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OSCILLATORY STRUCTURE OF THE pe+d → de+p TOTAL CHARGE- TRANSFER CROSS SECTION

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1. Introduction

The study of the one-electron diatomic systems is very fruitful in bringing to light in a simple case a number of phenomena which arise in dealing with more complicated systems. In such simple systems not only the electronic energy as a function of inter-nuclear distance but also the matrix elements representing interaction between the electronic states can be computed.

The equations of the perturbed stationary state method (P.S.S.) or adiabatic representation for collision problem [1,2,3] result from these computations. In its turn solving of the equations in question gives some opportunity to study the peculiarities of the adiabatic or any related to it representation [3,4]. In this paper the cross section of the charge-transfer process

$$(pe)_{1s} + d \to (de)_{1s} + p \qquad (1)$$

has been calculated. For energy region $E \leq 1$ eV (in c.m.s.) the two-state approximation of the P.S.S. method is a good one when the reaction (1) is considered. Recently [5] we have already used the same approximation for the calculation of the process

$$(p\mu^-)_{1s} + d \to (d\mu^-)_{1s} + p \qquad (1a)$$

but some technical details due to the large reduced mass in the case of the reaction (1) have forced us to look for some new algorithm. First of all it proved to be useful to convert the adiabatic representation into the diabatic

one.[3] Further the wave function of the nuclear motion was parametrized in the sense of the phase function method [6]. The resulting equations were integrated numerically and the happy choice of the parameters helped us to overcome the above-mentioned difficulties.

All the potentials used are widely accessible and the technical details given in appendix are sufficient to reproduce our computations.

2. Adiabatic Representation

In the case of the process (1) two-state approximation of the P.S.S. method gives the system of the radial Schrödinger equations[5]

$$\left(\frac{d^2}{dR^2} + k_1^2 - \frac{\ell(\ell+1)}{R^2}\right)\chi_1 = K_{11}\chi_1 + K_{12}\chi_2 + 2Q_{12}\frac{d\chi_2}{dR}$$

$$\left(\frac{d^2}{dR^2} + k_2^2 - \frac{\ell(\ell+1)}{R^2}\right)\chi_2 = K_{22}\chi_2 + K_{21}\chi_1 - 2Q_{12}\frac{d\chi_1}{dR}, \qquad (2)$$

where

$$K_{11}(R) = M(W_g + W_u) + (K_{gg} + K_{uu} - K_{gu} - K_{ug})/2$$

$$K_{12}(R) = M(W_g - W_u) + (K_{gg} - K_{ug} + K_{gu} - K_{uu})/2$$

$$K_{21}(R) = M(W_g - W_u) + (K_{gg} - K_{uu} - K_{gu} + K_{ug})/2 \qquad (3)$$

$$K_{22}(R) = M(W_g + W_u) + (K_{gg} + K_{uu} + K_{gu} + K_{ug})/2$$

$$Q_{12}(R) = -Q_{gu}$$

Matrix elements $K_{gg}, \ldots K_{ug}, Q_{gu}$ are given by the equations

$$K_{ij} = \langle i | -\Delta_{\vec{R}} | j \rangle$$

$$Q_{ij} = \frac{\vec{R}}{R}\langle i | -\nabla_{\vec{R}} | j \rangle, \quad i,j = g,u \qquad (4)$$

These are calculated when the electronic two-center problem for W_g, W_u (terms) is being solved. The other quantities are defined by the notation

$$1/M = 1/M_p + 1/M_d, \quad 1/m = 1/m_e + 1/(M_p + M_d)$$

$$k_1^2 = 2ME, \quad k_2^2 = k_1^2 + (M_d - M_p)/(M_d + M_p). \qquad (5)$$

Here E is a collision energy in c.m.s. and the units $e = \hbar = m = 1$ are used. The terms and matrix elements of the two-center problem are given in the paper[5]. The effective potentials resulting from the definition (3) are pictured in Figs. 1,2. The characteristic feature of the adiabatic equations is the presence of the first derivatuve of the wave function in the wave equations (2). As a result of it the matrix (3) is not symmetric.

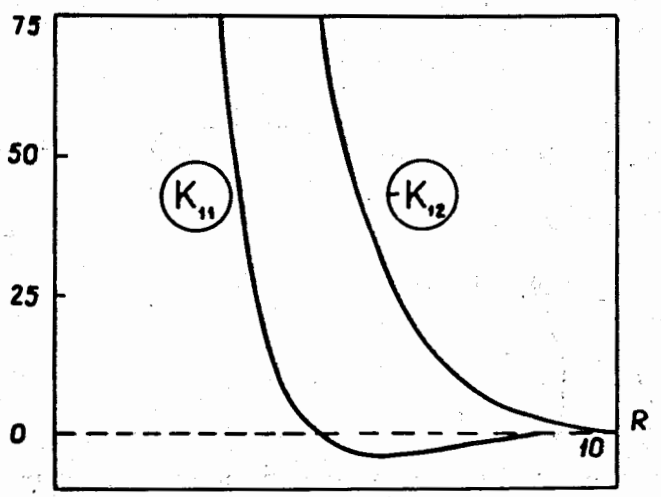

Fig. 1. Adiabatic matrix elements $K_{11}(R) = K_{22}(R)$, $K_{12}(R) = K_{21}(R)$ defined by formula (3).

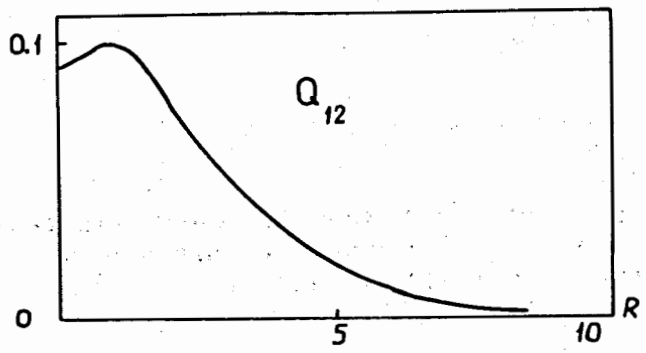

Fig. 2. Adiabatic matrix element $Q_{12}(R)$.

3. Diabatic Representation

We rewrite in matrix form the equations (2)

$$L\chi = K\chi + 2Q\,d\chi/dR, \tag{6}$$

where the free motion operator is given by

$$L=\left(-\frac{d^2}{dR^2}+\frac{\ell(\ell+1)}{R^2}\right)\begin{pmatrix}1&0\\0&1\end{pmatrix}+\begin{pmatrix}k_1^2&0\\0&k_2^2\end{pmatrix}, \tag{6a}$$

and convert the adiabatic representation into new one defined by the transformation

$$\chi(R)=W(R)\psi(R). \tag{7}$$

The unitary matrix $W(R)$ is as follows

$$W(R)=\begin{pmatrix}\cos q & \sin q\\ -\sin q & \cos q\end{pmatrix}, \tag{8}$$

where the function $q(R)$ can be found if matrix element $Q_{12}(R)$ is known

$$q(R)=\int_R^\infty Q_{12}(x)\,dx. \tag{9}$$

The given transformation reduces the first derivative in the wave equation (6) and makes the potential energy matrix symmetric. The transformed equation takes the form

$$L\psi=\bar{K}\psi, \tag{10}$$

where matrix $\bar{K}$ is given by the formula

$$\bar{K}=W^{-1}\left[K-\frac{dQ}{dR}-Q^2-\begin{pmatrix}k_1^2&0\\0&k_2^2\end{pmatrix}\right]W+\begin{pmatrix}k_1^2&0\\0&k_2^2\end{pmatrix}. \tag{11}$$

The equation (10) is the two-state approximation for the scattering problem (1) in diabatic representation, and matrix (8) defines the connection between diabatic and adiabatic representations in this approximation [3]. It is clear that the system of equations (10) is completely equivalent to the system (6) but for different problems one of the two can appear to be more convenient. In this paper we have chosen the diabatic basis because of the symmetry of the potential matrix $\bar{K}$. The characteristic feature of the diabatic representation is the fact that matrix $\bar{K}$ depends on the linear momenta k_1 and k_2. Matrix elements $\bar{K}_{ij}$ are plotted against internuclear distance R in Fig. 3.

4. Phase Function Method

Let us try the solution of the matrix equation (10) in the form [6]

$$\psi=(uS_1-vS_2)A \tag{12}$$

with the first derivative

$$\psi'_R=(u'S_1-v'S_2)A. \tag{13}$$

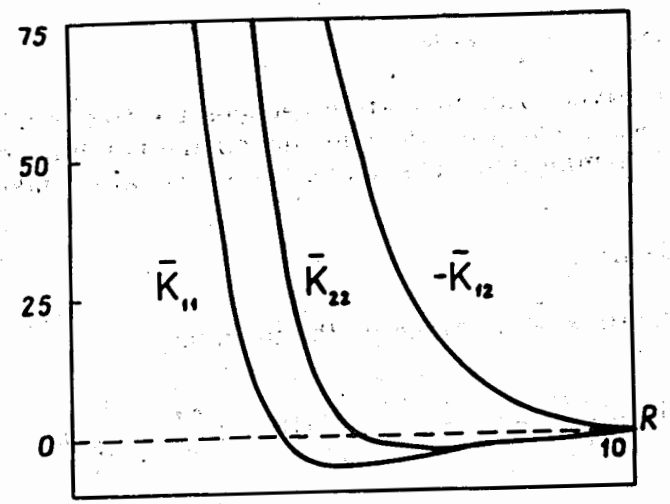

Fig. 3. Diabatic matrix elements defined by formulae (8,9,11).

Here

$$u=\begin{pmatrix} u_1 & 0 \\ 0 & u_2 \end{pmatrix}, \qquad v=\begin{pmatrix} v_1 & 0 \\ 0 & v_2 \end{pmatrix} \tag{14}$$

are the regular and irregular at $R=0$ solutions of the free equation

$$L\phi = 0 \tag{15}$$

normalized so that

$$uv' - u'v = 1. \tag{16}$$

Matrices $S_1(R)$ and $S_2(R)$ define the parametrization of the wave function and $A(R)$ is a coefficient matrix. Suppose that the equality

$$S_1^t S_2 - S_2^t S_1 \equiv 0 \tag{17}$$

is fulfilled then putting the solution (12) in equation (10) and making use of equations (13), (16) and (17) we receive the equation

$$S_1^t \frac{dS_2}{dR} - S_2^t \frac{dS_1}{dR} = (S_1^t u - S_2^t v)\bar{K}(uS_1 - vS_2). \tag{18}$$

The transformation of the initial problem (10) to the equation of the type (18) is known in the physical literature as phase function method. The choice of the matrices S_1, S_2 defines the type of the phase functions used and in its turn gives some parametrization of the scattering matrix S or reaction matrix T. The latter is evidently got from (12) by

$$T = S_2(\infty)S_1^{-1}(\infty). \tag{19}$$

5. Production Parameters

In the problem (1) the phase functions $\delta_1(R)$, $\delta_2(R)$ and $\epsilon(R)$ given by

$$S_1 = \begin{pmatrix} \cos\epsilon & \cos\delta_1 & -\sin\epsilon & \sin\delta_2 \\ -\sin\epsilon & \sin\delta_1 & \cos\epsilon & \cos\delta_2 \end{pmatrix} \tag{20}$$

$$S_2 = -\begin{pmatrix} \cos\epsilon & \sin\delta_1 & \sin\epsilon\cos\delta_2 \\ \sin\epsilon & \cos\delta_1 & \cos\epsilon\sin\delta_2 \end{pmatrix}$$

were used. In this case one easily gets for the left-hand side of equation (18)

$$S_1^t S_2' - S_2^t S_1' = \begin{pmatrix} \delta_1' & \epsilon' \cos(\delta_1 - \delta_2) \\ \epsilon' \cos(\delta_1 - \delta_2) & \delta_2' \end{pmatrix}. \qquad (21).$$

In the problem considered the chosen parameters have the useful property: $\cos(\delta_1 - \delta_2) \neq 0$ for $0 < R < \infty$. This means that equations (18) can be easily handled in all the region of integration. Such a circumstance is evidently a chance, but one could look forward to it keeping in mind the quasisymmetry of the reaction (1).

6. Results and Discussion

The total charge-transfer cross section of (1) versus the velocity of the relative nuclear motion is given in Fig. 4. Its general appearance is rather ordinary. The cross section strongly increases untill $v \simeq 0.2$, then it goes through characteristic maximum $v \sim 0.4$ and decreases slowly with increasing v (v in 10^6 cm/sec.).

The oscillations are much more interesting. They arise at $v \sim 0.3$ ($\ell_{max} \simeq 25$), its amplitude growing at first. It gets a maximum at $v \sim 0.5$ ($\ell_{max} = 40$) and then decreases. The period of oscillations increases with velocity from $\Delta v = 0.09$ to $\Delta v = 0.11$ for the interval $0.3 \leq v \leq 1.2$. The low frequency oscillations can also be detected from minimum at $v = 0.565$ ($\ell_{max} = 45$) and from less pronounced maximum at $v = 0.76$ ($\ell_{max} = 55$).

The partial wave analysis can be used to explain the high frequency oscillations. In Fig. 5 the partial cross sections are plotted for $v = 0.565$ (maximum) and $v = 0.590$ (minimum). It is easily seen that in the latter case the waves with $\ell = 30, 31, 32$ practically do not participate in

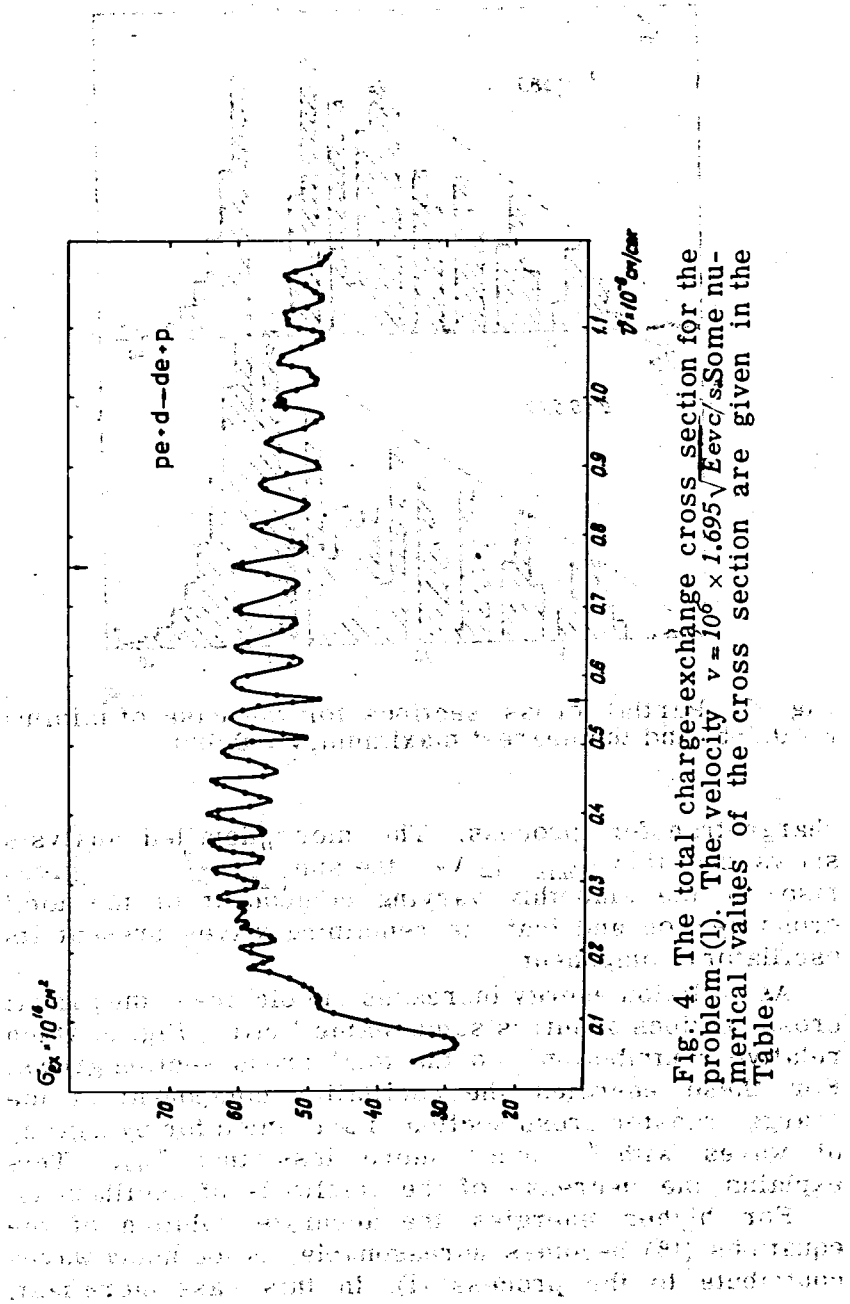

Fig. 4. The total charge-exchange cross section for the problem (1). The velocity $v = 10^6 \times 1.695 \sqrt{E_{evc}}$. Some numerical values of the cross section are given in the Table.

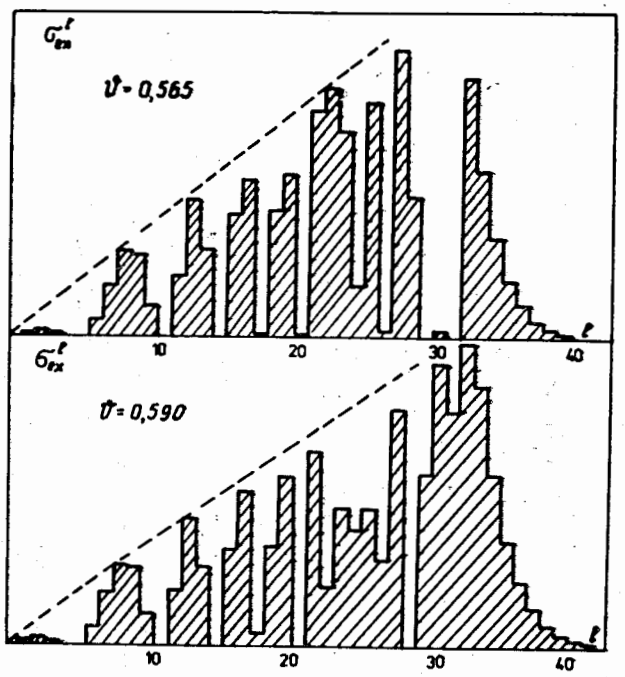

Fig. 5. Partial cross sections for the case of minima $v = 0.565$, and the nearest maximum, $v = 0.590$.

charge-transfer process. The more detailed analysis shows that if $|v - v_{min}| \leq \Delta v$ the sum $\sum_{\ell=0}^{30} \sigma_{ex}^{\ell}$ gives rise to the smoothly varying component of the total cross section and that the remaining waves present its oscillatory component.

As collision energy increases the picture of the partial cross sections acquires some stable "tail", Fig. 6, which relative contribution into the total cross section grows. For these energies the oscillation component of the charge-transfer cross section is accounted for by a group of waves with ℓ much more less than ℓ_{max}. This explains the decrease of the amplitude of oscillations.

For higher energies the accurate solution of the equations (18) becomes unreasonable, as too many waves contribute to the process (1). In this case more fast,

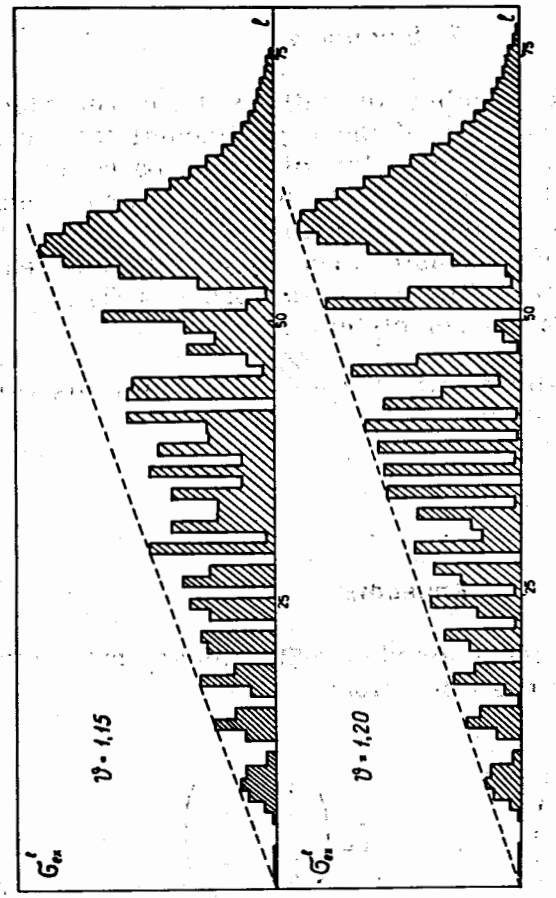

Fig. 6. The picture of the partial cross sections acquires some stable "tail" which makes the amplitude of the oscillation to decrease.

though less accurate, methods of computation can be recommended[4]. The largest E, for which the calculations have been completed equals 1 eV, $\ell_{max} \sim 100$, $v = 1.7$.

The Table lists the velocity positions of the peaks and minima of the total cross sections and its values.

7. Summary

Recently a number of authors have reported the oscillatory structure of the experimental total charge-transfer cross sections for different pairs of atoms, including alkali atoms[8]. We hope that our calculations will contribute to the understanding of the general features of charge-transfer reactions. To this end the experimental investigation of the process (1) in the low energy region is extremely urgent.

I am grateful to Dr. L.I.Ponomarev for his valuable comments and critics.

Appendix

Phase function method calculations are more simpler and faster with basic functions

$$\bar{u} = \begin{pmatrix} \bar{u}_1 & 0 \\ 0 & \bar{u}_2 \end{pmatrix}, \qquad \bar{v} = \begin{pmatrix} \bar{v}_1 & 0 \\ 0 & \bar{v}_2 \end{pmatrix} \tag{A.1}$$

$$\bar{u}_i = \frac{1}{\sqrt{k_i}} \sin k_i R, \quad \bar{v}_i = -\frac{1}{\sqrt{k_i}} \cos k_i R$$

which are the solutions of the free equations

$$\bar{L}\phi = \left[\frac{d^2}{dR^2}\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} + \begin{pmatrix} k_1^2 & 0 \\ 0 & k_2^2 \end{pmatrix}\right]\phi = 0. \tag{A.2}$$

In this case $\ell(\ell+1)/R^2$ is put into the potential energy matrix $\bar{K}$ and the production system of equations looks like

$$\begin{pmatrix} \delta_1' & \epsilon' \cos(\delta_1 - \delta_2) \\ \epsilon' \cos(\delta_1 - \delta_2) & \delta_2' \end{pmatrix} = \tag{A.3}$$

$$= (\bar{u}S_1 - \bar{v}S_2)^t \left(\bar{K} + \frac{\ell(\ell+1)}{R^2}\right)(\bar{u}S_1 - \bar{v}S_2),$$

$$\delta_1(0) = \delta_2(0) = \epsilon(0) = 0.$$

With $R \to 0$ matrix $\bar{K}$ has the following behaviour

$$\bar{K}_{11} = \frac{1}{R^2}(\cos q + \sin q)^2 + \frac{2M}{R} + 2Q(\cos^2 q - \sin^2 q)/R$$

$$\bar{K}_{12} = \bar{K}_{21} = -\frac{1}{R^2}(\cos^2 q - \sin^2 q) + \frac{2Q}{R}\sin 2q \tag{A.4}$$

$$\bar{K}_{22} = \frac{1}{R^2}(\cos q - \sin q)^2 + \frac{2M}{R} - 2Q(\cos^2 q - \sin^2 q)/R.$$

In these formulae and everywhere in Appendix

$$Q = Q_{12}(0), \qquad q = \int_0^\infty \bar{Q}_{12}(x)\,dx. \tag{A.5}$$

The expressions (A.4) and (A.5) define the asymptotic form of the phase functions $\delta_1(R)$, $\delta_2(R)$, $\epsilon(R)$. Really in the $R \to 0$ limit it can be written

$$S_1 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

$$S_2 = \begin{pmatrix} \sqrt{k_1} & 0 \\ 0 & \sqrt{k_2} \end{pmatrix} W^{-1} (AR+BR^2) W \begin{pmatrix} \sqrt{k_1} & 0 \\ 0 & \sqrt{k_2} \end{pmatrix}, \qquad (A.6)$$

where

$$A = \begin{pmatrix} a_1 & a_2 \\ a_2 & a_1 \end{pmatrix}$$

$$B = Q D_1 \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} D_1 + D_2 \,. \qquad (A.7)$$

Matrix D_1 is defined through

$$D_1 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} - A$$

and for D_2 we take the form

$$D_2 = - \begin{pmatrix} d_1 & d_2 \\ d_3 & d_4 \end{pmatrix}.$$

Finally for A we have

$$a_1 = -a_2 = 0.25 \quad \text{if} \quad \ell = 0$$

otherwise

$$\begin{aligned} a_1 - a_2 &= (\mathfrak{L}+1)(1-a_1+a_2)^2 \\ a_1 + a_2 &= (\mathfrak{L}-1)(1-a_1-a_2)^2 \end{aligned} \qquad (A.8)$$

with

$$\mathfrak{L} = \ell(\ell+1)+1$$

and for the calculation of the D_2 -matrix we have the system of equations

$$\begin{aligned} (d_1+d_4)+(d_2+d_3) &= \frac{2M(1-a_1+a_2)^2}{1+(\mathfrak{L}-1)(1-a_1-a_2)} \\ (d_1+d_4)-(d_2-d_3) &= \frac{2M(1-a_1-a_2)^2}{1+(\mathfrak{L}+1)(1-a_1+a_2)} \\ d_1-d_4 &= \frac{2Q[(1-a_1)^2 - a_2(1+a_2)]}{1+\mathfrak{L}(1-a_1)+a_2} \\ d_2-d_3 &= -\frac{2Q(1-a_1)}{1+\mathfrak{L}(1-a_1)+a_2}. \end{aligned} \qquad (A.9)$$

The numerical integration proceeds untill R_{max} and it is stopped if the conjunction of the numerical solution of system (A.3)

$$\bar{\psi} = (\bar{u}\bar{S}_1 - \bar{v}\bar{S}_2)\bar{A} \qquad (A.10)$$

with the physical solution of the equation (10) in the form

$$\psi = (u - vT)A \qquad (A.11)$$

due to the formula

$$\bar{\psi}\cdot\bar{\psi}^{-1} = \psi\cdot\psi^{-1} = D \qquad (A.12)$$

produces the T -matrix

$$T = (Dv - v')^{-1}(Du - u') \qquad (A.13)$$

independent of K for all $R > R_{max}$.

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Table

$\nu \times 10^{-6}$ cm/sec	0,51	0,54	0,565	0,59	0,62	0,64	0,675	0,695	0,73	1,5	1,7
$\sigma_{ex} \times 10^{16}$ cm^2	50	61	48	61	51	60	52	60	51	48	46