

and therefore each particular level from which a transition occurs has a small population.

The BiS molecule, which we have considered as an example, is evidently not the best one from the experimental point of view, even among molecules with $\omega = \frac{1}{2}$. In it the effect is suppressed by about an order of magnitude because of the large angular momentum of the Bi nucleus. Most molecules, indeed, have $\omega = 0$ in the ground state. However, if the excited state to which the transition goes has $\omega = 1$, the case is one in which the effect will be of the same order as in a molecule with $\omega = \frac{1}{2}$. In fact, for $\omega = 1$ the matrix element of the mixing is of the form

$$\frac{\langle 1|H_w|0\rangle\langle 0|H_B|-1\rangle}{E_1 - E_0} \sim \left\langle \frac{1}{2}|H_w|-\frac{1}{2}\right\rangle \frac{B}{\varepsilon} J, \quad (15)$$

where H_B is the centrifugal energy operator; Eq. (2). However, the smallness of the factor B/ε in the matrix element is compensated by a similar smallness of the splitting of levels of different parities (see the Introduction).

We call attention to the fact that the optical activity of molecules can also be studied in the rf range in transitions between rotational levels and between hyperfine-structure levels.

In conclusion we remark that a two-center system similar to a molecule in a definite rotational state is formed during nuclear fission. In such a system, as shown in this paper, T -odd effects are greatly enhanced. As for P -odd effects in fission, the mechanism we have considered here cannot be directly transferred to this phenomenon because of the strong spin-spin interaction.

We are grateful to I. B. Khriplovich, L. M. Barkov, M. S. Zolotarev, V. F. Dmitriev, and V. G. Zelevinskiĭ for many discussions.

¹We point out that if, owing to nonsphericity of the nucleus, there is a tensor interaction $H_w = T_{ik} I_i I_k$, it may be enhanced relative to the vector interaction by 4 or 5 more orders of magnitude. The point is that $\langle \Omega | T_{ik} | -\Omega \rangle \neq 0$ for $\omega = 1$, and the splitting for a level with $\omega = 1$ is 5 orders of magnitude smaller than that of one with $\omega = \frac{1}{2}$.

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Dielectronic recombination of electrons in collisions with ions

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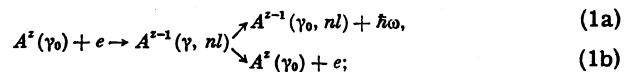
Zh. Eksp. Teor. Fiz. 75, 1214-1221 (October 1978)

A simple expression is obtained for the dielectronic recombination coefficient of electrons colliding with partly ionized ions. The results are in good agreement with numerical calculations of the dielectronic recombination coefficients carried out by other authors.

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1. INTRODUCTION

Dielectronic recombination (DR) is known¹⁻⁵ to occur in the course of radiative stabilization [described by Eq. (1a) below] of an autoionizing state of an ion $A^{z-1}(\gamma, nl)$ formed on collision of an electron with an ion in a state $A^z(\gamma_0)$:



here, z is the ionic charge; γ_0 and γ are the quantum numbers of the ground and excited states of the A^z ion.

The important role played by DR in a high-tempera-

ture low-density plasma¹⁾ was first pointed out by Burgess,¹ who showed that the DR coefficient may be considerably greater than the photorecombination coefficient. Burgess carried out also² a large number of numerical calculations of the DR coefficients and approximated the results by a formula depending in a complex and physically unclear manner on the parameters of the recombining ions. The Burgess formula was used by several authors^{6,7} in specific calculations of the DR rates. Tucker and Gould³ obtained an analytic expression for the DR coefficient but—as pointed out earlier^{4,6} they made fairly rough approximations. Beigman *et al.*⁴ reported the results of numerical calculations of the DR coefficients as a function of the ionic charge for several isoelectronic sequences from He to Ne and for all the degrees of ionization of iron. The results obtained by Beigman *et al.*⁴ were insufficient to describe the dynamics of stripping of multiply charged multielectron ions of heavy impurities (of the Mo and W type) encountered in currently used high-temperature systems.⁸ Donaldson and Peacock⁵ recently tabulated the results of numerical calculations of the DR coefficients of hydrogen-like ions. Some work^{4,9} has been done on the influence of the electron density and radiation on DR.

We shall obtain a simple and physically clear expression for the DR coefficient. A shortcoming of the earlier investigations³⁻⁵ has been the absence of comparison of the results of calculations with earlier results. Therefore, we shall also compare (in the case of hydrogen-like ions and various iron ions) the DR coefficients reported in Refs. 2-5 and in the present paper. We shall use the atomic system of units, unless specifically stated otherwise.

2. PRINCIPAL FORMULAS

The DR coefficient which can be obtained from the theory of resonance scattering or the equilibrium conditions for the formation and decay of autoionizing states is⁴

$$\alpha_e = \left(\frac{2\pi}{T}\right)^{\frac{1}{2}} \frac{g(\gamma)}{g(\gamma_0)} \sum_n \sum_{l=0}^{n-1} \frac{(2l+1)\Gamma_r \Gamma_{nl}}{\Gamma_{nl} + \Gamma_r} \exp\left(-\frac{\omega}{T} + \frac{z^2}{2n^2 T}\right), \quad (1)$$

where

$$\Gamma_r = \frac{2\omega^2}{c^3} f_{\gamma\gamma_0}, \quad f_{\gamma\gamma_0} = \frac{2\omega}{3g(\gamma)} \sum_{\pi_0} |\langle \Psi_{\gamma_0} | \mathbf{r} | \Psi_{\gamma} \rangle|^2, \quad (2)$$

Γ_{nl} and Γ_r are the autoionization and radiative decay widths; $g(\gamma)$ and $g(\gamma_0)$ are the statistical weights of the states $A^z(\gamma)$ and $A^z(\gamma_0)$; ω and $f_{\gamma\gamma_0}$ are the energy and oscillator strength of the $\gamma \rightarrow \gamma_0$ transition; c is the velocity of light.

Since the radiative decay width is small, $\sim 1/c^3$, the main contribution to DR is made by the strongly excited autoionizing states $A^{z-1}(\gamma, nl)$ with a principal quantum number n much greater than $n_f = (z+1)/(2I_f)^{1/2}$, which is the effective principal quantum number of the excited state $A^z(\gamma)$; I_f is the ionization potential of the $A^z(\gamma)$ ion. In this case a weakly bound electron can be described by purely Coulomb wave functions for a charge z (we shall use the same functions to describe an electron in a continuous spectrum) ignoring the influence of a weak-

ly bound electron on an internal strongly bound excited electron and also neglecting the exchange effects; in the calculation of the autoionization decay width we have to allow for $\mathbf{r}_1 \cdot \mathbf{r}_2 / r_2^3$, which is the first nonvanishing dipole-dipole term of the expansion of the electron-electron interaction in terms of the reciprocal powers of the distance from the nucleus of a weakly bound electron. Applying the well-known rules for the calculation of the dipole matrix elements,¹⁰ we obtain the following expression for the autoionization decay width:

$$\begin{aligned} &= \frac{2\pi}{g(\gamma)(2l+1)} \sum_{\pi_0} \sum_{m'l'm'} \left| \langle \Psi_{\gamma}(r_1) \varphi_{nlm}(r_2) \left| \frac{1}{r_{12}} \right| \Psi_{\gamma_0}(r_1) \varphi_{n'l'm'}(r_2) \rangle \right|^2 \\ &= \frac{2\pi}{g(\gamma)(2l+1)} \left(\sum_{\pi_0} |\langle \Psi_{\gamma} | \mathbf{r}_1 | \Psi_{\gamma_0} \rangle|^2 \right) \left(\sum_{l'=|\pm 1, m} \left| \langle \varphi_{nlm} \left| \frac{\mathbf{r}_2}{r_2^3} \right| \varphi_{n'l'm'} \rangle \right|^2 \right) \\ &= \frac{f_{\gamma\gamma_0} \pi}{\omega(2l+1)} \left(\sum_{l'=|\pm 1} l_{\max} \langle R_{nl}^z \left| \frac{1}{r^2} \right| R_{n'l'}^z \rangle \right)^2. \end{aligned}$$

Here, R_{nl}^z and $R_{n'l'}^z$ are the radial Coulomb wave functions for a nuclear charge z . The dipole approximation in the calculation of the decay width corresponds to the Bethe-Born-Coulomb approximation in the theory of excitation of ions by electron impact. This is the approximation used in all the DR calculations (with the exception of those of Beigman *et al.*,⁴ who used the Born-Coulomb approximation) of the partial excitation cross sections near the threshold, in terms of which the autoionization decay widths are expressed in Refs. 1-5. We shall use the proportionality of the autoionization decay width to the photoionization cross section rather than to the excitation cross section near the threshold.

Going over to the Coulomb wave functions for a unit nuclear charge, we obtain

$$\Gamma_{nl} = \frac{z^2 f_{\gamma\gamma_0} \pi}{\omega(2l+1)} \sum_{l'=|\pm 1} l_{\max} \langle R_{nl}^1 \left| \frac{1}{r^2} \right| R_{n'l'}^1 \rangle^2. \quad (3)$$

We shall now find the dependence of Γ_{nl} on the principal quantum number. We can show¹¹ that in the case of strongly excited states the radial Coulomb wave functions are

$$R_{nl}^1(r) \rightarrow \frac{1}{n^{\frac{1}{2}}} \left(\frac{2}{r}\right)^{\frac{1}{2}} J_{2l+1}((8r)^{\frac{1}{2}}). \quad (4)$$

It follows from Eq. (4) that the autoionization width (3) can be written in the form

$$\Gamma_{nl} = \frac{z^2 f_{\gamma\gamma_0}}{\omega n^2} g_l\left(\frac{v}{z}\right), \quad \frac{v}{z} = \frac{(2\omega)^{\frac{1}{2}}}{z} = \frac{(\omega |eV| / Ry)^{\frac{1}{2}}}{z}, \quad (5)$$

where the function $g_l(v, z)$ is

$$g_l\left(\frac{v}{z}\right) = \lim_{n \rightarrow \infty} n^3 \frac{\pi}{(2l+1)} \sum_{l'=|\pm 1} l_{\max} \langle R_{nl}^1 \left| \frac{1}{r^2} \right| R_{n'l'}^1 \rangle^2$$

and depends on just one parameter: v/z .

The function $g_l(v/z)$ can be found if we know the photoionization cross sections, given by¹⁰

$$\sigma(nl, E) = \frac{4\pi^2 \omega}{3c(2l+1)} \sum_{l'=|\pm 1} l_{\max} \langle R_{nl}^z | \mathbf{r} | R_{n'l'}^z \rangle^2. \quad (6)$$

Using the properties of the Coulomb wave functions, we shall transform Eq. (6) to

$$\sigma(nl, E) = \frac{4\pi z^4}{3c\omega^2 n^2} g_l\left(\frac{v}{z}\right). \quad (7)$$

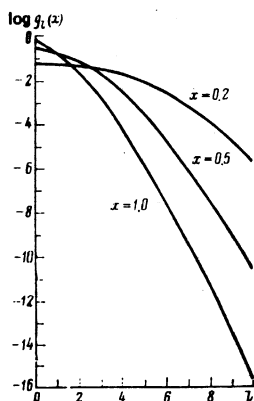


FIG. 1. Function $g_l(x)$.

In the calculation of the DR coefficient one might use analytic expressions for the photoionization cross sections. However, even in the quasiclassical approximation these cross sections¹² are far too complex.²⁾

Therefore, it is more convenient and reliable to use the results of the exact numerical calculations of the photoionization cross sections of the hydrogen atom¹³ carried out for the states with $n \leq 15$ and electron energies in a continuous spectrum up to 13 eV.

The functions $g_l(x)$ decrease rapidly on increase of l (see Fig. 1) and the main contribution of the DR coefficient comes from the first few moments, so that the upper limit in the sum over the moments in Eq. (1) can be replaced with ∞ . Excluding the case $\omega \gg T$, which is of little practical interest and in which the DR coefficient is exponentially small compared with the photorecombination coefficient, we may assume that the binding energies of strongly excited states dominating DR satisfy the condition

$$\frac{z^2}{2n^2} \ll T,$$

and we can also assume the factor $\exp(z^2/2n^2T)$ in Eq. (1) to be unity. Altering the order of summation in Eq. (1), replacing the summation over n with integration, and using Eqs. (2) and (5), we obtain the following expression for the DR coefficient:

$$\alpha_d = \left(\frac{2\pi}{T}\right)^{1/2} \frac{2^{1/2} \pi \omega z^{1/2} f_{l0T}}{3c^2 \sin \pi/3} D\left(\frac{v}{z}\right) \exp\left(-\frac{\omega}{T}\right), \quad (9)$$

$$\alpha_d [\text{cm}^3/\text{sec}] = \frac{5.15 \cdot 10^{-14} \omega [\text{eV}] z^{1/2} f_{l0T}}{T^{1/2} [\text{eV}]} D\left(\frac{v}{z}\right) \exp\left(-\frac{\omega}{T}\right), \quad (9a)$$

$$D\left(\frac{v}{z}\right) = \sum_{l=0}^{\infty} (2l+1) g_l^{1/2}\left(\frac{v}{z}\right), \quad \frac{v}{z} = \frac{(\omega [\text{eV}]/Ry)^{1/2}}{z}. \quad (10)$$

Thus, the DR coefficient can be expressed in terms of a universal function $D(v/z)$ which depends on just one natural parameter v/z . The cases defined by $0.1 \leq v/z \leq 1$ are of practical interest. The values of the function $D(v/z)$ for this range of the argument are:

z	0.1	0.2	0.3	0.4	0.5	0.6	0.7	0.8	0.9	1.0
$D(x)$	17.5	14.5	11.5	9.63	8.30	7.33	6.61	6.02	5.56	5.16

In the numerical summation of the series (10) use is made of the moments with $l \leq 14$. With a high degree of accuracy (see Fig. 2) the function $D(x)$ can be represented by³⁾

$$D(x) \approx 5.0x^{-1/6}. \quad (11)$$

In this case we obtain the following formula convenient for practical use:

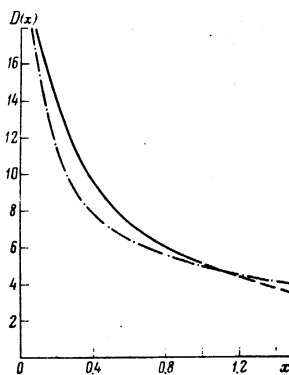


FIG. 2. Function (10) $D(x)$. The continuous curve represents exact calculations, the dashed part is extrapolated, and the chain line is the approximation based on Eq. (11).

$$\alpha_d [\text{cm}^3/\text{sec}] = \frac{4.94 \cdot 10^{-14} \omega^{1/2} [\text{eV}] z^{1/2} f_{l0T}}{T^{1/2} [\text{eV}]} \exp\left(-\frac{\omega}{T}\right). \quad (12)$$

The main assumption in the derivation of Eq. (9) is the hypothesis that the DR process is dominated by strongly excited states. It is clear from Eqs. (1), (2), and (5) that, for a given l , the DR process is dominated by states with a principal quantum number satisfying the condition

$$n \leq n_l = \frac{z^{3/2} g_l^{1/2} c}{2^{3/2} \omega}.$$

Therefore, the condition $n_l \gg n_r$ should be satisfied at least for the first few moments. If, by way of estimate, we use the average value $g_l \sim 0.25$ for the first few moments, we obtain the following condition for the validity of Eq. (9):

$$\frac{1.86 \cdot 10^4 z^{3/2}}{\omega [\text{eV}]} \gg n_l. \quad (13)$$

In particular, in the case of hydrogen-like ions we obtain a restriction on the ionic charge $z \leq 10$. In the case of multiply charged multielectron ions the restriction on the charge is usually much weaker, due to the relatively low energies of the transitions in which there is no change of the principal quantum number.⁴⁾ For example, in the case of the iron ions, Eq. (9) is valid right up to $z \leq 23$ (Table I). If the condition (13) is not satisfied or only partly satisfied, Eqs. (9) and (12) give, respectively, strongly overestimated or just overestimated values of the DR coefficients.

3. COMPARISON WITH THE RESULTS OF OTHER CALCULATIONS

For comparison, we shall now consider the results obtained by other authors. Burgess² approximated the

TABLE I. Values of coefficient in Eq. (17) for iron ions*

z	Transition $\gamma_0 - \gamma$	ω, eV	v/z	$f_{\gamma_0\gamma}$	$c(\gamma)$	$c_1(\gamma)$	$c_2(\gamma)$	$c_3(\gamma)$
1	4s-4p	4.9	0.60	1.00	1.37	1.38	1.71	23.2
6	3p ² 3d ² -3p ³ 3d ³	50.6	0.32	3.04	6.40	6.30	8.06	31.0
12	3s ² 3p ² -3s3p ³	34.0	0.13	0.6	5.46	5.25	4.59	22.0
18	2s ² 2p ⁴ -2s2p ⁵	93.8	0.15	0.086	0.53	0.48	0.49	1.38
23	2s-2p	43.8	0.08	0.05	0.82	0.87	0.57	2.90

*Here, $c(\gamma)$ are the values calculated by Beigman *et al.*,⁴ $c_1(\gamma)$ are those calculated using the Burgess formula (14) (Ref. 2), $c_2(\gamma)$ are calculated on the basis of Eq. (9) in the present paper, and $c_3(\gamma)$ are calculated using the Tucker-Gould formula (16) (Ref. 3). The transition energies and oscillator strengths are taken from Beigman *et al.*⁴

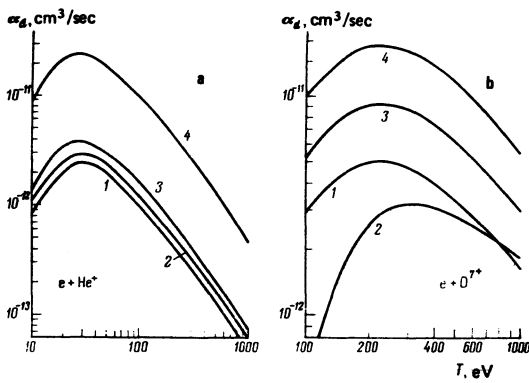


FIG. 3. Dielectronic recombination coefficients: a) He^+ ion; b) O^{7+} ion; 1) according to Burgess²; 2) according to Donaldson and Peacock³; 3) our results [$D(1.73) \approx 2.8$ for He^+]; 4) according to Tucker and Gould.³

numerical values of the DR coefficients by a formula which, subject to the condition (8), is

$$\alpha_d [\text{cm}^3/\text{sec}] = \frac{2.40 \cdot 10^{-9} B(z) A(x) f_{\text{TOT}} \exp\left(-\frac{\omega}{T}\right)}{T^{3/2} [\text{eV}]}, \quad \left. \begin{aligned} B(z) &= \left(\frac{z}{z^2+13.4}\right)^{1/2} (z+1)^{1/2}, \quad A(x) = x^{1/2} / (1+0.105x+0.015x^2), \\ x &= \frac{\omega [\text{eV}]}{(z+1) \text{Ry}}. \end{aligned} \right\} \quad (14)$$

As pointed out earlier, the Burgess formula does not depend in any clear manner on the parameters of the recombining ion. It follows from our results that a more natural approximation parameter is $\omega^{1/2}/z$ and not $\omega/(z+1)$.

Tucker and Gould³ obtained an analytic expression for the DR coefficient on the assumption that the autoionizing states with different moments but with a fixed value of n have the same average decay width

$$\Gamma_n = \frac{1}{n^2} \sum_{l=0}^{n-1} \Gamma_{nl} = \frac{2f_{\text{TOT}} z^2}{3^{1/2} \omega n^3}. \quad (15)$$

It should be noted that Eq. (15) is easily obtained applying Eqs. (5) and (7) and the Kramers quasiclassical autoionization cross section.¹⁰ Using Eqs. (1) and (15) and the condition (8), we obtain³

$$\alpha_d = \left(\frac{2\pi}{T}\right)^{3/2} \frac{2\pi z^{1/2} \omega^{1/2} f_{\text{TOT}} \exp\left(-\frac{\omega}{T}\right)}{5 \sin \frac{\pi}{5} \cdot 3^{1/2} c^{1/2}}, \quad (16)$$

or

$$\alpha_d [\text{cm}^3/\text{sec}] = \frac{1.83 \cdot 10^{-9} z^{1/2} \omega^{1/2} [\text{eV}] f_{\text{TOT}} \exp\left(-\frac{\omega}{T}\right)}{T^{3/2} [\text{eV}]}.$$

The formula (15) and the Kramers approximation for the photoionization cross section gives a result which is satisfactory only when averages are considered. Since in reality the autoionization decay width decreases rapidly on increase of l [see Eq. (5) and Fig. 1], it follows that Eq. (16) overestimates the contribution of the higher moments, so that it also overestimates (by a factor of 2–8) the value of the DR coefficient.

Beigman *et al.*⁴ represented the results of their numerical calculations of the DR coefficients in the form

$$\alpha_d [\text{cm}^3/\text{sec}] = c(\gamma) \cdot 10^{-19} (\omega/T)^{3/2} \exp(-\omega/T). \quad (17)$$

The values of $c(\gamma)$ are given in Table I.

The DR coefficients for the hydrogen-like ions He^+ and O^{7+} obtained in Refs. 2, 3, and 5 and in the present study are all plotted in Fig. 3. In the case of He^+ the results of Refs. 2 and 5 are in good agreement with one another and with our data. The Tucker–Gould formula (16) overestimates the result by a factor of about 7. In the case of O^{7+} the condition (13) ceases to be satisfied by a reasonable margin and the results begin to depend on the details of the calculations and agree with one another to within a factor of ~2.

Table I lists the coefficients $c(\gamma)$ in Eq. (17) for the iron ions with $z \leq 23$ calculated in Ref. 4 and obtained in the present study from Eqs. (9), (14), and (16). We can see that the results of Refs. 2 and 4 and our data are in good agreement (on the average to within ~25%). The Tucker–Gould formula gives a DR coefficient which is on the average overestimated by a factor of 4.

4. CONCLUSIONS

Our comparison shows that, in contrast to the Tucker–Gould formula,³ the results obtained using the Burgess expression² or Eqs. (9) and (12) in the present study are in good agreement with the results of numerical calculations reported by Beigman *et al.*⁴ and can be used to calculate the DR coefficients in cases of practical interest.

The function $D(v/z)$, governing the DR coefficient, is calculated in the present paper on the basis of numerically found photoionization cross sections¹³ and, therefore, within the range of their validity, our results are equivalent in respect of precision to numerical calculations of Burgess² and of Beigman *et al.*⁴ However, the expression (9) for the DR coefficient obtained above is almost analytic and it shows why the DR coefficient depends in this way on the parameters of the recombining ion and under which conditions this result applies. This is the advantage of the above analysis over the work of Burgess.²

The author is grateful to M. A. Lenontovich and participants of a seminar led by him for valuable discussions.

¹By a low-density plasma we mean a plasma in which triple recombination is weak compared with photorecombination or dielectronic recombination.

²It should also be pointed out that the partial photoionization coefficients in a range of practical interest $0.1 \leq v/z \leq 1$ vary extremely rapidly when l or v/z is altered and they cannot be represented accurately by any one asymptotic expression. Therefore, the use of any asymptotic representations for the photoionization cross sections reduces the range of validity of the results.

³According to the referee of the present paper, the approximation $D(x) \approx 5.0x^{-2/3}$ would be somewhat better. However, within the limits of the error, both approximations are almost equivalent and Eq. (12) is already used widely with Eq. (11) so that to avoid misunderstanding we shall retain Eq. (11).

⁴Dielectronic recombination via transitions involving a change in the principal quantum number under near-equilibrium conditions is weakened by the smallness of the exponential function in Eq. (12), although the preexponential factor is large.

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Translated by A. Tybulewicz

Influence of symmetry on the exchange of one and two electrons in atomic collisions

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A theoretical investigation is made of one- and two-electron charge exchange in collisions between an atom and an ion of the same element, the latter with two missing electrons. It is shown that the probability of one-electron exchange in the case when the initial term crosses the final ground-state term is half the usual probability for reasons of symmetry: the atom and ion are identical. The occurrence of term crossing in this system alters the physical nature of resonant two-electron exchange. There is a new channel for two-stage exchange of two electrons. The first electron is released on the first pseudocrossing of terms and the second on the second pseudocrossing. In the case of crossing with terms of the excited state, this exchange occurs if the excitation is transferred during the time between the two pseudocrossings. The experimental cross section for the exchange of two electrons in a collision of a negative hydrogen atom with a proton can be ascribed completely to this new channel.

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1. We shall consider the exchange of one and two electrons in slow ($v < 2 \times 10^8$ cm/sec) collisions between an atom and an ion of the same element but with two missing electrons:



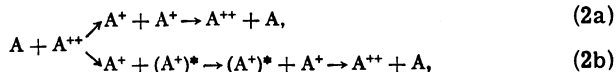
(1b)

It is found that the symmetry resulting from the fact that the particles A and A^{++} represent the same element has an important influence on the physical nature of these processes and their effective cross sections.

The exchange of one electron, process (1a), is non-resonant and due to the crossing of the energy terms of the initial and final states. The exchange of two electrons is a resonant process and its probability in the absence of one-electron term crossing has already been studied.¹⁻² However, the occurrence of such crossing greatly alters this process.

The absolute magnitude of the term repulsion responsible for the two-electron exchange^{2,3} is considerably less than the splitting in the one-electron exchange. Therefore, when an atom approaches an ion, the one-electron exchange may occur earlier. This would seem

to block the two-electron exchange channel (1b) to an extent increasing with the probability of the one-electron exchange during the collision time, i.e., the time interval between two passages of an atom through the same pseudocrossing. In fact, the situation is different. When the probability of the one-electron exchange is high, new ways of exchanging two electrons become possible:



(2b)

which will be investigated below; it should be noted that the chain of events (2) occurs during the same collision.

Let us assume that, in the process (2b), the probability of a nonadiabatic transition on pseudocrossing of one-electron terms is small. Then, after the first passage of the atom through this pseudocrossing, an electron is very likely (probability ~ 1) to be captured by the ion. If there is no event up to the second passage through the pseudocrossing, the probability of the electron returning to the atom as a result of the second pseudocrossing is equally high and the probability of one-electron charge exchange is low. If excitation is exchanged between the