Collisions of Fast Electrons with Positronium Atoms.

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(ricevuto il 20 Marzo 1995; approvato il 13 Luglio 1995)

Summary. — Elastic and inelastic collisions of fast non-relativistic electrons with positronium atoms have been studied in the Born-Ochkur approximation. It has been shown that exchange plays an important role for transitions between states with the same parity as in this case the direct scattering amplitude vanishes. Numerical results for the total and ortho-para conversion cross-sections for the $1s \rightarrow 1s$, $1s \rightarrow 2s$ and $1s \rightarrow 2p$ transitions have been presented for projectile energies varying from 0.1 to 10 keV. According to charge symmetry, presented results apply also to positron projectiles.

PACS 34.80.Bm – Elastic scattering of electrons by atoms and molecules.
PACS 34.80.Dp – Atomic excitation and ionization by electron impact.
PACS 36.10.Dr – Positronium, muonium, muonic atoms and molecules.
PACS 52.20.Hv – Atomic, molecular, ion, and heavy-particle collisions.

1. – Introduction.

Experimental detection of the positronium negative ion Ps^- [1] has stimulated considerable growth of interest in theoretical investigating various properties of the simplest «polyelectron» system $e^- e^- e^+$. So far an effort was mainly concentrated on the calculation of ground-state and resonant-state properties of this system and several dozens papers appeared dealing with the subject (for an extensive review see ref. [2]). On the contrary, only very few papers dealt with continuum properties of the considered system. For investigation of low-energy elastic $e^- + Ps$ scattering Baltenkov *et al.* [3,4] used the Born-Oppenheimer approximation, Ward *et al.* [5,6] employed the Kohn variational method, Melezhik and Vukajlović [7,8] applied the adiabatic method, while Kvitsinsky *et al.* [9-11] attacked the problem solving the Faddeev equations. In the high-energy region, Chen *et al.* [12-14] adopted the first-order Faddeev-Watson multiple-scattering approximation for investigation of the symmetric charge exchange in electron collision with the ground state of the positronium atom and Igarashi *et al.* [15] considered transfer of fast electrons to $1s$, $2s$

and $2p$ states of positronium in the second-order Born approximation. Moreover, Peach [16] calculated the first-order Born cross-section for the ionization of Ps by slow and fast electrons, Amusia *et al.* [17] investigated bremsstrahlung in $e^- + Ps$ scattering, while Bhatia and Drachman [18] and Ward *et al.* [19] performed calculations on photodetachment of the positronium negative ion.

On the experimental side, none $e^- + Ps$ scattering measurements have been carried out so far but in view of a recent experimental progress such investigations are likely to be performed in the nearest future [20].

In this paper, we apply the Born-Ochkur approximation to derive formulae for cross-sections describing elastic and inelastic collisions of fast non-relativistic electrons with positronium atoms. We present numerical results for the total and ortho-para conversion cross-sections for the $1s \to 1s$, $1s \to 2s$ and $1s \to 2p$ transitions for electron impact energies varying from 0.1 to 10 keV. According to charge symmetry, results presented below apply also to positron projectiles.

2. – Theory.

2'1. *Formulation of the problem.* – Let $\boldsymbol{r}_1$, $\boldsymbol{r}_2$ and $\boldsymbol{r}_3$ be the position vectors of the two electrons and the positron with respect to an origin of some coordinate system (here and below subscripts 1 and 2 correspond to the electrons and 3 corresponds to the positron). The non-relativistic Hamiltonian of the $e^- e^- e^+$ system has the form

$$H(\boldsymbol{r}_1, \boldsymbol{r}_2, \boldsymbol{r}_3) = -\frac{\hbar^2}{2m}\Delta_1 - \frac{\hbar^2}{2m}\Delta_2 - \frac{\hbar^2}{2m}\Delta^3 + \\ + \frac{e^2}{|\boldsymbol{r}_1 - \boldsymbol{r}_2|} - \frac{e^2}{|\boldsymbol{r}_1 - \boldsymbol{r}_3|} - \frac{e^2}{|\boldsymbol{r}_2 - \boldsymbol{r}_3|}. \tag{1}$$

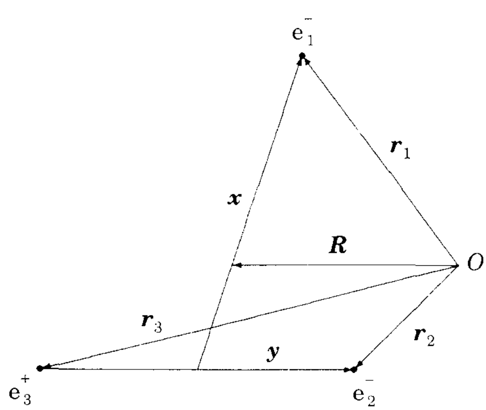

Fig. 1. – Coordinates for the e^- + Ps system.

We introduce a set of the Jacobi coordinates (see fig. 1)

$$R = \frac{1}{3}(r_1 + r_2 + r_3), \tag{2}$$

$$x = r_1 - \frac{1}{2}(r_2 + r_3), \tag{3}$$

$$y = r_2 - r_3 . \tag{4}$$

Obviously, $\boldsymbol{R}$ is the coordinate of the centre of mass of the system, $\boldsymbol{x}$ is the position vector of the electron 1 relative to the centre of mass of the $e_2^- e_3^+$ system, while $\boldsymbol{y}$ is the position vector of the electron 2 with respect to the positron. In terms of the new coordinates the Hamiltonian H may be written as

$$H(\boldsymbol{R}, \boldsymbol{x}, \boldsymbol{y}) = -\frac{\hbar^2}{2M}\Delta_R - \frac{\hbar^2}{2\tilde{\mu}}\Delta_x - \frac{\hbar^2}{2\mu}\Delta_y - \frac{e^2}{y} + \frac{e^2}{\left|\boldsymbol{x} - \frac{1}{2}\boldsymbol{y}\right|} - \frac{e^2}{\left|\boldsymbol{x} + \frac{1}{2}\boldsymbol{y}\right|}, \tag{5}$$

where

$$M = 3m, \qquad \tilde{\mu} = \frac{2}{3}m, \qquad \mu = \frac{1}{2}m. \tag{6}$$

Since interaction terms in the Hamiltonian are independent of $\boldsymbol{R}$, uniform motion of the centre of mass can be separated off and the Schrödinger equation becomes

$$\left(-\frac{\hbar^2}{2\tilde{\mu}}\Delta_x - \frac{\hbar^2}{2\mu}\Delta_y - \frac{e^2}{y} + \frac{e^2}{\left|\boldsymbol{x} - \frac{1}{2}\boldsymbol{y}\right|} - \frac{e^2}{\left|\boldsymbol{x} + \frac{1}{2}\boldsymbol{y}\right|} - E\right)\Psi(\boldsymbol{x}, \boldsymbol{y}) = 0, \tag{7}$$

where E is an internal energy of the considered system. In a standard manner [21] this equation may be converted into integral form:

$$\Psi(\boldsymbol{x}, \boldsymbol{y}) = \exp[i\boldsymbol{k}_i \cdot \boldsymbol{x}]\,\Phi_i(\boldsymbol{y})\,\chi_{(1/2)m_i}(1)\,\chi_{\sigma_i\mu_i}(2, 3) - \tag{8}$$

$$- \frac{\tilde{\mu}}{2\pi\hbar^2}\sum_f \Phi_f(\boldsymbol{y}) \int \mathrm{d}^3\boldsymbol{x}' \,\frac{\exp[ik_f|\boldsymbol{x} - \boldsymbol{x}'|]}{|\boldsymbol{x} - \boldsymbol{x}'|} \int \mathrm{d}^3\boldsymbol{y}'\, \Phi_f^*(\boldsymbol{y}')\,V(\boldsymbol{x}', \boldsymbol{y}')\,\Psi(\boldsymbol{x}', \boldsymbol{y}'),$$

which has built into it the correct asymptotic form to describe scattering. Here we have arbitrarily chosen r_1 and r_2 as the coordinates of the incident and bound electrons, respectively, and we have taken the direction of spin quantization to be the incident beam direction. In the above expression

$$V(\boldsymbol{x}, \boldsymbol{y}) = \frac{e^2}{\left|\boldsymbol{x} - \frac{1}{2}\boldsymbol{y}\right|} - \frac{e^2}{\left|\boldsymbol{x} + \frac{1}{2}\boldsymbol{y}\right|}, \tag{9}$$

$\Phi_f(\boldsymbol{y})$ is a spin-independent eigenfunction of the positronium atom with a corresponding eigenenergy E_f:

$$\left(-\frac{\hbar^2}{2\mu}\Delta_y - \frac{e^2}{y} - E_f\right)\Phi_f(\boldsymbol{y}) = 0\,, \tag{10}$$

where f stands collectively for positronium quantum numbers $n_f L_f M_f$, while $\boldsymbol{k}_i\,(\boldsymbol{k}_f)$ denotes the initial (final) wave vector of the projectile relative to the centre of mass of the positronium, with

$$\boldsymbol{k}_i^2 = \frac{2\tilde{\mu}}{\hbar^2}(E - E_i) \tag{11}$$

and similarly for $\boldsymbol{k}_f$. As regards spin variables, $\chi_{(1/2)m_i}(1)$ and $\chi_{\sigma_i\mu_i}(2, 3)$ describe initial spin states of the incident electron and the positronium atom, respectively, with $\sigma_1 = 0$ for the singlet state (para-positronium) and $\sigma_i = 1$ for the triplet state (ortho-positronium).

It follows from eq. (8) that the scattering amplitude for a transition $\gamma_i\sigma_i\mu_i m_i \to \to \gamma_f\sigma_f\mu_f m_f$ (with $\gamma_i = \boldsymbol{k}_i n_i L_i M_i$, $\gamma_f = \boldsymbol{k}_f n_f L_f M_f$) is

$$\begin{aligned} &A(\gamma_i\sigma_i\mu_i m_i \to \gamma_f\sigma_f\mu_f m_f) = \\ &= -\frac{\tilde{\mu}}{2\pi\hbar^2}\int \mathrm{d}^3\boldsymbol{x}\int \mathrm{d}^3\boldsymbol{y}\exp[-i\boldsymbol{k}_f\cdot\boldsymbol{x}]\,\Phi_f^*(\boldsymbol{y})\,V(\boldsymbol{x},\boldsymbol{y})\langle\chi_{(1/2)m_i}(1)\chi_{\sigma_i\mu_i}(2,3)|\Psi(\boldsymbol{x},\boldsymbol{y})\rangle \end{aligned} \tag{12}$$

and consequently a relevant differential cross-section is

$$Q(\gamma_i\sigma_i\mu_i m_i \to \gamma_f\sigma_f\mu_f m_f) = \frac{k_f}{k_i}|A(\gamma_i\sigma_i\mu_i m_i \to \gamma_f\sigma_f\mu_f m_f)|^2\,. \tag{13}$$

In eq. (12) $\langle\,|\,\rangle$ denotes integration over spin coordinates of the three particles.

In practice, one will be rather interested in the cross-section for the process of exciting the unpolarized beam of the positronium atoms by unpolarized electrons from the state $n_i L_i \sigma_i$ to $n_f L_f \sigma_f$. In this case we have to average eq. (13) over the initial magnetic quantum numbers $\mu_i m_i M_i$ and sum over the final magnetic quantum numbers $\mu_f m_f M_f$. This gives

$$\begin{aligned} &Q(\boldsymbol{k}_i n_i L_i \sigma_i \to \boldsymbol{k}_f n_f L_f \sigma_f) = \\ &= \frac{k_f}{k_i}\frac{1}{2(2\sigma_i+1)(2L_i+1)}\sum_{M_i M_f}\sum_{\substack{\mu_i m_i\\ \mu_f m_f}}|A(\gamma_i\sigma_i\mu_i m_i \to \gamma_f\sigma_f\mu_f m_f)|^2\,. \end{aligned} \tag{14}$$

When $\sigma_f \neq \sigma_i$, this formula gives the cross-section for the scattering with the spin-flip process. Finally, it additionally one is not aware of the initial and final total spin states of the positronium atom, the relevant cross-section is obtained averaging eq. (13) over $\sigma_i\mu_i m_i M_i$ and summing over $\sigma_f\mu_f m_f M_f$:

$$Q(\boldsymbol{k}_i n_i L_i \to \boldsymbol{k}_f n_f L_f) = \frac{k_f}{k_i}\frac{1}{8(2L_i+1)}\sum_{M_i M_f}\sum_{\substack{\sigma_i\mu_i m_i\\ \sigma_f\mu_f m_f}}|A(\gamma_i\sigma_i\mu_i m_i \to \gamma_f\sigma_f\mu_f m_f)|^2\,. \tag{15}$$

The total (integrated) cross-sections are then obtained by integrating eqs. (14) and

(15) over the scattering angle:

$$Q(n_iL_i\sigma_i \to n_fL_f\sigma_f) = \int \mathrm{d}^2\hat{k}_f\, Q(\boldsymbol{k}_i n_iL_i\sigma_i \to \boldsymbol{k}_f n_fL_f\sigma_f)\,, \tag{16}$$

$$Q(n_iL_i \to n_fL_f) = \int \mathrm{d}^2\hat{k}_f\, Q(\boldsymbol{k}_i n_iL_i \to \boldsymbol{k}_f n_fL_f)\,. \tag{17}$$

Since in eqs. (14) and (15) we have already averaged over initial magnetic quantum numbers M_i and μ_i, both cross-sections $Q(n_iL_i\sigma_i \to n_fL_f\sigma_f)$ and $Q(n_iL_i \to n_fL_f)$ are independent of the direction of incidence $\hat{k}_i$.

2'2. *The Born-Oppenheimer approximation.* – When interchanging the coordinates of the two electrons, $\boldsymbol{r}_1 \leftrightarrow \boldsymbol{r}_2$, the Jacobi coordinates $\boldsymbol{x}$ and $\boldsymbol{y}$ transform themselves in the following way:

$$\boldsymbol{x} \to \boldsymbol{x}' = \frac{3}{4}\boldsymbol{y} - \frac{1}{2}\boldsymbol{x}\,, \qquad \boldsymbol{y} \to \boldsymbol{y}' = \boldsymbol{x} + \frac{1}{2}\boldsymbol{y}\,. \tag{18}$$

Therefore, in the first-order Born-Oppenheimer approximation [21] one substitutes

$$\Psi(\boldsymbol{x}, \boldsymbol{y}) \simeq \exp[i\boldsymbol{k}_i\cdot\boldsymbol{x}]\,\Phi_i(\boldsymbol{y})\,\chi_{(1/2)m_i}(1)\,\chi_{\sigma_i\mu_i}(2, 3) - \tag{19}$$
$$-\exp\left[i\boldsymbol{k}_i\cdot\left(\frac{3}{4}\boldsymbol{y} - \frac{1}{2}\boldsymbol{x}\right)\right]\Phi_i\left(\boldsymbol{x} + \frac{1}{2}\boldsymbol{y}\right)\chi_{(1/2)m_i}(2)\,\chi_{\sigma_i\mu_i}(1, 3)$$

under the integral on the right-hand side of eq. (8). Then expression (12) for the scattering amplitude takes the form

$$A^{(\mathrm{BO})}(\gamma_i\sigma_i\mu_im_i \to \gamma_f\sigma_f\mu_fm_f) = F(\gamma_i \to \gamma_f)\,\delta_{\sigma_f\sigma_i}\delta_{\mu_f\mu_i}\delta_{m_fm_i} - \tag{20}$$
$$-G(\gamma_i \to \gamma_f)\langle\chi_{(1/2)m_f}(1)\,\chi_{\sigma_f\mu_f}(2, 3)\,|\,\chi_{(1/2)m_i}(2)\,\chi_{\sigma_i\mu_i}(1, 3)\rangle\,,$$

where

$$F(\gamma_i \to \gamma_f) = -\frac{\tilde{\mu}}{2\pi\hbar^2}\int \mathrm{d}^3\boldsymbol{x}\int \mathrm{d}^3\boldsymbol{y}\,\exp[-i\boldsymbol{k}_f\cdot\boldsymbol{x}]\,\Phi_f^*(\boldsymbol{y})\,V(\boldsymbol{x}, \boldsymbol{y})\exp[i\boldsymbol{k}_i\cdot\boldsymbol{x}]\,\Phi_i(\boldsymbol{y}) \tag{21}$$

is the direct scattering amplitude, while

$$G(\gamma_i \to \gamma_f) = -\frac{\tilde{\mu}}{2\pi\hbar^2}\int \mathrm{d}^3\boldsymbol{x}\int \mathrm{d}^3\boldsymbol{y}\,\exp[-i\boldsymbol{k}_f\cdot\boldsymbol{x}]\,\Phi_f^*(\boldsymbol{y})\,V(\boldsymbol{x}, \boldsymbol{y})\,\cdot \tag{22}$$
$$\cdot\exp\left[i\boldsymbol{k}_i\cdot\left(\frac{3}{4}\boldsymbol{y} - \frac{1}{2}\boldsymbol{x}\right)\right]\Phi_i\left(\boldsymbol{x} + \frac{1}{2}\boldsymbol{y}\right)$$

is the exchange scattering amplitude.

Both cross-sections (14) and (15) may be expressed in terms of the amplitudes $F(\gamma_i \to \gamma_f)$ and $G(\gamma_i \to \gamma_f)$. Carrying out summations over spin quantum numbers, after performing straightforward but tedious angular-momentum algebra, we obtain

$$Q^{(\mathrm{BO})}(\boldsymbol{k}_i n_i L_i \to \boldsymbol{k}_f n_f L_f) = \frac{k_f}{k_i}\frac{1}{(2L_i+1)}\cdot \tag{23}$$

$$\cdot \sum_{M_i M_f}\left(\frac{1}{2}|F(\gamma_i\to\gamma_f)|^2 + \frac{1}{2}|G(\gamma_i\to\gamma_f)|^2 + \frac{1}{2}|F(\gamma_i\to\gamma_f) - G(\gamma_i\to\gamma_f)|^2\right)$$

and

$$Q^{(\mathrm{BO})}(\boldsymbol{k}_i n_i L_i \sigma_i \to \boldsymbol{k}_f n_f L_f \sigma_f) = Q^{(\mathrm{BO})}(\boldsymbol{k}_i n_i L_i \to \boldsymbol{k}_f n_f L_f)\,\delta_{\sigma_i\sigma_f} + \tag{24}$$

$$+\frac{k_f}{k_i}\frac{1}{(2L_i+1)}\left(\frac{1}{4}(2\sigma_f+1) - \delta_{\sigma_i\sigma_f}\right)\sum_{M_i M_f}|G(\gamma_i\to\gamma_f)|^2 .$$

For practical reasons it may be sometimes useful to rewrite eq. (23) in another form:

$$Q^{(\mathrm{BO})}(\boldsymbol{k}_i n_i L_i \to \boldsymbol{k}_f n_f L_f) = \frac{k_f}{k_i}\frac{1}{(2L_i+1)}\cdot \tag{25}$$

$$\cdot \sum_{M_i M_f}\left(\frac{3}{4}|F(\gamma_i\to\gamma_f) - G(\gamma_i\to\gamma_f)|^2 + \frac{1}{4}|F(\gamma_i\to\gamma_f) + G(\gamma_i\to\gamma_f)|^2\right).$$

This expression receives a simple interpretation when one performs calculations in the representation which diagonalizes the total spin of the two electrons. In this representation one finds that $F-G$ and $F+G$ are the scattering amplitudes for the cases when the electrons are in the triplet and singlet states, respectively, and the cross-section is a weighted sum (with respective weights $3/4$ and $1/4$) of the cross-sections describing scattering in these two modes.

2·3. *Evaluation of scattering amplitudes. The Ochkur approximation.* – Evaluation of the direct scattering amplitude (21) is straightforward and gives

$$F(\gamma_i\to\gamma_f) = -\frac{2\tilde{\mu}e^2}{\hbar^2}\frac{1}{q^2}\left(S_{fi}\left(\frac{1}{2}\boldsymbol{q}\right) - S_{fi}\left(-\frac{1}{2}\boldsymbol{q}\right)\right), \tag{26}$$

where $\boldsymbol{q}$ is the momentum transfer

$$\boldsymbol{q} = \boldsymbol{k}_i - \boldsymbol{k}_f \tag{27}$$

and $S_{fi}(\boldsymbol{q})$ is the target form factor defined as

$$S_{fi}(\boldsymbol{q}) = \int \mathrm{d}^3\boldsymbol{y}\exp[i\boldsymbol{q}\cdot\boldsymbol{y}]\,\Phi_f^*(\boldsymbol{y})\,\Phi_i(\boldsymbol{y}). \tag{28}$$

As

$$S_{fi}(-\boldsymbol{q}) = (-)^{L_i+L_f}S_{fi}(\boldsymbol{q}), \tag{29}$$

eq. (26) can be rewritten in the form

$$F(\gamma_i \to \gamma_f) = -\frac{2\tilde{\mu}e^2}{\hbar^2}(1 + (-)^{L_i + L_f + 1})\frac{1}{q^2}S_{fi}\left(\frac{1}{2}\boldsymbol{q}\right). \tag{30}$$

It is seen that when $L_i + L_f$ is an even number the direct scattering amplitude vanishes and the transition $\gamma_i \to \gamma_f$ takes place only through electron exchange. The same selection rule for positronium-atom collisions has been derived by Mrówczyński [22].

Evaluation of the exchange amplitude (22) is lengthy and leads to a long and rather intractable formula. However, in the high-energy region these calculations can be greatly simplified without significant loss of accuracy by using an approximation suggested by Ochkur [23]. The idea is to isolate a leading term of the exchange amplitude for large k_i and use it as an approximation. Let us change the variable of integration in eq. (22) from $\boldsymbol{x}$ to

$$\boldsymbol{x}' = \boldsymbol{x} + \frac{1}{2}\boldsymbol{y}. \tag{31}$$

Then

$$G(\gamma_i \to \gamma_f) = G_1(\gamma_i \to \gamma_f) - G_0(\gamma_i \to \gamma_f), \tag{32}$$

where

$$G_n(\gamma_i \to \gamma_f) = -\frac{\tilde{\mu}e^2}{2\pi\hbar^2}\int d^3\boldsymbol{x}' \int d^3\boldsymbol{y} \exp[i\boldsymbol{a}\cdot\boldsymbol{y}]\,\Phi_f^*(\boldsymbol{y})\frac{1}{|\boldsymbol{x}' - n\boldsymbol{y}|}\exp[-i\boldsymbol{b}\cdot\boldsymbol{x}']\,\Phi_i(\boldsymbol{x}'), \tag{33}$$

with

$$\boldsymbol{a} = \boldsymbol{k}_i + \frac{1}{2}\boldsymbol{k}_f, \qquad \boldsymbol{b} = \boldsymbol{k}_f + \frac{1}{2}\boldsymbol{k}_i. \tag{34}$$

Writing

$$\frac{1}{|\boldsymbol{x}' - n\boldsymbol{y}|} = \frac{1}{2\pi^2}\int d^3\boldsymbol{p}\, p^{-2}\exp[i\boldsymbol{p}\cdot(\boldsymbol{x}' - n\boldsymbol{y})] \tag{35}$$

and denoting by $\tilde{\Phi}$ the Fourier transform of the function Φ, we have

$$G_n(\gamma_i \to \gamma_f) = -\frac{2\tilde{\mu}e^2}{\hbar^2}\int d^3\boldsymbol{p}\, p^{-2}\,\tilde{\Phi}_f^*(n\boldsymbol{p} - \boldsymbol{a})\,\tilde{\Phi}_i(\boldsymbol{p} - \boldsymbol{b}). \tag{36}$$

Changing the variable of integration to

$$\boldsymbol{t} = \boldsymbol{p} - \boldsymbol{k}_i \tag{37}$$

and noting that for large k_i, $p^2 = |\boldsymbol{t} + \boldsymbol{k}_i|^2$ in eq. (36) can be replaced by k_i^2, we obtain

$$G_1(\gamma_i \to \gamma_f) \simeq -\frac{2\tilde{\mu}e^2}{\hbar^2} k_i^{-2} S_{fi}\left(\frac{1}{2}\boldsymbol{q}\right) \tag{38}$$

and

$$G_0(\gamma_i \to \gamma_f) \simeq -(2\pi)^{3/2} \frac{2\tilde{\mu}e^2}{\hbar^2} k_i^{-2} \Phi_i(0) \tilde{\Phi}_f^*(-\boldsymbol{a}). \tag{39}$$

As $\tilde{\Phi}_f$ is a square-integrable function, it vanishes rapidly for large a (*i.e.* large k_i). Thus the leading term of the exchange amplitude is given by eq. (38) and in the Ochkur approximation one replaces $G(\gamma_i \to \gamma_f)$ by $G_1(\gamma_i \to \gamma_f)$.

2·4. *Evaluation of cross-sections.* – From eqs. (30) and (38) we see that evaluation of the cross-sections (23)-(25) requires knowledge of the expression

$$B_{fi}(q) = \frac{1}{(2L_i + 1)} \sum_{M_i M_f} |S_{fi}(\boldsymbol{q})|^2 . \tag{40}$$

After performing the necessary angular-momentum algebra we obtain

$$B_{fi}(q) = (2L_f + 1) \sum_{L=0}^{\infty} (2L + 1) \begin{bmatrix} L_f & L & L_i \\ 0 & 0 & 0 \end{bmatrix}^2 \langle n_f L_f | j_L(q) | n_i L_i \rangle^2 , \tag{41}$$

where $\begin{bmatrix} a & b & c \\ d & e & f \end{bmatrix}$ denotes the 3-j symbol [24] and

$$\langle n_f L_f | j_L(q) | n_i L_i \rangle = \int_0^\infty \mathrm{d}y \, P_{n_f L_f}(y) j_L(qy) P_{n_i L_i}(y) . \tag{42}$$

Here $P_{n_k L_k}$ stands for a radial part of the positronium wave function

$$\Phi_k(\boldsymbol{y}) = \frac{1}{y} P_{n_k L_k}(y) Y_{L_k M_k}(\hat{y}) \tag{43}$$

normalized to unity

$$\int_0^\infty \mathrm{d}y \, P_{n_1 L_1}(y) P_{n_2 L_2}(y) = \delta_{n_1 n_2} \qquad \text{for } L_1 = L_2 \tag{44}$$

and j_L is the spherical Bessel function. Because of selection rules for the 3-j symbols [24] the sum in eq. (41) contains only a finite number of terms. For transitions between states for which $L_i = 0$ or $L_f = 0$ further simplification is possible and one finds

$$B_{fi}(q) = \begin{cases} (2L_f + 1)\langle n_f L_f | j_{L_f}(q) | n_i 0 \rangle^2 & \text{for } L_i = 0 , \\ \langle n_f 0 | j_{L_i}(q) | n_i L_i \rangle^2 & \text{for } L_f = 0 . \end{cases} \tag{45}$$

The first few $B_{n_f L_f, 1s}(q)$ functions are given explicitly in the appendix.

The differential cross-sections for the spin-unresolved and spin-resolved scattering processes in the Ochkur approximation are thus

(46) $$Q^{(\mathrm{Och})}(\boldsymbol{k}_i n_i L_i \to \boldsymbol{k}_f n_f L_f) = \frac{k_f}{k_i}\left(\frac{2\tilde{\mu}e^2}{\hbar^2}\right)^2 (2q^{-2}\tau(L_i, L_f, 1)(2q^{-2} - k_i^{-2}) + k_i^{-4}) B_{fi}\left(\frac{1}{2}q\right),$$

(47) $$Q^{(\mathrm{Och})}(\boldsymbol{k}_i n_i L_i \sigma_i \to \boldsymbol{k}_f n_f L_f \sigma_f) = Q^{(\mathrm{Och})}(\boldsymbol{k}_i n_i L_i \to \boldsymbol{k}_f n_f L_f)\,\delta_{\sigma_i\sigma_f} + \left(\frac{1}{4}(2\sigma_f + 1) - \delta_{\sigma_i\sigma_f}\right)\left(\frac{2\tilde{\mu}e^2}{\hbar^2}\right)^2 k_f k_i^{-5} B_{fi}\left(\frac{1}{2}q\right),$$

where

(48) $$\tau(L_1, L_2, L_3) = \begin{cases} 1 & \text{for } L_1 + L_2 + L_3 \text{ even}, \\ 0 & \text{for } L_1 + L_2 + L_3 \text{ odd}. \end{cases}$$

The total (integrated) cross-sections can be obtained from eqs. (46) and (47) by integrating them over the scattering angle (see eqs. (16) and (17)) or, equivalently, over the values of the momentum transferred during the collision

(49) $$Q^{(\mathrm{Och})}(n_i L_i \sigma_i \to n_f L_f \sigma_f) = \frac{2\pi}{k_i k_f}\int_{q_{\min}}^{q_{\max}} \mathrm{d}q\, q\, Q^{(\mathrm{Och})}(\boldsymbol{k}_i n_i L_i \sigma_i \to \boldsymbol{k}_f n_f L_f \sigma_f),$$

(50) $$Q^{(\mathrm{Och})}(n_i L_i \to n_f L_f) = \frac{2\pi}{k_i k_f}\int_{q_{\min}}^{q_{\max}} \mathrm{d}q\, q\, Q^{(\mathrm{Och})}(\boldsymbol{k}_i n_i L_i \to \boldsymbol{k}_f n_f L_f),$$

where $q_{\min}$ and $q_{\max}$ are the values of the minimal and maximal momentum transfer given by

(51) $$q_{\min} = |k_i - k_f|, \qquad q_{\max} = k_i + k_f.$$

Therefore, for $Q^{(\mathrm{Och})}(n_i L_i \sigma_i \to n_f L_f \sigma_f)$ we have

(52) $$Q^{(\mathrm{Och})}(n_i L_i \sigma_i \to n_f L_f \sigma_f) \simeq \frac{\pi}{2}\left(\frac{2\tilde{\mu}e^2}{\hbar^2}\right)^2 (2\sigma_f + 1) k_i^{-6} \int_{q_{\min}}^{q_{\max}} \mathrm{d}q\, q\, B_{fi}\left(\frac{1}{2}q\right)$$

for $\sigma_i = \sigma_f$ and $L_i + L_f$ even,

(53) $$Q^{(\mathrm{Och})}(n_i L_i \sigma_i \to n_f L_f \sigma_f) \simeq 8\pi\left(\frac{2\tilde{\mu}e^2}{\hbar^2}\right)^2 k_i^{-2} \int_{q_{\min}}^{q_{\max}} \mathrm{d}q\, q^{-3} B_{fi}\left(\frac{1}{2}q\right)$$

for $\sigma_i = \sigma_f$ and $L_i + L_f$ odd, and

(54) $$Q^{(\mathrm{Och})}(n_i L_i \sigma_i \to n_f L_f \sigma_f) \simeq \frac{\pi}{2}\left(\frac{2\tilde{\mu}e^2}{\hbar^2}\right)^2 (2\sigma_f + 1) k_i^{-6} \int_{q_{\min}}^{q_{\max}} \mathrm{d}q\, q\, B_{fi}\left(\frac{1}{2}q\right)$$

for $\sigma_i \neq \sigma_f$. For $Q^{(\mathrm{Och})}(n_i L_i \to n_f L_f)$ we have

$$Q^{(\mathrm{Och})}(n_i L_i \to n_f L_f) \simeq 2\pi \left(\frac{2\tilde{\mu} e^2}{\hbar^2} \right)^2 k_i^{-6} \int_{q_{\min}}^{q_{\max}} \mathrm{d}q \, q \, B_{fi}\left(\frac{1}{2} q \right) \tag{55}$$

for $L_i + L_f$ even and

$$Q^{(\mathrm{Och})}(n_i L_i \to n_f L_f) \simeq 8\pi \left(\frac{2\tilde{\mu} e^2}{\hbar^2} \right)^2 k_i^{-2} \int_{q_{\min}}^{q_{\max}} \mathrm{d}q \, q^{-3} \, B_{fi}\left(\frac{1}{2} q \right) \tag{56}$$

for $L_i + L_f$ odd.

2.5. *Numerical results.* – We have carried out numerical calculations of the total cross-sections for the $1s \to 1s$, $1s \to 2s$ and $1s \to 2p$ transitions for projectile energies varying in the laboratory system from 0.1 to 10 keV. Since the ortho-Ps to para-Ps conversion is expected to be one of the most effective quenching processes shortening the lifetime of the ortho-Ps in plasma and could be used for determining free-electron concentration [3, 4, 25], we also present cross-sections for the scattering accompanied by this process. Our results are shown in fig. 2. Notice that for transitions with $L_i + L_f$ even the ortho-para conversion cross-section (54) can be obtained from the total cross-section (55) multiplying the latter by 1/4 (see also eqs. (23) and (24)). For the ortho-para conversion in the $1s \to 1s$ transition we compare our results with results deduced from the electron-transfer cross-section calculated in the first-order Faddeev-Watson multiple-scattering approximation by Chen *et al.* [12, 14].

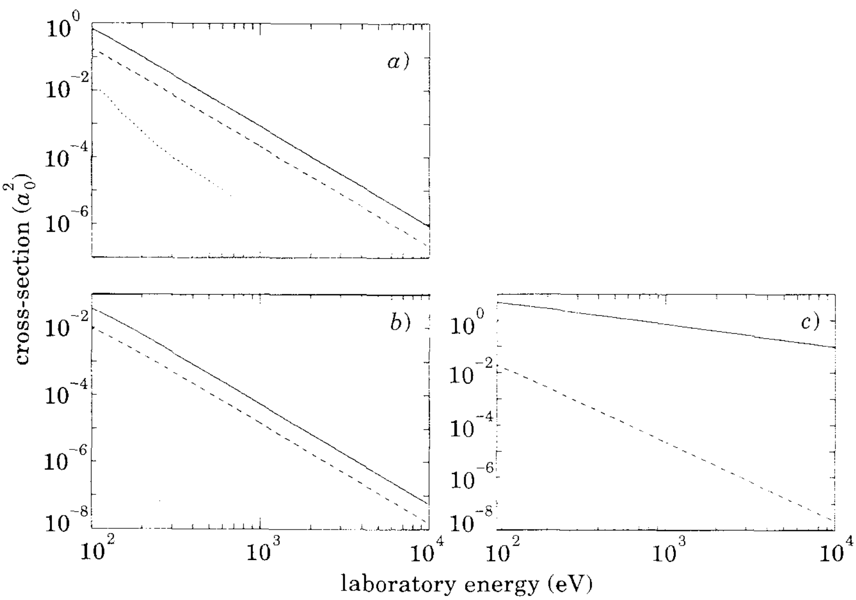

Fig. 2. – Total and ortho-para conversion cross-sections for the $1s \to 1s$ (*a*)), $1s \to 2s$ (*b*)) and $1s \to 2p$ (*c*)) transitions in $e^- + Ps$ collisions. Total: —— present results (eqs. (55) and (56)). Ortho-para conversion: – – – present results (eq. (54)); ····· results deduced from calculations of Chen *et al.* [12, 14].

3. – Conclusions.

We have applied the Born-Ochkur approximation to derive formulae for differential and total cross-sections describing scattering of fast non-relativistic electrons (positrons) from positronium atoms. It has been shown that the direct scattering amplitude vanishes for transitions between states with the same parity and consequently such transitions can take place only through electron exchange. Particularly, it applies to elastic scattering. It contrasts with the case of collisions of fast electrons with hydrogen atoms when the direct scattering amplitude dominates the exchange one independently of parities of initial and final states. Numerical calculations of total and ortho-para conversion cross-sections have been performed for the $1s \to 1s$, $1s \to 2s$ and $1s \to 2p$ transitions for projectile energies varying in the laboratory system from 0.1 to 10 keV. For elastic scattering the present results are much higher than results deduced from the electron-transfer cross-section calculated in the first-order Faddeev-Watson multiple-scattering approximation by Chen *et al.* [12, 14] which are the only total scattering data available in this energy region.

APPENDIX

The first few $B_{n_f L_f,\,1s}(q)$ functions are given explicitly by

$$B_{1s1s}(q) = 256(q^2 a_0^2 + 4)^{-4}\,, \tag{A.1}$$

$$B_{2s1s}(q) = 32 q^4 a_0^4 \left(q^2 a_0^2 + \frac{9}{4}\right)^{-6}, \tag{A.2}$$

$$B_{2p1s}(q) = 72 q^2 a_0^2 \left(q^2 a_0^2 + \frac{9}{4}\right)^{-6}, \tag{A.3}$$

$$B_{3s1s}(q) = \frac{256}{27} q^4 a_0^4 \left(q^2 a_0^2 + \frac{16}{27}\right)^2 \left(q^2 a_0^2 + \frac{16}{9}\right)^{-8}, \tag{A.4}$$

$$B_{3p1s}(q) = \frac{2048}{81} q^2 a_0^2 \left(q^2 a_0^2 + \frac{16}{27}\right)^2 \left(q^2 a_0^2 + \frac{16}{9}\right)^{-8}, \tag{A.5}$$

$$B_{3d1s}(q) = \frac{131\,072}{19\,683} q^4 a_0^4 \left(q^2 a_0^2 + \frac{16}{9}\right)^{-8}, \tag{A.6}$$

where a_0 is the Bohr radius.

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