with accuracy of 25% can be represented in the form of a function  $R$  of a single variable which is the same for all media. By using the function  $r$  and the cross sections obtained in the Brinkman-Kramers approximation, we obtain the charge-exchange

cross sections for protons in hydrogen, helium, lithium, nitrogen, neon, argon, and krypton.

## 2. CROSS SECTIONS FOR THE CAPTURE OF AN ELECTRON FROM COMPLETELY FILLED ATOMIC SHELLS

According to the energy and momentum conservation laws, when an electron goes over from an atom with mass  $m_a + \mu$  (where  $\mu$  is the mass of the electron in question) to a fast ion with mass  $m$ , a change must take place in the momenta of the particles with masses  $m_a$  and  $m$ , respectively, by amounts  $-\hbar\mathbf{A}$  and  $\hbar\mathbf{B}$ ; the electron momentum changes by an amount  $\hbar\mathbf{A} - \hbar\mathbf{B}$ . The absolute values of these quantities, with a relative accuracy of the order of  $\mu/m_a$  and  $\mu/m$ , are given by the following expressions:

$$\hbar^2 A^2 = \hbar^2 A_0^2 + 4m^2 m_a^2 (m + m_a)^{-2} v^2 \sin^2 \theta / 2,$$

$$\hbar^2 B^2 = \hbar^2 B_0^2 + 4m^2 m_a^2 (m + m_a)^{-2} v^2 \sin^2 \theta / 2, \quad (1)$$

with  $\hbar A_0 = (\epsilon - \epsilon_a)/v + \mu v/2$  and  $\hbar B_0 = (\epsilon - \epsilon_a)/v - \mu v/2$ , where  $v$  is the relative velocity of the colliding particles,  $\epsilon_a$  and  $\epsilon$  are the binding energies of the electron in the initial and final states, and  $\theta$  is the particle scattering angle in the c.m.s. From this we see that  $\hbar^2 A^2 + 2\mu\epsilon_a = \hbar^2 B^2 + 2\mu\epsilon$ .

Thus, owing to the "recoil" effect, the momenta of the fast ion and of the atomic remnant should change during the course of electron capture by amounts not smaller than  $\hbar B_0$  and  $\hbar A_0$ . These quantities are of the order of  $\mu v/2$  and are those impact characteristics on which the cross section for electron capture depends essentially.

The electron capture cross section  $\sigma(i|k)$  from the initial state  $i$  of the atom into the final state  $k$  of the fast ion is expressed in terms of the interaction matrix element  $U$ :<sup>[22]</sup>

$$\sigma(i|k) = [m m_a / (m + m_a)]^2 (2\pi\hbar^2)^{-2} \int |\langle i|U|k \rangle|^2 d\Omega, \quad (2)$$

where  $d\Omega$  is the solid-angle element.

In the Brinkman-Kramers approximation, in which  $U$  is assumed equal to the Coulomb interaction of the ion with the captured electron, the square of the modulus of the matrix element, as follows from the work of Jackson and Schiff,<sup>[23]</sup> can be represented for the cases when the electron is captured from a single-electron ion as follows (in atomic units):

$$|\langle i|U|k \rangle|^2 = 2^4 \pi^6 (B^2 + 2\epsilon)^2 |\psi_i(\mathbf{A})|^2 |\psi_k(\mathbf{B})|^2, \quad (3)$$

<sup>2)</sup>In accordance with the terminology adopted in the widely known handbooks which we use, namely by Moore<sup>[20]</sup> and Wapstra et al.<sup>[21]</sup>, we define the atomic shell here as an aggregate of electrons in states with equal values of the principal quantum number  $n$ .

where  $\psi_i(\mathbf{p})$  and  $\psi_k(\mathbf{p})$  are the wave functions of the initial state of the electron relative to the atom of the medium and the final state of the electron relative to the fast ion in the momentum representation.

The total cross section for the capture of the electron in several final states  $k_j$  corresponds to a summary square of the modulus of the matrix element:

$$\begin{aligned} & \left| \langle i | U | \sum_j k_j \rangle \right|^2 \equiv \sum_j |\langle i | U | k_j \rangle|^2 \\ & = 2^4 \pi^6 \sum_j (B_j^2 + 2\varepsilon_j)^2 |\psi_i(\mathbf{A})|^2 |\psi_{k_j}(\mathbf{B})|^2. \end{aligned} \quad (4)$$

For cases of capture of an electron by atoms of a medium with several electrons, we shall have in place of (4) in the simplest single-electron variant of the Brinkman-Kramers approximation

$$\begin{aligned} & \left| \langle \sum_s i_s | U | \sum_j k_j \rangle \right|^2 = 2^4 \pi^6 \\ & \times \sum_s \sum_j (B_{sj}^2 + 2\varepsilon_{sj})^2 |\psi_{i_s}(\mathbf{A})|^2 |\psi_{k_j}(\mathbf{B})|^2. \end{aligned} \quad (5)$$

When an electron is captured by atomic nuclei, the final states of the electron are described by hydrogen like wave functions  $F_{nlm}(\mathbf{p})$ , for which, as can be readily established for example from May's paper,<sup>[24]</sup> the following relation is satisfied:

$$\sum_{l=0}^{n-1} \sum_{m=-l}^l |F_{nlm}(\mathbf{p})|^2 = \frac{32}{\pi} \frac{b^5}{(p^2 + b^2)^4} n^2 \quad (6)$$

with  $b = Z/n$ , where  $n$ ,  $l$ ,  $m$  are respectively the principal, orbital, and magnetic quantum numbers and  $Z$  is the charge of the nucleus (in units of electron charge  $e$ ). In addition

$$\varepsilon = (\mu e^2 / \hbar) (b^2 / 2) \quad (7)$$

so that for the summary cross section of the capture of the electron in all the states with specified value of the principal quantum number we have

$$\left| \langle \sum_s i_s | U | n \rangle \right|^2 = 2^9 \pi^5 b^5 n^2 \sum_s |\psi_{i_s}(\mathbf{A})|^2 (B_s^2 + b^2)^{-2}. \quad (8)$$

The hydrogen-like wave functions can be used also to describe states of electrons in multi-electron atoms of a medium.<sup>[25]</sup> In this case the parameter  $b = Z/n$ , on which the wave function depends, should be replaced by the quantity  $b_a = Z_a^*/n_a^*$ , where  $Z_a^*$  and  $n_a^*$  are the effective values of the charge of the nucleus and of the principal quantum number for the atomic electron.

The quantity  $b_a$ , just as the binding energy  $\varepsilon_a$  of the atomic electron, depends on the orbital quantum number  $l_a$ . However, in order to obtain first the simplest expression for the cross sections for electron capture, we shall assume that for all the electrons situated in states with given value of the principal quantum number  $n_a$ , the values of  $b_a$  and  $\varepsilon_a$  are identical, i.e., they depend only on  $n_a$ .

In such a case, when summing in (8) over the electrons making up a completely filled shell ( $K$  or  $L$ , or  $M$  etc.), a relation similar to (6) is satisfied, so that for the corresponding square of the modulus of the matrix element we have

$$|\langle n_a | U | n \rangle|^2 = 2^{14} \pi^4 b^5 b_a^5 n^2 N_a (A^2 + b_a^2)^{-4} (B^2 + b^2)^{-2}, \quad (9)$$

where  $N_a$  is the number of electrons in the atomic shell.

From (2) and (9), taking (1) into account, we obtain for the cross section for the capture by the atomic nucleus of an electron in the state with principal quantum number  $n$  from a completely filled shell, characterized by a principal quantum number  $n_a$ , the following expression:

$$\begin{aligned} \sigma(n_a | n) &= \pi a_0^2 \frac{2^8}{5} N_a n^2 \left( \frac{v_0}{v} \right)^2 \gamma^5 \eta^5 \\ &\times (1 + \beta)^{5/2} (1 + \beta\gamma)^{-3} \Phi_4(\beta\gamma), \end{aligned} \quad (10)$$

where  $a_0 = \hbar^2/e^2$  and  $v_0 = e^2/\hbar$  are the atomic units of length and velocity,

$$\begin{aligned} \gamma &= 4V^{-2} [1 + 2(1 + \eta^2)V^{-2} + (1 - \eta^2)^2 V^{-4}]^{-1}, \\ V &= v/u, \quad u = (2\varepsilon_a/\mu)^{1/2}, \\ \eta_n &= (\varepsilon/\varepsilon_a)^{1/2} = Zv_0/nv, \\ \beta &= 2\varepsilon_a/\mu v_0^2 b_a^2 - 1. \end{aligned}$$

The function  $\Phi_4(\beta\gamma)$  belongs to the class of functions

$$\begin{aligned} \Phi_k(t) &= \frac{k+1}{t} \left\{ 1 - \frac{k}{t} \left[ \left( 1 + \frac{1}{t} \right)^{k-1} \right. \right. \\ &\times \left. \left. \ln(1+t) - \sum_{\nu=1}^{k-1} \frac{1}{\nu} \left( 1 + \frac{1}{t} \right)^{k-1-\nu} \right] \right\}, \end{aligned} \quad (11)$$

which can be represented when  $t \lesssim 1$  in the form of a series

$$\Phi_k(t) = \sum_{\nu=0}^{\infty} (-1)^\nu \frac{(k+1)!(\nu+1)!}{(k+1+\nu)!} t^\nu. \quad (11a)$$

In all cases of capture of an electron by protons in collisions with different atoms, the values of  $\beta$ ,  $\gamma$ , and  $\eta$  stay within the following limits:  $0 \leq \beta$

$\leq 5$ ,  $0 < \gamma \leq 1$ ,  $0 < \eta \leq 1$ . The relatively cumbersome expression for  $\Phi_4(\beta\gamma)$  when  $\beta\gamma < 5$  is approximated within 10% by the function  $(1 + \beta\gamma)^{-0.46}$ , and when  $\beta\gamma \leq 1$  it is approximated accurate to 3% by the binomial  $1 - 0.25\beta\gamma$ .

Formula (10) is the simplest generalization of the widely known Brinkman-Kramers formula for the cross sections for capture of electrons by atomic nuclei from the ground state of a hydrogen-like ion<sup>[11, 26, 61]</sup> to include the case of capture of an electron from completely filled atomic shells with arbitrary values of  $n_a$  and  $\beta$ . If the expression for the cross sections given by the Brinkman-Kramers formula<sup>[11, 26, 61]</sup> is represented as a function of the parameters  $\gamma$  and  $\eta$  introduced here, then the resultant formula will differ from (10) in the absence of the factor  $N_a(1 + \beta)^{5/2} \times (1 + \beta\gamma)^{-3}\Phi_4(\beta\gamma)$ , which becomes equal to  $N_a$  when  $\beta = 0$ . Thus, we have introduced in the generalization of the well known Brinkman-Kramers formula presented here only one additional parameter  $\beta$ , which characterizes the external screening. The quantity  $\beta$  is connected with the usually employed screening parameter  $\Theta$ <sup>[27]</sup> by the relation  $\beta = \Theta^{-1} - 1$ .

Regarding formula (10) as a first trial approximation, we have calculated with its aid, in the velocity region  $v > 2 \times 10^8$  cm/sec, the cross sections for the capture of an electron by protons in collisions with atoms of helium, neon, argon, krypton, xenon, and molecules of hydrogen and nitrogen, i.e., we used it not only for completely filled shells, but also as a trial approximation for unfilled atomic shells. The choice of the foregoing media is explained by the fact that in practice the experimental values of the cross sections at  $v > 2 \times 10^8$  cm/sec are known only for these gases.<sup>[28, 15]</sup>

The values of  $b_a$  were obtained by the Slater rules.<sup>[29, 21]</sup> The binding energy for the internal-

shell electrons was taken from the tables of Wapstra et al.,<sup>[21]</sup> while those for the electrons in the outer shell were taken for simplicity from the ionization potentials of the atoms.<sup>[21]</sup> (Allowance for the difference between the binding energy of the s and p electrons of the outer shells changes the cross sections obtained by formula (10) by  $\lesssim 10\%$ .) The binding energy of the external electrons in the molecules  $H_2$  and  $N_2$  was determined from the ionization potentials of these molecules, and the values of  $\beta$  were assumed to be the same as for the isolated atoms. In the calculation of the cross sections for the capture of the electron by any shell we used the values of  $\epsilon_a$  and  $\beta$  averaged over all the electrons of the shell. The values of  $\epsilon_a$ ,  $b_a$ ,  $\eta_1$ , and  $\beta$  for the individual atomic shells, used in the calculations, are listed in the table.

It follows from (10) that when  $v > v_0$  the cross section for the capture of an electron in the ground state of the produced hydrogen atom amounts to 60–85% of the total cross section for the capture in all states, for all the media considered. On the other hand, if account is taken of the conclusions presented at the end of the article, then it must be assumed that in practice this cross section amounts to about 80% of the total charge exchange cross section in all cases. In this connection, to compare the theory with the experiment, Fig. 1 shows the ratios  $R'$  of the experimental charge exchange cross sections of protons and different gases<sup>[28, 15]</sup> to the calculated cross sections for electron capture in the ground state of the hydrogen atom. It is seen from Fig. 1 that the general character of the variation of these ratios  $R'$  with  $v$  and the maximum values of  $R'$  in different media turn out to be the same. The only exception is the dependence of  $R'$  on  $v$  in the case of proton charge exchange in argon, for which an apprecia-

	Medium	configuration	$\epsilon_a$ , eV	$b_a$	$\eta_1$	$\beta$
Outer electron shell	H <sub>2</sub>	1s	15.4	1.07	0.94	0
	He	1s <sup>2</sup>	14.6	1.70	0.74	0.59
	Li	2s	5.4	0.65	1.59	0.06
	N <sub>2</sub>	2s <sup>2</sup> 2p <sup>3</sup>	15.6	2.10	0.93	2.57
	Ne	2s <sup>2</sup> 2p <sup>6</sup>	21.5	2.93	0.79	4.45
	Ar	3s <sup>2</sup> 3p <sup>6</sup>	15.8	2.25	0.93	3.35
	Kr	4s <sup>2</sup> 4p <sup>6</sup>	14.0	2.22	0.98	3.77
	Xe	5s <sup>2</sup> 5p <sup>6</sup>	12.1	2.06	1.06	3.80
	Deeper shell	Li	1s <sup>2</sup>	55	2.7	0.497
N <sub>2</sub>		1s <sup>2</sup>	400	6.7	0.184	0.52
Ne		1s <sup>2</sup>	867	9.7	0.125	0.47
Ar		2s <sup>2</sup> 2p <sup>6</sup>	257	6.9	0.230	1.53
Kr		3s <sup>2</sup> 3p <sup>6</sup> 3d <sup>10</sup>	153	6.6	0.298	2.88
Still deeper shell	Ar	1s <sup>2</sup>	3200	17.7	0.065	0.33
	Kr	2s <sup>2</sup> 2p <sup>6</sup>	1750	15.9	0.088	0.96

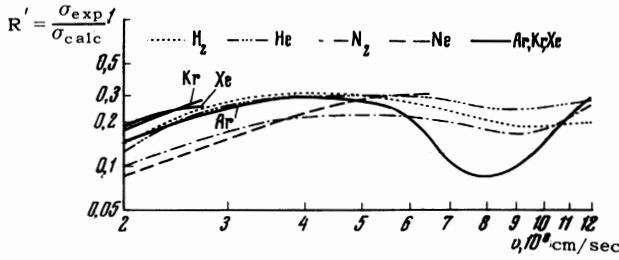


FIG. 1. Ratio  $R'$  of the experimental charge exchange cross sections for protons in different gases to those calculated by formula (10), the cross sections for the capture of an electron in the ground state of the hydrogen atom as a function of the proton velocity  $v$ .

ble decrease in the ratios  $R'$  is observed at  $v \sim (7-9) \times 10^8$  cm/sec. This decrease, as will be shown below, is completely due to the incomplete filling of the external electron shell of the argon atom, i.e., to the fact that in the external shell of these atoms there are only 3s and 3p electrons and there are no electrons in the 3d states.

### 3. CROSS SECTION FOR THE CAPTURE OF AN ELECTRON FROM SOME FILLED SUBSHELLS

Among the atoms mentioned above, nitrogen, argon, krypton, and xenon have incompletely filled external shells. The outer external shell of the nitrogen atom can be regarded as consisting of a filled shell with  $n_a = 2$ , in which are contained four electrons with parallel spins, and one electron in the state 2s with oppositely directed spin. In the outer shells of the atoms of argon, krypton, and xenon in the states with principal quantum number  $n_a = 3, 4$  and 5 there are only eight s and p electrons each. In this connection, we calculate the cross section for the capture of the electron from the states 2s, 3s<sup>2</sup>3p<sup>6</sup>, and 4s<sup>2</sup>4p<sup>6</sup> in nitrogen, argon, and krypton.

For the hydrogen-like wave functions the sum

$\sum_{m=-l}^l |F_{nlm}(p)|^2$  does not depend on the angle variables and is determined only by the absolute values of  $p$  and  $b_a$ , as can be seen, for example, from May's paper.<sup>[24]</sup> According to<sup>[30]</sup>, for the cases of interest to us we shall have

$$|F_{200}(p)|^2 = 4 \left[ 1 - \frac{4b_a^2 p^2}{(p^2 + b_a^2)^2} \right] \frac{32}{\pi} \frac{b_a^5}{(p^2 + b_a^2)^4}, \quad (12a)$$

$$|F_{300}(p)|^2 + \sum_{m=-1}^1 |F_{31m}(p)|^2 = 9 \left[ 1 - \frac{128b_a^4 p^4}{9(p^2 + b_a^2)^4} \right] \frac{32}{\pi} \frac{b_a^5}{(p^2 + b_a^2)^4}, \quad (12b)$$

$$|F_{400}(p)|^2 + \sum_{m=-1}^1 |F_{41m}(p)|^2 = 16 \left[ 1 - \frac{64b_a^4 p^8 - 76.8b_a^6 p^6 + 64b_a^8 p^4}{(p^2 + b_a^2)^6} \right] \times \frac{32}{\pi} \frac{b_a^5}{(p^2 + b_a^2)^4}. \quad (12c)$$

From (2), (8), and (12), taking (1) into account for the corresponding cross sections for the capture of an electron, we obtain the following expressions:

$$\sigma(2,0|n) = N_a(2,0) \frac{4\sigma(2|n)}{N_a(2)} \times \left\{ 1 - \frac{10(1+\beta)\gamma}{3(1+\beta\gamma)^2 \Phi_4(\beta\gamma)} \left[ \chi_6(\beta\gamma) - \frac{6}{7} \gamma \Phi_6(\beta\gamma) \right] \right\}, \quad (13a)$$

$$\sigma(3,01|n) = N_a(3,01) \frac{9\sigma(3|n)}{4N_a(3)} \times \left\{ 1 - \frac{640(1+\beta)^2 \gamma^2}{63(1+\beta\gamma)^4 \Phi_4(\beta\gamma)} \times \left[ 1 - \frac{7}{4} \gamma \chi_8(\beta\gamma) + \frac{7}{9} \gamma^2 \Phi_8(\beta\gamma) \right] \right\}, \quad (13b)$$

$$\sigma(4,01|n) = N_a(4,01) \frac{4\sigma(4|n)}{N_a(4)} \left\{ 1 - \frac{320(1+\beta)^2 \gamma^2}{7(1+\beta\gamma)^4 \Phi_4(\beta\gamma)} \times \left[ 1 - \frac{7(5.2 + 3.2\beta)\gamma}{8(1+\beta\gamma)} + \frac{7(10.6 + 10.8\beta + 3.2\beta^2)\gamma^2}{9(1+\beta\gamma)^2} - \frac{7(9.6 + 7.6\beta + 2\beta^2)\gamma^3}{10(1+\beta\gamma)^2} \chi_{10}(\beta\gamma) + \frac{7(3.2 + 3.2\beta + \beta^2)\gamma^4}{11(1+\beta\gamma)^2} \Phi_{10}(\beta\gamma) \right] \right\}, \quad (13c)$$

Where  $N_a(n_a, l_a, l'_a)$  is the number of atomic electrons in states with principal quantum number  $n_a$  and orbital quantum numbers  $l_a$  and  $l'_a$ ; the values of  $\sigma(n_a|n)$  are given by formula (10), and the values of  $\Phi_6(\beta\gamma)$  and  $\Phi_8(\beta\gamma)$  by (11) and (11a). The functions  $\chi_6(\beta\gamma)$ ,  $\chi_8(\beta\gamma)$ , and  $\chi_{10}(\beta\gamma)$  are defined as follows:

$$\chi_k(t) = \frac{k}{t} \left[ \left( 1 + \frac{1}{t} \right)^{k-1} \ln(1+t) - \sum_{v=1}^{k-1} \frac{1}{v} \left( 1 + \frac{1}{t} \right)^{k-1-v} \right]. \quad (14)$$

When  $t \leq 1$  the following expansion holds:

$$\chi_k(t) = \sum_{v=0}^{\infty} (-1)^v \frac{k!v!}{(k+v)!} t^v. \quad (14a)$$

When  $\beta\gamma \leq 5$ , the functions  $\chi_k(\beta\gamma)$  and  $\Phi_k(\beta\gamma)$  are approximated, accurate to 5%, by the binomials  $(1 + \beta\gamma)^{-\alpha_k}$  with exponents  $\alpha_6 = 0.22$ ,  $\alpha_8 = 0.17$ ,  $\alpha_{10} = 0.16$  for  $\chi_k(\beta\gamma)$  and exponents  $\alpha_6 \approx 0.37$ ,  $\alpha_8 \approx 0.33$ , and  $\alpha_{10} \approx 0.28$  for  $\Phi_k(\beta\gamma)$ .

Since

$$\begin{aligned}\sigma(2|n) &= \sigma(2,0|n) + \sigma(2,1|n), \\ \sigma(3|n) &= \sigma(3,0|n) + \sigma(3,2|n), \\ \sigma(4|n) &= \sigma(4,0|n) + \sigma(4,23|n),\end{aligned}\quad (15)$$

we obtain directly from (10) and (13) expressions for  $\sigma(2, 1|n)$ ,  $\sigma(3, 2|n)$ , and  $\sigma(4, 23|n)$ . In particular, for  $\sigma(2, 1|n)$ , taking into consideration the fact that  $N_a(2, 0) = N_a(2)/4$ , we obtain

$$\begin{aligned}\sigma(2,1|n) &= \sigma(2|n) \frac{10(1+\beta)\gamma}{3(1+\beta\gamma)^2\Phi_4(\beta\gamma)} \\ &\times \left[ \chi_6(\beta\gamma) - \frac{6}{7}\gamma\Phi_6(\beta\gamma) \right].\end{aligned}\quad (16)$$

Formulas (13a), (13b), and (16) are generalizations of the formulas of May and Lodge<sup>[10]</sup> for the cross sections for the capture of an electron from excited hydrogen atoms in states with different  $l_a$  at  $n_a = 2$  and 3, and for arbitrary values of  $\beta$ . When  $\beta = 0$  formulas (13a), (13b), and (16), coincide with the corresponding formulas of May and Lodge.<sup>[10]</sup>

Figure 2 shows the ratios of the cross sections given by formula (13) to the cross sections calculated by formula (10), for the values of  $\epsilon_a$ ,  $\beta$ , and  $\eta_1$  corresponding to the capture of an electron in the ground state of a hydrogen atom from the outer shell of nitrogen, argon, and krypton (see the table). A similar picture (with a rather insignificant shift in the velocity  $v$ ) holds also for the case of capture of an electron in states with  $n > 1$ . From Fig. 2 we see that allowance for the incomplete filling of the shell leads to either increase or de-

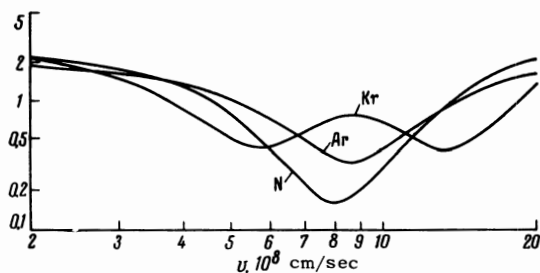


FIG. 2. Ratio of the cross sections given by formulas (13) to the cross sections calculated by formula (10), at values of  $\epsilon_a$ ,  $\eta_1$ , and  $\beta$  corresponding to the capture of an electron in the ground state of the hydrogen atom from the outer shell of the atoms of nitrogen, argon, and krypton, as a function of the proton velocity  $v$ .

crease of the cross sections, by a factor up to 2–6. The decrease in the proton charge exchange cross section in argon at  $v = (6-12) \times 10^8$  cm/sec, shown in Fig. 2, agrees fully with that observed in experiment (Fig. 1). In the case of nitrogen atoms, the considered change in the cross section pertains only to one of the five L electrons, therefore for the summary cross section of electron capture from the L shell of nitrogen this correction does not exceed  $\pm 25\%$ .

From the calculation results shown in Fig. 2 it follows that in the region of  $V$  between  $\sim 2$  and  $\sim 5$  the cross section for the capture of the 2s electron is smaller (and for  $V \approx 3-4$ , appreciably smaller) than the average cross section for the capture of the L electron. Therefore for  $v = (5-13) \times 10^8$  cm/sec, more than 80% of the cross section for the capture of an electron from the completely filled L shell is due to the capture of the p electrons. The ratio cross sections for capture of electrons making up the configuration  $2s2p^3$ , to the cross section for the capture of only  $2p^3$  electrons of nitrogen, is shown in Fig. 3.

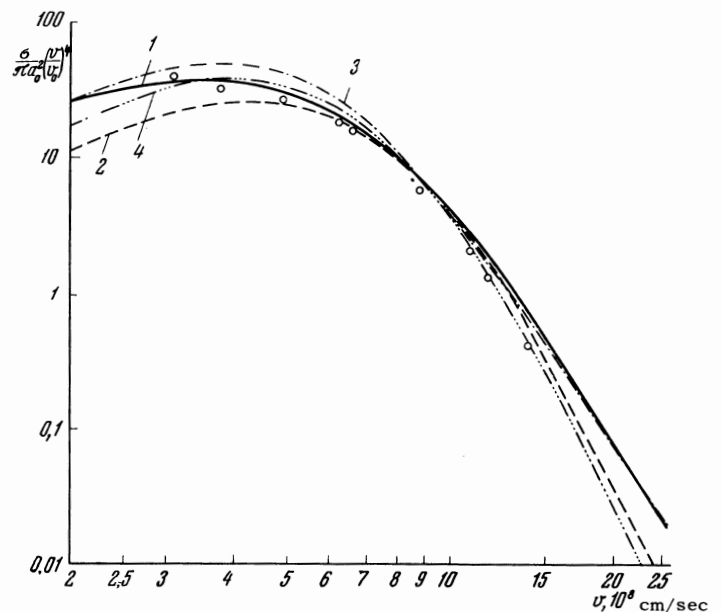


FIG. 3. Cross section for the capture of an electron in the ground state of the hydrogen atom from the L-shell of the nitrogen atom: 1—cross section for the capture of  $2s2p^3$  electrons as given by formula (10) with  $u/v_0 = 1.08$ ,  $\beta = 3.55$  (after Slater); 2—cross section for the capture of  $2p^3$  electrons according to formula (13a) for the same values of  $u$  and  $\beta$ ; 3—cross section for the capture of  $2s2p^3$  electrons as given by (13a) and (16) with  $u/v_0 = 1.41$  and  $\beta = 1.55$  for 2s electrons and  $u/v_0 = 1.08$  and  $\beta = 1.92$  for  $2p^3$  electrons (after Hartree-Fock); 4—Cross section for the capture of  $2p^3$  electrons, according to (13a), with  $u/v_0 = 1.08$  and  $\beta = 1.92$ ; points—cross sections for the capture of  $2p^3$  electrons as obtained by Mapleton<sup>[18]</sup>.

The same figure shows for comparison the cross section for the capture of  $2p^3$  electrons and the summary cross sections for the capture of the  $2s2p^3$  electrons, calculated for values  $u/v_0 = 1.41$  and  $\beta = 1.55$  for the  $2s$  electron, and  $u/v_0 = 1.08$ ,  $\beta = 2.92$  for the  $2p^3$  electrons. The value  $u/v_0 = 1.41$  corresponds to the average binding energy of the  $2s$  electrons in the nitrogen atom, obtained from spectroscopic data,<sup>[20]</sup> while the values of  $\beta$  correspond to the parameters  $b_a = a_a^*/n_a^*$ , obtained from calculations of the wave function of the nitrogen atom by the Hartree-Fok method.<sup>[25]</sup> Figure 3 shows also the cross section for the capture of  $2p^3$  electrons of nitrogen atoms, calculated by Mapleton<sup>[18]</sup> by using a better analytic wave function.

When comparing Mapleton's results with ours, it must be borne in mind that in the case of protons colliding with nitrogen atoms, the cross sections for the capture of the electrons from the outer shell should, according to formula (10), in the region of  $v$  from  $\sim 6 \times 10^8$  to  $15 \times 10^8$  cm/sec, be  $\sim 20\%$  smaller than in collisions with nitrogen molecules.

It is seen from Fig. 3 that the use of a better wave function for more exact values of  $u$  and  $\beta$  does not lead as a rule to any serious changes in the values of the obtained cross sections. In addition, within the framework of the comparatively crude Brinkman-Kramers approximation, it is meaningless to aim at high calculation accuracy. Therefore in calculating the cross sections for the charge exchange of protons in the Brinkman-Kramers approximation, the state of the atoms of the medium can be described by hydrogen-like functions with values of  $u$  and  $\beta$  averaged for the shell, and use formulas (10), (13), and (16).

#### 4. SEMI-EMPIRICAL METHOD OF CALCULATING THE CROSS SECTIONS FOR CHARGE EXCHANGE OF PROTONS IN DIFFERENT MEDIA

The ratio of the experimental cross sections for charge exchange of protons in hydrogen, helium, nitrogen, neon, argon, and krypton to the calculated cross sections for the capture of an electron from the outer shells of the corresponding atoms in the ground state of the hydrogen atom is shown in Fig. 4 as a function of the quantity  $v/v_0\sqrt{b_a}$ . It is seen from Fig. 4 that for identical values of  $v/v_0\sqrt{b_a}$ , in the region of  $v/v_0\sqrt{b_a}$  from 0.6 to 3-5, these ratios  $R$ , for all the media under consideration, turn out to be practically the same and do not differ within approximately 20% from

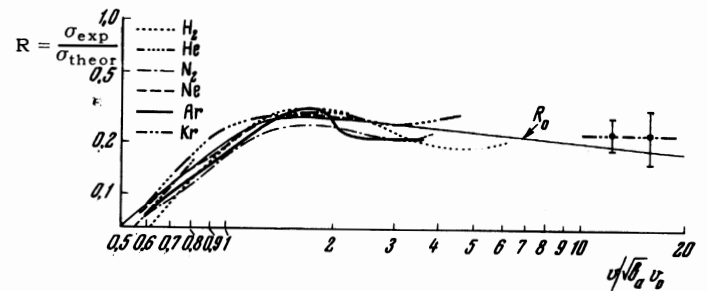


FIG. 4. Ratio  $R$  of the experimental cross sections for charge exchange of protons in different gases, to the calculated cross sections for the capture of electrons from the outer shell of the corresponding atoms in the ground state of the hydrogen atom.

the values of  $R_0(v/v_0\sqrt{b_a})$  given by the formula

$$R_0(t) = 0.3[(7/9t)^{-8} + 7/9t]^{-0.2} \quad (17)$$

with  $t = v/v_0\sqrt{b_a}$ .

It should be noted that the error in the experimental charge exchange cross sections amounts as a rule to 10-20%.

For cases of charge exchange for which the ratios  $R$  are given in Fig. 4, the values of  $\beta$  change from zero to 4.5, and those of  $\epsilon_a$  from 14

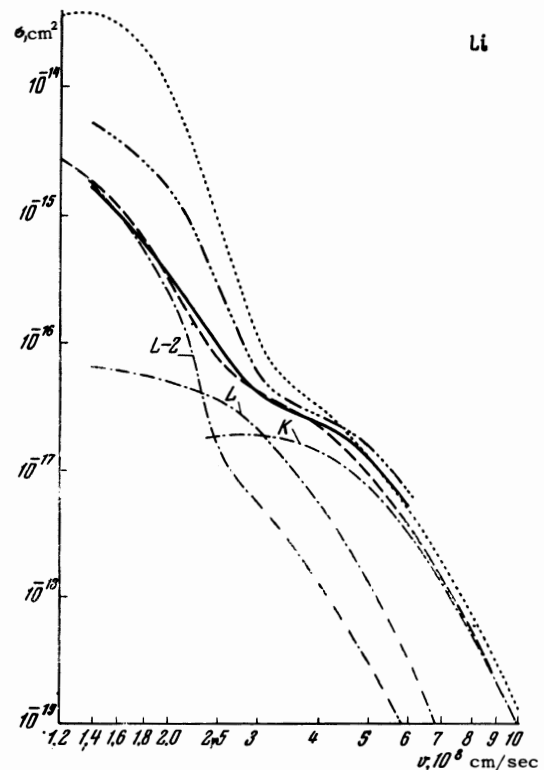


FIG. 5. Cross sections for the charge exchange of protons in lithium as a function of the proton velocity  $v$ ; continuous curve—experimental data, dashed—calculated; the curves K, L, and L-2 indicate respectively:  $\sigma(1|1)R_0(v/1.64v_0)$ ,  $\sigma(2|1)R_0(v/0.8v_0)$ , and  $\sigma(2|2)R_0(v/0.8v_0)$ . The values of  $n3\sigma_n$  for  $n \geq 10$  are shown as follows: dash-dot curves—experimental, dotted curves—calculated.

to 24 eV, corresponding to a change of  $\eta_1$  from  $\sim 1$  to  $\sim 0.75$ . For any other atom, the values of  $\beta$  lie in the same interval, while the values of the binding energy  $\epsilon_a$  of the electrons, even if we consider only the outer shell of the atoms, go beyond the indicated interval. In order to check the suitability of formula (17) for small values of  $\epsilon_a$ , we calculated the cross sections for the charge exchange of protons in collisions with lithium atoms. The cross sections for the capture of K and L electrons, calculated from formulas (10) and (13a) with the values of  $\epsilon_a$  and  $\beta$  listed in the table, were multiplied by the correcting function (17).

It follows from these calculations (Fig. 5) that when  $\epsilon_a = 5.4$  eV, i.e.,  $e/v_0 = 0.363$ , unlike the case of capture of electrons with  $\epsilon_a \geq 14$  eV, when  $u/v_0 > 1$ , in the region  $v \approx (1-2) \times 10^8$  cm/sec the main contribution to the total charge-exchange section of the protons is made by the cross section for the capture of the electron in the excited state of the hydrogen atom with  $n = 2$ . (Processes of electron capture in all other states given not more than 40% of the total cross section.) In this connection, in order to obtain the total charge-exchange cross section of the protons in lithium, we took the sum  $\sigma(1|1)R_0(v/1.64v_0) + [\sigma(2|1) + \sigma(2|2)]R_0(v/0.8v_0)$ . The cross section obtained, as seen from Fig. 5, agrees well with the experimental value.<sup>[31]</sup>

Assuming that the function (17) is valid in the case of capture of an electron from arbitrary atomic shells, we have calculated for  $v$  from  $2 \times 10^8$  to  $5 \times 10^9$  cm/sec the cross sections for charge exchange of protons in hydrogen, helium, nitrogen, neon, argon, and krypton. The cross sections for the capture of electrons from individual atomic shells in the ground state of the hydrogen atom, calculated by means of formulas (10) and (13), were multiplied by the correcting function  $R_0$  of  $v/v_0\sqrt{b_a}$  and summed. The values of  $\epsilon_a$ ,  $b_a$ ,  $\eta_1$ , and  $\beta$  used in these calculations are listed in the table. The results of the calculations, together with the available experimental data<sup>[28, 15]</sup>, are shown in Fig. 6, from which we see that there is good agreement between experiment and the calculation results.

From the calculations it follows (see Fig. 6) that  $v \sim v_0$  the proton charge exchange cross sections are determined practically completely by the capture of electrons from the outer shell of the atoms. The electrons in the next shell, i.e., the M electrons of the krypton atom, the L electron of the argon atom, and the K electrons of the nitrogen and neon atoms, begin to make a noticeable contribution ( $\sim 20\%$ ) to the cross sections at  $v \approx 7$ ,

9, 12, and  $18 \times 10^8$  cm/sec respectively. With further increase in the proton velocity, the role of these electrons increases rapidly: an increase of their contribution to the total cross section from 20 to 80% takes place when the velocity  $v$  is increased by a factor 1.7–2. The electrons of the deeper shells, i.e., the L electrons of the krypton atoms and the K electrons of the argon atoms begin to exert a noticeable influence on the total cross section at  $v = 30-40 \times 10^8$  cm/sec.

In all cases, the electrons of the internal atomic shells play an appreciable role in the charge exchange of the protons when  $v > u$ , and  $v/v_0\sqrt{b_a} > 1$  and the correcting function  $R_0$  depends little on  $v$ :  $R_0 = 0.3(7v/9v_0\sqrt{b_a})^{-1/5}$ . The good agreement between the calculated and the experimental charge exchange cross sections for protons and nitrogen and in argon for  $v$  equal to  $1.4 \times 10^9$ ,  $3.5 \times 10^9$ , and  $4.4 \times 10^9$  cm/sec, indicates that the correcting function (17) can be used not only for the capture of an electron from the outer shells with  $\epsilon_a$  of the order of 10–20 eV, when  $\eta_1 \sim 1$ , but also in cases of capture of an electron from internal shells, when the values of  $\eta_1$  turn out to be close to zero.

Thus, we can assume that for all the values of  $\eta$  and  $\beta$  realized in practice, corresponding to transitions which make the main contribution to the total cross section for proton charge exchange, the single-electron Brinkman-Kramers approximation employed in this paper, together with the correcting function (17), will give values close to actual values of the cross section of the charge exchange of protons colliding with any atom or simple molecule. This procedure can be regarded as a semi-empirical method of calculating proton charge exchange cross sections, with an accuracy estimated at 20–25%.

In view of the great interest recently shown in processes of electron capture in highly excited states of the hydrogen atom with  $n \sim 10$ , the method proposed here, i.e., formulas (10), (13), and (17), was used to calculate the cross section for the capture of an electron in highly excited states of the hydrogen atom with  $n \sim 10$  in hydrogen, helium, lithium, nitrogen, neon, and argon. From (10) and (13), and also from experiment,<sup>[31, 32]</sup> it follows that these cross sections  $\sigma_n$  are proportional to  $n^3$ , and therefore the results of the calculations and the experimental data<sup>[31, 32]</sup> are presented in Figs. 5 and 6 in the form of the product  $n^3\sigma_n$ .

It is seen from Figs. 5 and 6 that in the region of small velocities, the calculated values of  $n^3\sigma_n$  are as a rule larger than  $\sigma_1$ . Furthermore, whereas in helium and neon with  $u/v_0 = 1.35$  and 1.26 the ratio of these quantities does not exceed



1.5–1.7, in media such as hydrogen, nitrogen, and argon, for which  $u/v_0 \approx 1.08$ , these ratios reach 2.5–3, and in lithium ( $u/v_0 = 0.63$ ) they turn out to be larger than 10. The increase in the calculated values of  $n^3\sigma_n$  on going from  $n \sim 1$  to  $n \gtrsim 10$  is

due to the decrease in the lower limit  $\hbar A_0$  of the momenta of the captured atomic electrons. With increasing velocity  $v$ , the relative difference between the values of  $A_0$  for  $n = 1$  and  $n \gtrsim 10$  decreases, and when  $v < u (1 - \eta_k^2/2)^{1/2}$ , where  $k \sim 1$ ,

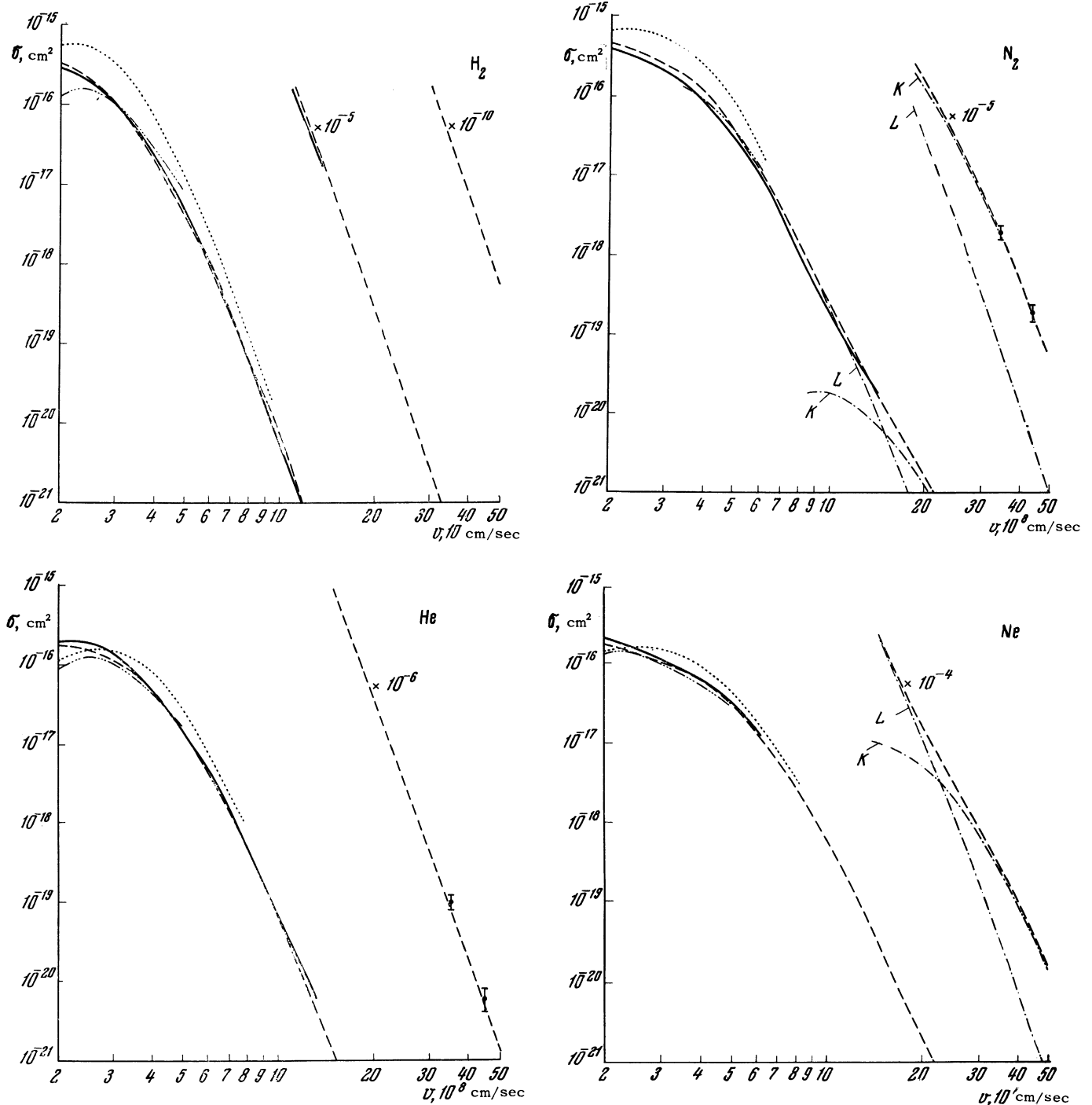


FIG. 6. Cross sections for the charge exchange of protons in hydrogen, helium, nitrogen, neon, argon, and krypton as functions of the proton velocity  $v$ : continuous curves—experimental from [28], points— experimental from [15], dashed curves—calculated. The curves K, L, and M indicate the cross sections for the capture of electrons from the individual (respective) shells. The values of  $n^3\sigma_n$  for  $n \geq 10$  are shown as follows: dash-dot curves—experimental, dashed curve—calculated. (continued)

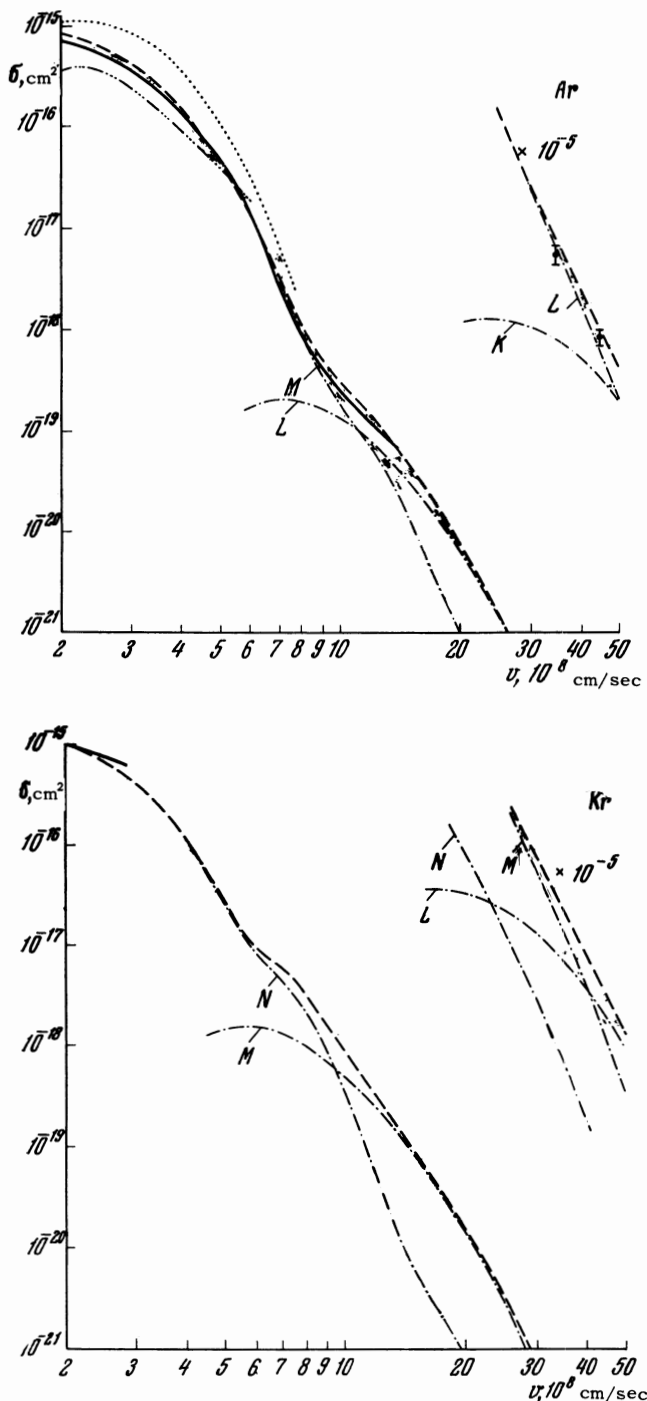


FIG. 6 (continued)

the quantity  $A_0$  for  $n \geq 10$  becomes smaller than for  $n = k \sim 1$ , therefore in the region of high velocities the values of  $n^3 \sigma_n$  for different  $n$  come closer together, while in the region of small velocities the values of  $n^3 \sigma_n$  for  $n \geq 10$  becomes smaller than  $\sigma_1$ .

The experimental values of  $n^3 \sigma_n$  for  $n \sim 1$  do not exceed as a rule the total charge exchange cross sections  $\sigma$ , and amounts to  $(4-5)\sigma$  in the case of a lithium target with  $v \lesssim 2 \times 10^8$  cm/sec, when the main contribution to the total cross sec-

tion  $\sigma$  is made by collisions with capture of an electron in states with  $n = 2$ . In other words, the  $\sigma_n$  are proportional to  $n^3$  starting with  $n = 1$ , and for a lithium target starting with  $n = 2$ . Thus, the difference in the values of  $A_0$  for  $n \sim 1$  and  $n \sim 10$ , which according to (10) and (13) should lead to an essential increase in the values of  $n^3 \sigma_n$  when  $n$  increases from  $\sim 1$  to  $\sim 10$ , actually exerts no influence on the value of the cross sections when  $v \sim v_0$ . This means that there is such a strong decrease in the probability for the capture of electrons possessing small momenta, that these electrons make no noticeable contribution to the charge exchange cross section.

The sharp decrease in the probability of capturing electrons with small momenta is apparently connected with an interaction, not accounted for in the Born approximation, between the captured electron and the atom of the medium in the final state, and should also influence the value of the cross sections for the capture of an electron in states with  $n \sim 1$ . In this connection it should be noted that in the region of  $v$  from  $v_0$  to  $1.2v_0\sqrt{b_a}$ , where a decrease in the value of  $R$  is observed (Fig. 4), the total cross sections for the charge exchange of protons are proportional to  $v^{-2}$ , i.e., they depend on  $v$  in the same manner as for a constant value of  $A_0$ , whereas the energy and momentum conservation laws lead to values of  $A_0$  which decrease with decreasing  $v$ , and consequently the cross sections calculated from (10) and (13) turn out to be approximately proportional to  $v^{-3.5}$ . It follows therefore that if the decrease in the values of  $R$  at  $v = v_0 - 1.2v_0\sqrt{b_a}$  is due to the strong decrease of the probability for the capture of electrons with small momenta, then the upper limit  $p'$  of these momenta is determined by the values  $\hbar A_0 = (\mu v/2)[1 - (1-\eta^2)(u/v)^2]$  for  $v \approx 1.3v_0\sqrt{b_a}$ , i.e.,  $p' \sim (0.5-1)\mu v_0$ . Thus, if we assume that electrons with  $p < p'$  make no essential contribution to the cross section of electron capture, then it is necessary to take in place of the correcting function (17) the quantity  $R \sim 0.3$ , which depends little on  $v$ . Within the framework of the approximation considered here, we can then obtain also agreement with experiment for the cross sections for the capture of an electron in states with different values of  $n$ .

The author is deeply grateful to O. B. Firsov and G. F. Drukarev for valuable remarks during the discussion of the present work.

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Translated by J. G. Adashko  
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#### ERRATUM

In the article by N. Y. Delyagin et al., "Magnetic Hyperfine Structure of the Gd<sup>155</sup> Levels in Metallic Gadolinium and in the Intermetallic Compound GdAl<sub>2</sub>" *Soviet Phys. JETP* **24**, 64 (1967), in the second paragraph of the Introduction (right-hand column, 14th line from the bottom), the phrase "temperature of liquid helium" should read "temperature of liquid nitrogen." This is a translation error and does not appear in the original Russian.