SOVIET PHYSICS JETP VOLUME 24, NUMBER 6 JUNE, 1967

MOLECULAR TERM SPLITTING IN TWO-ELECTRON EXCHANGE

I. V. KOMAROV and R. K. YANEV[1)]

Leningrad State University

Submitted to JETP editor April 18, 1966

J. Exptl. Theoret. Phys. (U.S.S.R.) 51, 1712-1721 (December, 1966)

The asymptotic behavior of molecular terms connected with exchange of electron pairs between atoms is considered. An asymptotically exact formula is derived for the splitting corresponding to large internuclear distances. The effect of the spins of the electrons that do not participate in the transition is taken into account. The cross section for double resonance charge exchange in inert gases is calculated and the results are compared with those of previous calculations and experiments.

1. Resonant processes occuring in slow collisions of heavy particles (charge exchange, excitation transfer, spin exchange) are determined by the asymptotic behavior of the terms of the quasimolecules. The magnitude of the separation of the symmetrical and antisymmetrical terms at large internuclear distances is exponentially small and can be calculated by perturbation-theory methods only accurate to the pre-exponential factor. It therefore becomes necessary to refine the wave function in the deep subbarrier region, solving the Schrödinger equation anew in this region. The asymptotic behavior of the splitting $E_g - E_u$ with the correct pre-exponential factor was obtained for the H_2^+ system in[1-3]. Gor'kov and Pitaevskiĭ[4], and also Herring and Flicker[5], found the singlet-triplet splitting for the ground state of the hydrogen molecule. The exchange coupling of two different atoms was discussed by Ovchinnikova[6].

The purpose of the present paper is to obtain an asymptotic expression for the splitting $E_g - E_u$ for the case when two atoms exchange a pair of electrons. Such a splitting was calculated by a variational method by Fetisov and Firsov[7], who used it to estimate the cross section for double resonance charge exchange. However, we shall show that they obtained an incorrect argument in the exponential, owing to the poor trial function employed. The terms of the quasimolecule He_2^{2+} were also calculated with account of the overlap of the configurations by Ferguson and Moiseiwitsch[8], and more accurately by Brown[9]. Although the latter calculation is sufficiently reliable at medium internuclear distances, the region of large R calls for a special analysis.

Let us consider a system of two identical atomic cores A^{2+}, one of which contains a pair of electrons. We shall characterize the atomic core by means of an effective potential, so that the total function of the system will be regarded as dependent only on the coordinates of the transferred electrons. The transition of two electrons to one of the centers as the atoms move apart corresponds to the terms Σ_g and Σ_u of the molecule A_2^{2+}. Following the standard procedure[4], we express the splitting $E_g - E_u$ in terms of the surface potential in configuration space (see Fig. 1). To this end we make up linear combinations of the molecular functions Ψ_g and Ψ_u; when the atoms move apart these go over into localized two-electron functions of the atoms situated at the points ± a (a = R/2):

$$\Psi_{\mp a} = 2^{-1/2}(\Psi_g \pm \Psi_u). \tag{1}$$

Let us consider the integral $J = (E_g - E_u) \times \int_\Omega \Psi_g \Psi_u d\tau$ over the domain Ω. This integral can be transformed by means of the Schrödinger equation into a surface integral

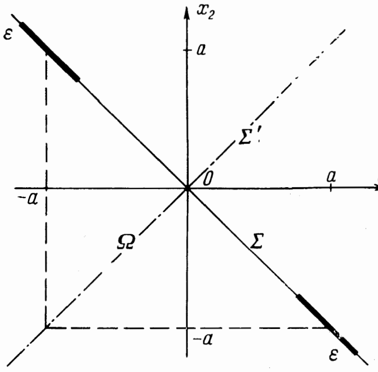

FIG. 1

[1)] Institute of Nuclear Sciences "Boris Kidric," Belgrade, Yugoslavia.

$$J=(E_g-E_u)\int\limits_{\Omega}\Psi_g\Psi_u d\tau=\int\limits_{\Sigma}\Psi_a\nabla_6\Psi_{-a}dS, \qquad (2)$$

where ∇_6 is the six-dimensional gradient. In the domain Ω the wave function is essentially concentrated near the center (−a), so that with exponential accuracy $\int\limits_{\Omega}\Psi_g\Psi_u d\tau = 1/2$, and finally

$$J=\frac{1}{2}(E_g-E_u)=\int\limits_{\Sigma}\Psi_a\nabla_6\Psi_{-a}dS. \qquad (3)$$

When the internuclear distances are sufficiently large, the most important in this integral are the two cylindrical regions $x_1 = -x_2 \sim \pm(a \pm \epsilon)$ (see Fig. 1), which correspond physically to electrons located at different centers. The wave function is largest there and changes most strongly, therefore the flux through the plane is largest in these regions. In the case of very large internuclear distances it can be assumed that the entire flux is determined by these two regions, so that it is sufficient to construct a function Ψ_{-a}, which goes over into the atomic function when $|\mathbf{r}_1 + \mathbf{a}|$, $|\mathbf{r}_2 + \mathbf{a}| \ll R$, $R \to \infty$, only in these regions.

As the zeroth approximation function in the domain Ω it is necessary to choose, if not the function of the isolated atom itself, at least its asymptotic value. At the present time, however, there is no known two-electron function which is uniform over $\mathbf{r}_1$ and $\mathbf{r}_2$. In the cylindrical regions of interest to us, however, one of the electrons is close to the "nucleus," therefore we choose, say for $|\mathbf{r}_1 + \mathbf{a}| > |\mathbf{r}_2 + \mathbf{a}|$,

$$\Psi_{-a}^0=N_{-a}e^{-\alpha_2|\mathbf{r}_2+\mathbf{a}|}|\mathbf{r}_1+\mathbf{a}|^{\beta}e^{-\alpha_1|\mathbf{r}_1+\mathbf{a}|}. \qquad (4)$$

In this formula $-\alpha_1^2/2$ and $-\alpha_2^2/2$ are the first and second ionization potentials, β is a parameter of the theory, characterizing the external electron, with $\beta \approx (1-\alpha_1)/\alpha_1$, and N_{-a} is a normalization coefficient. The latter would have been obtainable by making the chosen function continue into the exact atomic function, but since such functions are unknown, N_{-a} is in practice a parameter of the theory. An asymptotic behavior of this type was analyzed by Fock[10].

The wave function (4) is constructed in such a way that the internal electron is in the ground state of a Coulomb field with energy $-\alpha_2^2/2$, and the outer electron is in a potential which is Coulomb-like at large distances and has an energy $-\alpha_1^2/2$. There exist, however, real atomic systems of the K^- type, in which the inner electron is not in the ground state but in an excited state. In this case it is necessary to take into account in (4) polynomials of $|\mathbf{r}_2 + \mathbf{a}|$, and this alters somewhat the final expressions, but does not influence the reasoning. We note also that the situation under consideration (distinguishable electrons) eliminates the need for symmetrization within the transferred pair, so that the difference $E_g - E_u$ will be determined by the same formulas for the ortho and para states.

The splitting $E_g - E_u$ in (3) is connected with the flux through the hyperplane Σ (see Fig. 1), unlike the singlet-triplet splitting in the H_2 molecule, which is connected with the flux through Σ'. Since the electron interaction is maximal on this hyperplane, allowance for it is essential in the calculation of the singlet-triplet splitting. In our situation, however, the interaction of the electrons is strongest when both electrons are at one nucleus, and this interaction has already been effectively accounted for in the atomic function (4). Therefore, to take into account the influence of the second center it is sufficient to refine the wave function of the external electron. The latter is in the field of two Coulomb centers with different charges Z_1 and Z_2 (Z_1 and Z_2 are the effective charges of the summary field of the core and internal electron, and of the core alone, respectively). The quantity Z_1 is expressed in terms of β and α_1, namely $Z_1 = \alpha_1(\beta + 1)$, and $Z_2 = \alpha_2$.

The Schrödinger equation for a molecular ion with charges Z_1 and Z_2 is

$$\left(-\frac{\Delta}{2}-\frac{Z_1}{|\mathbf{r}_2+\mathbf{a}|}-\frac{Z_2}{|\mathbf{r}_1-\mathbf{a}|}+\frac{Z_1Z_2}{R}\right)\varphi=E\varphi. \qquad (5)$$

It was investigated by Gershteĭn and Krivchenkov[7]. The variables in this equation separate in the elliptic coordinates $\xi = (r_1 + r_2)/R$, $\eta = (r_1 - r_2)/R$, and $\Phi = \tan^{-1}(y/x)$, namely $\varphi = X(\xi)Y(\eta)\exp(im\Phi)$, with

$$\frac{d}{d\xi}\left[(\xi^2-1)\frac{dX}{d\xi}\right] + \left[-\frac{m^2}{\xi^2-1}+R(Z_1+Z_2)\xi-p^2\xi^2+A\right]X=0, \qquad (6a)$$

$$\frac{d}{d\eta}\left[(1-\eta^2)\frac{dY}{d\eta}\right] + \left[-\frac{m^2}{1-\eta^2}+R(Z_2-Z_1)\eta+p^2\eta^2-A\right]Y=0, \qquad (6b)$$

where $p^2 = -(R^2W)/2$, $W = E - (Z_1Z_2)/R$, and A is the separation constant. The energy of the molecule is usually obtained by equating the separation constants from (6a) and (6b)

$$A_{n_\xi}(R,p,m)=A_{n_\eta}(R,p,m).$$

Let us consider the transformation of the molecular functions φ into atomic functions $\varphi_{\pm a}$. At large internuclear distances (6a) takes the form (with the change of variables $\xi \rightarrow \nu = (\xi - 1)R = |\mathbf{r}_1 + \mathbf{a}| + |\mathbf{r}_1 - \mathbf{a}| - R$)

$$\nu X'' + X' + \left[-\frac{p^2}{R}\nu + \frac{A - p^2 + R(Z_1 + Z_2)}{2R}\right] X = 0 \tag{7}$$

(We henceforth put m = 0).

The solution which is finite on the axis of the molecular ion, i.e., at $\nu \rightarrow 0$, is expressed in terms of the confluent hypergeometrical function

$$X = e^{-p\nu/R} F\left(\frac{1}{2} - \frac{A - p^2 + R(Z_1 + Z_2)}{4p}, 1; \frac{2p\nu}{R}\right) \tag{8}$$

For the function to be finite at large distances from the axis, we must set the first argument equal to zero or to a negative integer

$$\frac{1}{2} - \frac{A - p^2 + R(Z_1 + Z_2)}{4p} = -n_1 = 0, \ -1, -2, \ldots$$

In accordance with formula (4), we have $n_1 = 0$ (we are considering a spherically symmetrical state of the external electron).

Let us transform the equation for Y. We introduce the variable $\mu = (\eta + 1)R = |\mathbf{r}_1 + \mathbf{a}| - |\mathbf{r}_1 - \mathbf{a}| + R$. Small values of μ denote localization of the electron near the "nucleus" Z_1, and when $\mu \ll R$ and $R \gg 1$ Eq. (6b) is similar to the just-considered equation for X:

$$\mu Y'' + Y' + \left[-\frac{p^2}{R}\mu + \frac{-A + p^2 - R(Z_2 - Z_1)}{2R}\right] Y = 0. \tag{9}$$

Its solution is also a confluent hypergeometric function, but unlike (8) it is necessary to choose a solution that decreases exponentially at infinity:

$$Y = e^{-p\mu/R}\Psi(-\beta', 1; 2p\mu/R), \tag{10}$$

where

$$-\beta' \equiv \frac{1}{2} + \frac{A - p^2 + R(Z_2 - Z_1)}{4p}.$$

By equating A_ξ to A_η we can express A and p/R in terms of the already fixed parameters of the problem α_1, α_2, and β'. The complete function for $1 \ll |\mathbf{r}_1 + \mathbf{a}| \ll R$ can be written by using the asymptotic expression for Y:

$$\text{fo} \quad \varphi_{-a} \sim e^{-\alpha_1|\mathbf{r}_1 + \mathbf{a}|}(\alpha_1|\mathbf{r}_1 + \mathbf{a}|)^{\beta'}$$

or, comparing with Ψ^0_{-a} from (4),

$$\varphi_{-a} = N_{-a}|\mathbf{r}_1 + \mathbf{a}|^{\beta} e^{-\alpha_1|\mathbf{r}_1 + \mathbf{a}|}. \tag{11}$$

Near the other center we must replace η by $\mu_1 = (1 - \eta)R = -|\mathbf{r}_1 + \mathbf{a}| + |\mathbf{r}_1 - \mathbf{a}| + R$, and when $\mu_1 \ll R$ Eq. (6b) goes over into

$$\mu_1 Y'' + Y' + \left[-\frac{p^2}{R}\mu_1 + \frac{-A + p^2 + R(Z_2 - Z_1)}{2R}\right] Y = 0, \tag{12}$$

and it is necessary to choose a solution which is finite at zero. Noting that the parameters A and p/R have already been determined, we obtain

$$Y = e^{-\frac{1}{2}\alpha_1\mu_1}F(\gamma, 1; \alpha_1\mu_1), \quad \gamma = 1 - \alpha_2/\alpha_1. \tag{13}$$

We assume that γ is not equal to a negative integer. This means physically that the considered terms Σ_g, and Σ_u do not coincide at $R \rightarrow \infty$ with any other term of the system. Multiplying X from (8) by Y from (13) we obtain the function near the foreign center:

$$\varphi_{+a} = N_{+a}F(\gamma, 1; \alpha_1\mu_1)\, e^{-\alpha_1|\mathbf{r}_1 - \mathbf{a}|}. \tag{14}$$

The coefficient N_{+a} has not yet been determined, but it can be expressed in terms of the parameters of the problem by considering the transition from φ_{-a} to φ_{+a} in the intermediate region. Let us carry out this transition, solving in this region Eq. (6b) by the usual semiclassical method, putting $Y = \exp(S_0 + S_1 + \ldots)$ and confining ourselves to the S_1 terms. Leaving out the straightforward intermediate steps, we obtain

$$N_{+a} = (2R)^{\beta + \alpha_2/\alpha_1}e^{-\alpha_1 R}N_{-a}. \tag{15}$$

This allows us to write down the two-electron wave function in the region of interest to us when the external (first) electron is close to the foreign core, and the internal (second) electron remains at its own core

$$\Psi_{-a} = N_{-a}(2R)^{\beta + \alpha_2/\alpha_1} e^{-\alpha_1 R} e^{-\alpha_1|\mathbf{r}_1 - \mathbf{a}| - \alpha_2|\mathbf{r}_2 + \mathbf{a}|} \times F[\gamma, 1; \alpha_1(|\mathbf{r}_1 - \mathbf{a}| - (x_1 - a))]. \tag{16}$$

We took account here of the fact that $\mu_1 \approx |\mathbf{r}_1 - \mathbf{a}| - (x_1 - a)$ when $R \gg 1$.

Let us use the function (16) to calculate the integral J. We change the notation somewhat, introducing $|\mathbf{r}_1 - \mathbf{a}| \rightarrow r_1$, $|\mathbf{r}_2 + \mathbf{a}| \rightarrow r_2$, and $x_1 - a = -(x_2 + a) \equiv z$; then, in the new variables

$$\begin{aligned} J &= \int_\Sigma \Psi_{+a}\boldsymbol{\nabla}_6\Psi_{-a}dS = 2\int_\varepsilon \Psi_{+a}\nabla_6\Psi_{-a}dS \\ &= 8\pi^2 N_{+a}\left[\int_0^\varepsilon dr_2\int_0^{r_2} dr_1\int_{-r_1}^{r_1} dz + \int_0^\varepsilon dr_1\int_0^{r_1} dr_2\int_{-r_2}^{r_2} dz\right] \\ &\times \{e^{-(\alpha_1+\alpha_2)(r_1+r_2)}F(\gamma, 1; \alpha_1(r_2 + z))[z(\alpha_2 r_1 - \alpha_1 r_2) \\ &\times F(\gamma, 1; \alpha_1(r_1 - z)) - \alpha_1(r_2 z + r_1 r_2)F'(\gamma, 1; \alpha_1(r_1 - z))]\}. \end{aligned} \tag{17}$$

The integral (17) can be calculated for sufficiently large ϵ in terms of elementary functions (see the appendix). It turns out to be

$$J = A(\alpha_1, \alpha_2, N)(2R)^{2(\beta + \alpha_2/\alpha_1)}e^{-2\alpha_1 R}, \tag{18}$$

where

$$A(\alpha_1, \alpha_2, N) = (2\pi N)^2 \frac{\alpha_2 - \alpha_1}{\alpha_2^5}\left(\frac{\alpha_2}{\alpha_1 + \alpha_2}\right)^{2\alpha_2/\alpha_1}$$
$$\times\left[5 - \frac{37}{6}\left(\frac{\alpha_2}{\alpha_1 + \alpha_2}\right) + \left(\frac{\alpha_2}{\alpha_1 + \alpha_2}\right)^2\right], \quad (N \equiv N_{-a}).$$

The difference $E_g - E_u$ is positive, corresponding to the well known fact that the ${}^1\Sigma_g^*$ term lies higher than the ${}^1\Sigma_u$ term. In the derivation we made use of the fact that $\exp(-\alpha_1 R) \gg \exp(-\alpha_2 R)$ for sufficiently large R. But this inequality does not impose any limitations on α_1 and α_2, since $\alpha_1 < \alpha_2$ always. Therefore the only criterion for the applicability of (18) is $\alpha_1 R/2 \gg 1$. Under this condition this formula gives an asymptotic exact value of the splitting. We note that formula (18) differs from the corresponding expression of Fetisov and Firsov even in the argument of the exponential.

2. In the derivation of (18) it was assumed that the atomic residue has zero spin. As shown by Firsov and Smirnov[9], using single-electron charge exchange as an example, if the core has spin 1/2 the difference $E_g - E_u$, is half as large for the case considered by them as for the electrons in the field of spinless nuclei. This is connected with the fact that the splitting $E_g - E_u$ depends on the symmetry properties with respect to permutations of all the electrons. Let us take these symmetry properties into account.

We consider the transition of a group of electrons between two identical centers. We shall describe the atomic residue by means of a total spin $S_1^{\pm a}$ with projection $\sigma_1^{\pm a}$, in the transferred group of electrons by a spin S_2 with projection σ_2. Such a transition corresponds to complete functions Σ_g and Σ_u, which depend on the coordinates of the transferred electrons and on the values of $S_{1,2}$ and $\sigma_{1,2}$. We draw in configuration space a symmetry plane that divides this space into two parts; then, integrating to the left of this plane and transforming the integral into a surface integral, we obtain in analogy with (2)

$$(E_g - E_u)\int\limits_\Omega \Psi_g\Psi_u d\tau = \frac{1}{2}\int\limits_\Sigma (\Psi_g\nabla\Psi_u - \Psi_u\nabla\Psi_g)dS \quad (19)$$

(summation over the spins is implied in this formula).

At large internuclear distances, $\Psi_{g,u}$ go over into the functions $\Psi_{\pm a} = 2^{-1/2}(\Psi_g \pm \Psi_u)$, which are localized on the centers ±a and which are eigenfunctions for the spin operator and can be represented in the form

$$\Psi_{\pm a} = \varphi_{\pm a}\chi_{\pm a}. \quad (20)$$

Here φ_a is the coordinate function, centered on the nucleus (a), and

$$\chi_{\pm a} = |S_1^{\mp a}, \sigma_1^{\mp a}\rangle|S_1^{\pm a}, S_2, S, \sigma\rangle, \quad (21)$$

where S and σ are the spin and its projection for the isolated atom. The spin characteristics of the atoms coincide, since we are considering the case of the symmetrical initial and final states. The dependence on the quantities S and σ is manifest in terms of the symmetry properties in the coordinate functions $\varphi_{\pm a}$. We introduce the functions $\varphi_{g,u} = 2^{-1/2}(\varphi_a \pm \varphi_{-a})$, which describe a molecule with zero-spin nuclei. Let us compare the splitting $(E_g - E_u)^0$ in such a molecule with $E_g - E_u$. To this end we relate $\Psi_{g,u}$ with $\varphi_{g,u}$:

$$\Psi_g = \tfrac{1}{2}\{\varphi_g(\chi_a + \chi_{-a}) + \varphi_u(\chi_a - \chi_{-a})\},$$
$$\Psi_u = \tfrac{1}{2}\{\varphi_g(\chi_a - \chi_{-a}) + \varphi_u(\chi_a + \chi_{-a})\}. \quad (22)$$

It is easy to see that the integral in the left side of (19) is equal to

$$\int\limits_\Omega \Psi_u\Psi_g d\tau = \frac{1}{2}(\chi_a^2 + \chi_{-a}^2)\int\limits_\Omega \varphi_u\varphi_g d\tau = \int\limits_\Omega \varphi_u\varphi_g d\tau,$$

and the right side of (19) yields

$$\int\limits_\Sigma (\Psi_g\nabla\Psi_u - \Psi_u\nabla\Psi_g)dS$$
$$= \langle\chi_a|\chi_{-a}\rangle \int\limits_\Sigma (\varphi_g\nabla\varphi_u - \varphi_u\nabla\varphi_g)dS. \quad (23)$$

Thus, the splitting in the case of a core with spin is connected with the spinless splitting by the relation

$$E_g - E_u = \langle\chi_a|\chi_{-a}\rangle(E_g - E_u)^0. \quad (24)$$

We express the matrix element in terms of the Clebsch-Gordan coefficient. To this end we represent χ_a in the form

$$\chi_a = \sum_{\sigma_1'^a\sigma_2'} C^{S\sigma}_{S_1^a\sigma_1'^a S_2\sigma_2'}|S_2\sigma_2'\rangle|S_1^a\sigma_1'^a\rangle|S_1^{-a}\sigma_1^{-a}\rangle. \quad (25)$$

The expression for χ_{-a} is similar and, using the orthonormality of $|S\sigma\rangle$, we obtain

$$\langle\chi_a|\chi_{-a}\rangle = [C^{S\sigma}_{S_1^a\sigma_1^a S_2\sigma_2}]^2. \quad (26)$$

If the spins cancel out in the transferred group or in the cores, i.e., $S_2 = \sigma_2 = 0$ or $S_1 = \sigma_1 = 0$, then, as expected, $\langle\chi_a|\chi_{-a}\rangle = 1$.

We note also that for the case of exchange of one electron at a core spin 1/2 and S = 0 we get $\langle\chi_a|\chi_{-a}\rangle = 1/2$, which coincides with the result of Smirnov and Firsov[12].

A relation similar to (24) for spin charge exchange is

$$E_g - E_u = \langle\chi_a|\chi_{-a}\rangle(E_g - E_u)^0,$$

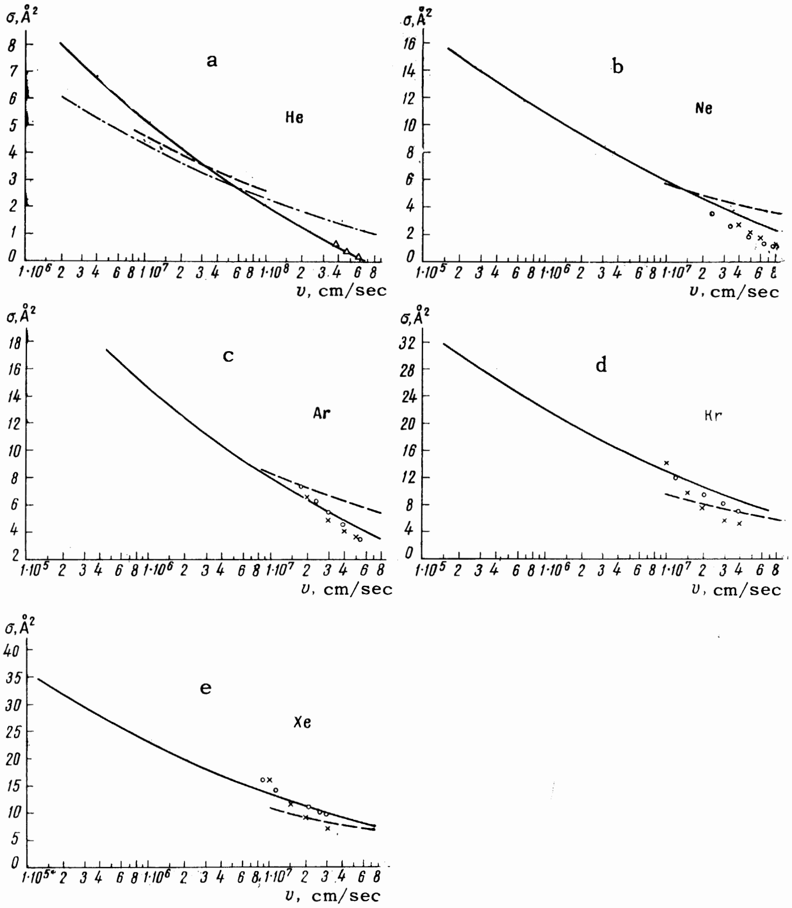

FIG. 2. Cross sections for double resonant charge exchange in inert gases. The solid line shows the result of the present work; △, ○, × – experimental data from [13], [14], and [15], respectively. Dashed curves–calculation from [7]; dash-dot–calculation from [8].

where

$$\langle\chi_a|\chi_{-a}\rangle = C^{S+\sigma+}_{S_1\sigma_1S_2\sigma_2}C^{S+\sigma'+}_{S_1\sigma_1S_2\sigma_2'}C^{S-\sigma-}_{S_1\sigma_1S_2\sigma_2}C^{S-\sigma'-}_{S_1\sigma_1S_2\sigma_2'}, \tag{27}$$

$$\sigma^{\pm} = \sigma_1 \pm \sigma_2, \quad \sigma'^{\pm} = \sigma_1 \pm \sigma_2'.$$

In this case the degeneracy in the spin projections of the transferred electrons is lifted.

The foregoing analysis enables us to write an asymptotically exact formula for the splitting of the terms in two-electron exchange. Using (18), (24), and (26) we obtain ultimately

$$\frac{1}{2}(E_g - E_u) = [C^{S\sigma}_{S_1\sigma_1S_2\sigma_2}]^2 A\,(2R)^{2(\beta+\alpha_2/\alpha_1)}\,e^{-2\alpha_1 R}, \tag{28}$$

where $S_2 = 0$, 1 and the spin of the atomic residue can be arbitrary.

3. Knowing the asymptotic behavior of the term splitting, let us estimate the cross section for double resonant charge exchange in inert gases. In the adiabatic approximation it is equal to

$$\sigma = {}^1\!/_2\pi\rho_0^2, \tag{29}$$

where the critical impact parameter ρ_0 is determined most naturally from the condition

$$\int\limits_{\rho_0}^{\infty} \frac{E_g - E_u}{2\hbar v}\,\frac{R\,dR}{\sqrt{R^2-\rho_0^2}} = \exp(-2C). \tag{30}$$

Here C is Euler's constant.

The splitting $E_g - E_u$, determined by (28), contains the parameter N, which is the normalization coefficient of the asymptotic atomic wave function. We have determined it by using the experimental data of[15].

Figure 2 shows the double charge exchange cross sections calculated from (28), (29), and (30), as functions of the velocity. The same figure shows the results of the calculations of[7,8] and of the experiments[13-15]. The comparison shows that our curves have a slope which is closer to the experimental value. We note that the use of (28) for the calculation of the cross sections in Ne, Ar, Kr, and Xe is by way of a crude estimate, since we have assumed in the derivation of (28) that the transferred electrons are in the s-state. Since the existing experimental data pertain to a velocity region which is at the upper limit of applicability of the present theory, it is very desirable to carry out experiments at lower velocities.

The authors consider it their pleasant duty to thank Yu. N. Demkov for interest in the work and useful discussions.

APPENDIX

The integral (17) can be readily transformed into

$$J \doteq M \int_0^{\varepsilon} dr_2 \int_0^{r_2} dr_1 \int_{-r_1}^{r_1} dz e^{-\varkappa(r_1+r_2)} \{\varkappa (zr_1 - zr_2)$$
$$\times F(\gamma, 1; \alpha_1(r_1 - z)) F(\gamma, 1; \alpha_1(r_2 + z))$$
$$- \alpha_1 (r_1 r_2 + r_1 z) F(\gamma, 1; \alpha_1(r_1 - z))$$
$$\times F'(\gamma, 1; \alpha_1(r_2 + z)) - \alpha_1 (r_1 r_2 - r_2 z) F'(\gamma, 1; \alpha_1(r_1 - z))$$
$$\times F(\gamma, 1; \alpha_1(r_2 + z))\} = M(I_1 + I_2 + I_3) \equiv MI, \qquad (A.1)$$

where $\kappa = \alpha_1 + \alpha_2$ and $M = 8\pi^2 N_{+a}^2$.

We use an integral representation for the confluent hypergeometric function:

$$F(\gamma, 1; x) = \frac{1}{B} \int_{(0)}^{(1)} e^{xu} K(u) du, \qquad (A.2)$$

where $K(u) = u^{\gamma-1}(1-u)^{-\gamma}$, B is a beta function, and the integration must be carried out in the complex u plane, choosing a contour which is regular in its dependence on γ and which circles around the points 0 and 1. By changing the order of integration we obtain for the integrals I_1, I_2, and I_3 the expressions

$$I_1 = \frac{\varkappa}{B^2} \iint_{(0)}^{(1)} du\, dv K(u) K(v) (J_{zr_1} - J_{zr_2}),$$

$$I_2 = \frac{\alpha_1}{B^2} \iint_{(0)}^{(1)} v\, du\, dv\, K(u) K(v) (-J_{r_1 r_2} - J_{r_1 z}),$$

$$I_3 = \frac{\alpha_1}{B^2} \iint_{(0)}^{(1)} u\, du\, dv\, K(u) K(v) (-J_{r_1 r_2} + J_{r_2 z}). \qquad (A.3)$$

We put here

$$J_{pq} = \int_0^{\varepsilon} dr_2 \int_0^{r_2} dr_1 \int_{-r_1}^{+r_1} dz\, pq \exp\{\lambda r_1 + \mu r_2 + (\mu - \lambda) z\}, \qquad (A.4)$$

where $\lambda = \alpha_1 u - \kappa$ and $\mu = \alpha_1 v - \kappa$.

Taking into account the fact that $\lambda, \mu \neq 0$ and $\exp(\lambda, \mu, \epsilon) \ll 1$, these integrals are equal to

$$J_{r_1 z} = \frac{\mu^2 - \lambda^2}{4\lambda^3\mu^4}, \quad J_{r_2 z} = \frac{\mu^2 + \lambda\mu - 2\lambda^2}{4\lambda^3\mu^4},$$
$$J_{r_1 r_2} = -\frac{\mu^2 + 2\lambda\mu + 2\lambda^2}{4\lambda^3\mu^4}. \qquad (A.5)$$

Substitution of these expressions into (A.3) leads to

$$I = \frac{1}{2B^2} \iint_{(0)}^{(1)} du dv K(u) K(v) \left\{ \frac{3}{\lambda\mu^3} + \frac{2}{\lambda^2\mu^2} + \frac{2\varkappa}{\lambda\mu^4} + \frac{2\varkappa}{\lambda^2\mu^3} + \frac{\varkappa}{\lambda^3\mu^2} \right\}. \qquad (A.6)$$

Integration with respect to u and z is independent, and thus (A.6) breaks up into products of integrals of the type

$$C_m = \frac{1}{B} \int_{(0)}^{(1)} du\, u^{\gamma-1} (1-u)^{-\gamma} \left(1 - \frac{\alpha_1}{\varkappa} u\right)^{-m}. \qquad (A.7)$$

It is easy to see that C_m is the hypergeometric function ${}_2F_1(\gamma, m, 1; \alpha_1/\kappa)$. Noting that

$${}_2F_1(a, c, c; x) = (1 - x)^{-a},$$

and using the recurrence formula

$${}_2F_1(a - 1, b, c; x) = {}_2F_1(a, b - 1, c; x)$$
$$+ \frac{a - b}{c} x\, {}_2F_1(a, b, c + 1; x),$$

we obtain the required expression for I:

$$I = \frac{1}{2} \frac{\alpha_2 - \alpha_1}{\alpha_2^5} \left(\frac{\alpha_2}{\alpha_1 + \alpha_2}\right)^{2\alpha_2/\alpha_1} \left[5 - \frac{37}{6} \left(\frac{\alpha_2}{\alpha_1 + \alpha_2}\right) \right.$$
$$\left. + \left(\frac{\alpha_2}{\alpha_1 + \alpha_2}\right)^2 \right]. \qquad (A.8)$$

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Translated by J. G. Adashko
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