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Charge transfer between atomic and ionic oxygen

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Résumé. — Nous avons calculé la section efficace de transfert de charge résonnant entre ion et atome d'oxygène. Les calculs ont été faits en utilisant la méthode du paramètre d'impact. Les coefficients des équations couplées ont été calculés sous forme analytique grâce à l'utilisation du développement des orbitales de Slater à deux centres de symétrie p et du potentiel atomique de Green, Sellin et Zachor (GSZ).

Abstract. — A calculation of a symmetric resonant charge exchange cross-section between atomic and ionic oxygen has been performed using the impact parameter method. The coefficients of the coupled equations are derived in an analytical form using a two centre expansion in the Slater orbitals of p-symmetry and the phenomenological atomic potential of Green, Sellin and Zachor (GSZ).

1. Introduction.

The resonant charge transfer cross-section has been calculated for a number of simple cases such as hydrogen and helium atoms but only a few papers have presented estimates of this cross-section for a more complex atom like oxygen (for review see [1-3]). In this case an extremely difficult experiment was performed by Stebbings *et al.* [4] using a cross-beam technique in the energy range 0.01-10 keV. The authors estimated the experimental error to be in the range $\pm 25\%$, mainly due to the possible presence of excited ions in the primary beam. Dalgarno [5] used a semi-empirical method to predict the charge transfer cross-section on the basis of experimental for ion mobilities in their parent gases at low field strengths.

As is shown in section 2 (formulae (6)-(9)). The cross section of a symmetric process in the two state-approximation depends only on the difference between the symmetric E_g and antisymmetric E_u stationary state energies, $\Delta E = E_u - E_g$, along the collision orbit.

Knof *et al.* [16] approximated this energy splitting for oxygen π states (as obtained directly from the fitted empirical curves for $X^2 \pi_g$ and $A^2 \pi_u$ states) by a single exponential term (1) with two fitting parameters. These results were compared to the data obtained on the

basis of the formulae of Rapp *et al.* [7], where the energy difference ΔE was also approximated by a single exponential, but with different parameters, which are in a rather rough correlation with the size of an electronic orbital through the ionization potential I (2)

$$\Delta E = 410 \exp(-3.489 R) [\text{eV}], \quad R > 1.95 \text{ \AA}, \quad (1)$$

$$\Delta E = 2 IR \exp(-\sqrt{I} R) [\text{eV}], \quad (2)$$

where R is the internuclear distance.

The above assumption concerning the form of ΔE for atoms other than hydrogen, is coarse approximation, especially when the outer electron is not in an s-state.

The purpose of the present work is to present a new calculation using the impact parameter method, in which the total wave function has been expressed as a set of atomic orbitals having the proper p-symmetry. The analytical forms of the coefficients of the coupled equations have been derived and evaluated in terms of the phenomenological atomic potential GSZ [9, 10] and the single-zeta functions of Clementi and Roetti [8], see also [16]. These functions have the correct radial dependence at large internuclear separations, which is the region of importance for the cross-section calculation.

On the basis of this evaluations preliminary results concerning the probabilities and the cross-sections have been calculated in the two-state approximation.

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2. Theory.

The collision between an ion O^+ and its parent atom O may be described as

where the nuclei A and B are assumed to be identifiable before and after collision. Within the impact parameter method it is assumed that the projectile moves along a rectilinear trajectory with a constant velocity $\bar{v}$ parallel to the fixed z axis (Fig. 1), so that the internuclear distance $2.R$ is given by

$$2.R = \sqrt{b^2 + v^2 t^2},$$

where b is the impact parameter, and where the time t varies from $-\infty$ to $+\infty$. The above assumption limits our approach to the intermediate relative velocity range (100 eV $\div$ 10 keV); down to zero energy the assumption of the straight-line paths is not valid, while at high energies not only the separation of the electronic and atomic motions becomes difficult but also the impact parameter becomes so small that the couplings to all other electronic states must be taken into account. The atomic wave-functions: $u_1(\bar{r}_{A,B}) = u_{p_z}(\bar{r}_{A,B})$, $u_2(\bar{r}_{A,B}) = u_{p_{x',y'}}(\bar{r}_{A,B})$, and the potentials $V(\bar{r}_A)$ and $V(\bar{r}_B)$ are defined in the rotating coordinate system (x', y', z') such that the z' axis coincides with $\bar{R}$ (Fig. 1).

The complete electronic wave-function of an active electron is written as a linear combination of traveling orbitals. Inserting this expansion into the Schrödinger equation leads to a set of coupled linear first-order differential equations for the expansion coefficients a_i , which are functions of the time, depending parametrically on the impact parameter b and the velocity v .

Fig. 1. — Coordinate systems used in the collision process : $(x' y' z')$ is the rotating coordinate system, (xyz) is the fixed coordinate system, $R(t)$ is half the internuclear distance, b is the impact parameter, A and B are the time dependent positions of the target (A) and the projectile (B) moving with constant velocity $\bar{v}$. The collision plane is chosen to be the xz plane.

Neglecting, in the final analysis, the momentum of the active electron (we assume $\exp(-i\bar{v}\bar{z})=1$) the coupled equations for the charge exchange have the following form [11] :

$$i\dot{a} = Aa, \quad (3)$$

here a is the vector of transition amplitudes ($a_1 = a_1^A$,

$$a_2 = a_2^A, a_3 = a_1^B, a_4 = a_2^B)$$

$\dot{a}$ is the time derivative of a ,

and the matrix of coefficients A is determined by the operation of the time dependent Hamiltonian $H = -\frac{1}{2}\Delta + V(\bar{r}_A) + V(\bar{r}_B)$ on the total electron wave-function ⁽¹⁾ :

$$A = \begin{vmatrix} \frac{S_1 J_1 - I_1}{S_1^2 - 1} & -i\beta & \frac{S_1 I_1 - J_1}{S_1^2 - 1} & 0 \\ i\beta & \frac{S_2 J_2 - I_2}{S_2^2 - 1} & 0 & \frac{S_2 I_2 - J_2}{S_2^2 - 1} \\ \frac{S_1 I_1 - J_1}{S_1^2 - 1} & 0 & \frac{S_1 J_1 - I_1}{S_1^2 - 1} & -i\beta \\ 0 & \frac{S_2 I_2 - J_2}{S_2^2 - 1} & i\beta & \frac{S_2 J_2 - I_2}{S_2^2 - 1} \end{vmatrix} \quad (4)$$

where :

$$\beta = \frac{bv}{4R} \quad (5)$$

and

$$\begin{aligned} J_1 &= \langle u_1(\bar{r}_A) | V(\bar{r}_B) | u_1(\bar{r}_B) \rangle \\ I_1 &= \langle u_1(\bar{r}_A) | V(\bar{r}_B) | u_1(\bar{r}_A) \rangle, \\ S_1 &= \langle u_1(\bar{r}_A) | u_1(\bar{r}_B) \rangle. \end{aligned}$$

The corresponding integrals with the subscript 2 are expressed by the functions u_2 . It is well known that the diagonal elements of (4) may be removed by an appropriate choice of new transition amplitudes which

⁽¹⁾ Atomic units have been used, except where otherwise mentioned.

only differ by a phase factor from the old ones. Then, in the two-state approximation, i.e. taking into account only 2 $p_{x,y}^{A,B}$ wave functions (3) and (4) reduce to :

$$\begin{aligned} i\dot{a}_2 &= A_{24} a_4, \\ i\dot{a}_4 &= A_{42} a_2, \end{aligned} \quad (6)$$

with $A_{24} = A_{42} = (S_2 I_2 - J_2)/(S_2^2 - 1)$. Uncoupling the two equations (6) by adding and subtracting them it may be seen that

$$|a_4(\infty)| = \left| \sin \int_{-\infty}^{+\infty} A_{24} dt \right|, \quad (7)$$

where A_{24} corresponds to the difference between the symmetric and antisymmetric stationary states energies calculated within the molecular orbital linear combinations of atomic orbitals (MO LCAO) approximation for π_g and π_u states. Having solved (6) for a_2 , a_4 and taking into account the initial condition : $a_2(-\infty) = 1$; $a_4(-\infty) = 0$, the charge transfer $A \rightarrow B$ probability is defined as

$$P(b) = |a_4(t = +\infty)|^2 \quad (8)$$

and the corresponding charge transfer cross-section Q is obtained by integrating P over all impact parameters b :

$$Q = 2\pi \int_0^\infty b P(b) db \quad (9)$$

3. Results and discussion.

As basis functions u_i we have used 2p oxygen single zeta functions [8] which are summarized in table I. A single zeta function is that approximation to the Hartree-Fock function, in which a given electron orbital is described by one Slater function. This function is more rudimentary than a double zeta function which is nearly as accurate as a Hartree-Fock function. In figure 2, we have compared both the above functions with the Hartree-Fock 2p wave function of the oxygen atom, which we have calculated self-consistently.

Fig. 2. — The radial parts of the oxygen 2p wave functions : (— — —) single zeta function [8], (•••••) double zeta function [8], (——) Hartree-Fock self-consistent wave function.

Table I. — The atomic orbitals (AO) of oxygen : single and double zeta functions [8] and the corresponding energies of the electronic level.

AO	Analytic form of AO of oxygen		Energy of state 2p (H)
	Radial function R_{nl}	Angular function Y_{lm}	
single $2p_x$	$8.5424 r \exp(-2.22662 r)$	$\sqrt{\frac{3}{4\pi}} \frac{x}{r}$	- 0.503
zeta $2p_y$		$\sqrt{\frac{3}{4\pi}} \frac{y}{r}$	
$2p_z$		$\sqrt{\frac{3}{4\pi}} \frac{z}{r}$	
double $2p_x$	$2.9875 r \exp(-1.82324 r) +$ $+ 8.3228 r \exp(-3.46668 r) +$ $+ 0.29042 r \exp(-1.15634 r) +$ $+ 2.9590 r \exp(-7.73305 r)$	$\sqrt{\frac{3}{4\pi}} \frac{x}{r}$	- 0.632
$2p_y$		$\sqrt{\frac{3}{4\pi}} \frac{y}{r}$	
zeta $2p_z$		$\sqrt{\frac{3}{4\pi}} \frac{z}{r}$	

The GSZ form [9] of the atomic potential has been chosen :

$$V(r_{A,B}) = \frac{-Z}{r_{A,B}} [(1-p)\omega(r_{A,B}) + p], \quad (10)$$

in order to evaluate the elements of the matrix A (4).

In the above formula Z is the atomic number, $p = \frac{\theta+1}{Z}$, θ — is the degree of ionization and the screening function ω may be written

$$\omega(r) = [Kd(\exp(r/d) - 1) + 1]^{-1}, \quad (11)$$

K and d being parameters.

The GSZ atomic potential has a particularly useful parametric and analytic form, which has proven to be successful in computing atomic properties to a very high accuracy [15]. It is easily applied to atoms and also to ions. The parameters K and d were calculated for all elements with atomic number $Z \leq 10$ [10].

$K = 2.41 (a_0^{-1})$ and $d = 0.735 (a_0)$ give the best fitting to the Hartree-Fock total energy for oxygen. The comparison of the self-consistent Hartree-Fock

Fig. 3. — The dependence of $r \cdot V(r)$ as a function of electron-nucleus distance r for : (—) GSZ atomic potential [9] (---) Hartree-Fock self-consistent potential.

(with Latter's correction [17]), and GSZ potentials, which are shown in figure 3, indicates a very good agreement of both potentials.

Then the integrals (5) can be calculated analytically in the prolate spheroidal coordinate system [13] :

$$\begin{aligned} J_1 = & \frac{N(Z-1)}{Kd-1} \sum_{\mu=1}^{\infty} \left\{ (-1)^{\mu-1} \left(\frac{Kd-1}{Kd} \right)^{\mu} \left\{ e^{-2aR} \left[\frac{1}{(2R)^3} \left(-\frac{6d^4}{s^3\mu^4} + \frac{6d^3}{s^4\mu^3} \right) \right. \right. \right. \\ & + \frac{1}{(2R)^2} \left(-\frac{12d^4}{s^3\mu^4} + \frac{12d^3}{s^3\mu^3} - \frac{3d^2}{s^4\mu^2} \right) + \frac{1}{(2R)} \left(-\frac{6d^4}{s\mu^4} + \frac{9d^3}{s^2\mu^3} - \frac{9/2d^2}{s^3\mu^2} + \frac{3/8d}{s^4\mu} \right) \\ & + \left(\frac{4d^3}{s\mu^3} - \frac{3d^2}{s^2\mu^2} + \frac{d}{s^3\mu} \right) + (2R) \left(-\frac{1/4d^2}{s\mu^2} + \frac{1/8d}{s^2\mu} \right) - (2R)^2 \left(\frac{3/2}{s\mu} \right) \left. \right] + \exp \left[-2R \left(a + \frac{\mu}{d} \right) \right] \\ & \times \left[\frac{1}{(2R)^3} \left(\frac{12d^4}{s^3\mu^4} - \frac{6d^3}{s^4\mu^3} \right) + \frac{1}{(2R)^2} \left(\frac{12d^4}{s^2\mu^4} - \frac{3d^2}{s^4\mu^2} \right) + \frac{1}{(2R)} \left(\frac{6d^4}{s\mu^4} + \frac{3d^3}{s^2\mu^3} - \frac{3/2d^2}{s^3\mu^2} - \frac{3/4d}{s^4\mu} \right) \right. \\ & + \left(\frac{2d^3}{s\mu^3} - \frac{1/2d}{s^3\mu} \right) + (2R) \left(-\frac{3/4d^2}{s\mu^2} + \frac{3/8d}{s^2\mu} \right) + (2R)^2 \left(\frac{d}{s\mu} \right) \left. \right] \left. \right\} \\ & + Ne^{-2aR} \left[\frac{1}{4a^4} + \frac{(2R)}{4a^3} - \frac{3(2R)^2}{8a^2} - \frac{11(2R)^3}{24a} \right] \end{aligned} \quad (12)$$

$$\begin{aligned} I_1 = & \frac{N(Z-1)}{Kd-1} \sum_{\mu=1}^{\infty} \left\{ (-1)^{\mu-1} \left(\frac{Kd-1}{Kd} \right)^{\mu} \left\{ -e^{-4aR} \left[\frac{1}{(2R)^3} \left(\frac{3/4}{s^4w^3} - \frac{3/4}{s^3w^4} \right) \right. \right. \right. \\ & + \frac{1}{(2R)^2} \left(+\frac{3/4}{s^4w^2} - \frac{3/2}{s^3w^3} + \frac{3/4}{s^2w^4} \right) + \frac{1}{(2R)} \left(\frac{3/8}{sw^4} - \frac{9/8}{s^2w^3} + \frac{9/8}{s^3w^2} - \frac{3/8}{s^4w} \right) + \left(\frac{1/2}{sw^3} + \frac{3/4}{s^2w^2} - \frac{1/2}{s^3w} \right) \\ & + (2R) \left(\frac{1/16}{sw^2} - \frac{5/16}{s^2w} \right) + R^2 \left(\frac{3/8}{sw} \right) \left. \right] + \exp \left(-2R \frac{\mu}{d} \right) \left[\frac{1}{(2R)^3} \left(\frac{3/4}{s^4w^3} - \frac{3/4}{s^3w^4} \right) \right. \\ & + \frac{1}{(2R)^2} \left(\frac{3/4}{s^2w^4} - \frac{3/4}{s^4w^2} \right) + \frac{1}{(2R)} \left(\frac{3/8}{sw^4} + \frac{3/8}{s^2w^3} - \frac{3/8}{s^3w^2} - \frac{3/8}{s^4w} \right) + \left(\frac{1/4}{sw^3} - \frac{1/4}{s^3w} \right) \\ & + (2R) \left(-\frac{3/16}{sw^2} - \frac{1/16}{s^2w} \right) + (2R)^2 \left(\frac{3/8}{sw} \right) \left. \right] \left. \right\} + Ne^{-4aR} \left[\frac{1}{(2R)^3} \left(\frac{-3/2}{a^7} \right) \frac{1}{(2R)} \left(\frac{3}{a^6} \right) - \frac{1}{(2R)} \left(\frac{3}{a^5} \right) \right. \\ & \times \left(\frac{7}{4a^4} \right) - \left(\frac{2R}{8a^3} \right) \left. \right] + \left[\frac{1}{(2R)^3} \left(\frac{3/2}{a^7} \right) - \left(\frac{3R}{8a^8} \right) \right] \end{aligned} \quad (13)$$

$$J_2 = \frac{N(Z-1)}{Kd-1} \sum_{\mu=1}^{\infty} \left\{ (-1)^{\mu-1} \left(\frac{Kd-1}{Kd} \right)^{\mu} \left\{ e^{-2Ra} \left[\frac{1}{(2R)^3} \left(-\frac{6d^3}{s^4\mu^3} + \frac{12d^4}{s^3\mu^4} \right) \right. \right. \right. \\ \left. \left. + \frac{1}{(2R)^2} \left(\frac{12d^4}{s^2\mu^4} - \frac{12d^3}{s^3\mu^3} + \frac{3d^2}{s^4\mu^2} \right) + \frac{1}{(2R)} \left(-\frac{8d^3}{s^2\mu^3} + \frac{4d^2}{s^3\mu^2} \right) + \frac{2d^2}{s^2\mu^2} \right] + \exp \left[-2R \left(a + \frac{\mu}{a} \right) \right] \right. \\ \left. \times \left[\frac{1}{(2R)^3} \left(\frac{6d^3}{s^4\mu^3} - \frac{12d^4}{s^3\mu^4} \right) + \frac{1}{(2R)^2} \left(-\frac{12d^4}{s^2\mu^4} + \frac{3d^2}{s^4\mu^2} \right) + \frac{1}{(2R)} \left(-\frac{4d^3}{s^2\mu^3} + \frac{2d^2}{s^3\mu^2} \right) \right] \right\} \right\} \\ + N e^{-2aR} \left[\frac{1}{2a^4} + \frac{(2R)}{2a^3} + \frac{(2R)^2}{6a^2} \right] \quad (14)$$

$$I_2 = \frac{N(Z-1)}{Kd-1} \sum_{\mu=1}^{\infty} \left\{ (-1)^{\mu-1} \left(\frac{Kd-1}{Kd} \right)^{\mu} \left\{ e^{-4aR} \left[\frac{1}{(2R)^3} \left(\frac{-3/4}{s^4w^3} + \frac{3/4}{s^3w^4} \right) \right. \right. \right. \\ \left. \left. + \frac{1}{(2R)^2} \left(\frac{3/4}{s^2w^4} - \frac{3/2}{s^3w^3} + \frac{3/4}{s^4w^2} \right) + \frac{1}{(2R)} \left(\frac{-1}{s^2w^3} + \frac{1}{s^3w^2} \right) + \left(\frac{1/2}{s^2w^2} \right) \right] \right. \\ \left. + \exp \left(-2R \frac{\mu}{d} \right) \left[\frac{1}{(2R)^3} \left(\frac{3/4}{s^4w^3} - \frac{3/4}{w^4s^3} \right) + \frac{1}{(2R)^2} \left(\frac{-3/4}{s^2w^4} + \frac{3/4}{s^4w^2} \right) + \frac{1}{2R} \left(\frac{-1/2}{s^2w^3} + \frac{1/2}{s^3w^2} \right) \right] \right\} \right\} \\ + N e^{-4aR} \left[\frac{1}{(2R)^3} \left(\frac{3}{2a^7} \right) + \frac{1}{(2R)^2} \left(\frac{3}{a^6} \right) + \frac{1}{(2R)} \left(\frac{1}{a^5} \right) + \left(\frac{1}{2a^4} \right) \right] + N \left[\frac{1}{(2R)^3} \left(\frac{-3}{2a^7} \right) + \frac{1}{(R \cdot 2)} \left(\frac{1}{a^5} \right) \right] \quad (15)$$

$$S_1 = N e^{-2aR} \left[\frac{1}{2a^5} + \frac{(2R)}{2a^4} - \frac{3/10(2R)^2}{a^3} - \frac{2/5(2R)^3}{a^2} - \frac{5/32(2R)^4}{a} \right] \quad (16)$$

$$S_2 = N e^{-2aR} \left[\frac{1}{a^5} + \frac{(2R)}{a^4} + \frac{2/5(2R)^2}{a^3} + \frac{1/15(2R)^3}{a^2} \right] \quad (17)$$

where $N = 54.729$ (au) is the normalization constant, a is an exponent of the atomic wave function (see Table I), $a = 2.22662(a_0^{-1})$, while $s = 2a + \mu/d$ and $w = -2a + \mu/d$.

The last parenthesis of each expression (12-15) corresponds to the part of the atomic potential (10) $V(r) \sim -1/r$, which is equivalent to the hydrogen atom potential. Therefore, this part of our results corresponds to the results of Rapp and Dinwiddie [14] for $2p_1$ hydrogen atom states.

The dependences of $J_{p_{xy}}$, $I_{p_{xy}}$ and $S_{p_{xy}}$ as on the internuclear distance are presented in figure 4.

It is evident from our calculations that even in the most simple case when we assume $S_2 = 0$, in the whole range of internuclear distances at least two exponential terms are necessary to describe $A_{24} = J_2$. The first one (for $\mu = 1$) describes the screening of the nucleus, particularly important for short and middle internuclear distances. The second exponential function describes the oxygen atom in terms of the hydrogen-like model, for large distances. In previous publications [6, 7], this difference between symmetric and antisymmetric stationary states energies was approximated by a single exponential term (1), (2).

All the above results (12-17) can be easily transformed if the double zeta function is used instead of the single zeta function. In this case the magnitudes J , I and S can be expressed as linear combinations of terms corresponding to the single zeta function, in which $2a$ should be replaced by a sum of two different

Fig. 4. — J_2 , I_2 and S_2 dependence on the internuclear distance $2R$. For further explanations see the text.

(in general) exponents $(a_1 + a_2)$ and N by the product of the coefficients in front of the exponentials (see Table I).

We have solved (3) in the two-state approximation using Hamming's predictor-corrector method [12]. Our results for the cross-sections as a function of the oxygen energy in the range 0.100-10 keV are presented in figure 5 as compared to the experimental data [4], and the previous theoretical results [6, 7].

Fig. 5. — The comparison of the experimental data of Stebbings [4] denoted by points with the semi-empirical results of Rapp *et al.* [14] (—●—) and Knof *et al.* [6] (—●—) and our theoretical results (—). Below the range 100 eV ÷ 10 keV, the theoretical results are denoted by a dashed curve.

The calculated data differ slightly from the experimental results. There are several reasons for this. First, our results based on the two-state approximation neglect all nonadiabatic transitions to higher O_2^+ states, whereas the actual experiment may probably involve charge exchange process with excitation. Furthermore, the initial ion beam used in experiment [4] contained excited states of O^+ which could react

analogously to the ground state of O^+ , but involving other states. Finally in the two-state approximation the rotational coupling terms were neglected as are, obviously all dynamic interactions.

4. Conclusions.

Contrary to approaches [6, 7] which were fitted to the experimental data, we have presented a fully theoretical model to calculate the charge exchange cross-sections for the p-electron atoms, in the intermediate energy region, where the semiclassical impact parameter method is applicable.

The total wave function of an active electron has been expressed as a set of atomic orbitals having a proper p-symmetry. Then the analytical forms of the coefficients of the coupled equations have been derived and evaluated in terms of a single zeta function and of the phenomenological atomic GSZ potential. These equations have been numerically solved using Hamming's predictor-corrector method for the transition amplitudes. The charge exchange cross-section for the oxygen resonant process which was calculated on the basis of these amplitudes shows a satisfactory agreement with the experimental data.

In order to obtain a better accuracy our model can be easily extended to take into account the double zeta function (see Fig. 2) and the additional states of s-symmetry. This more sophisticated and more time consuming extension of the calculations above is in progress.

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- There are errors in the formulae 21.5.1 and 21.5.2 : instead of : $c = \frac{1}{2}fk$ should be : $c = fk$.
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