Triple differential cross section of electron impact ionisation of Na(3s, 3p, 3d)

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Abstract. The fivefold differential cross section (5DCS) of the ionisation by electron impact of atomic sodium is determined theoretically for its fundamental $3s(^2S)$ state and the excited $3p(^2P)$ and $3d(^2D)$ states by a procedure which employs in the transition matrix element of the first order Born approximation, the correlated double continuum (3C) wave function. This permits us to determine the statistical M-state population and the orientation and alignment tensors in $(e, 2e)$ detection. It is also shown that, the use of Gamow correlation term, in the independent particle (2C) model, reproduces, only in some situations, the shape of the angular distribution of the 5DCS obtained by the (3C) wave function.

1 Introduction

Atomic sodium has been largely employed in ion-atom collisions [1–3]. These authors have studied the electron exchange and excitation in collisions involving excited and prepared sodium targets. In spite of the fact that, the manipulation, from the experimental point of view, of sodium seems to be easier than other alkali, it has been rarely employed in $(e, 2e)$ ionisation experiments [4], in which the incident electron is detected after scattering in coincidence with the ejected electron. Zheng *et al.* [5] have observed the momentum density profile of excited and oriented sodium atoms. Recently Dorn *et al.* [6] give the orientational dichroism in $(e, 2e)$ reactions with oriented Na(3p) atoms. These experiments present a large theoretical and experimental interest as they permit through the determination of the five fold differential cross section (5DCS) the study of the ionisation mechanisms and the verifications of the different theoretical models proposed for the description of the double continuum.

Sodium atoms present the particularity of having a fundamental $3s(^2S)$ state, which has, in contrast to atomic hydrogen, a distinct energy value from that of $3p(^2P)$ and $3d(^2D)$ states. From this point of view, it is the only target which permits the study of the $3s$ distribution in an $(e, 2e)$ experiment. More the preparation of the p states is relatively easier for sodium than for lithium.

Many approximate descriptions, of the electronic double continuum resulting from an $(e, 2e)$ reaction, where the ejected and the scattered electrons are subject to the

Coulomb field of the residual ion, are nowadays available (see for example [7]), such as those obtained by generalising the partial wave expansion to the two electron systems, or the independent particle model using a product of two monoelectronic exact Coulomb wave functions, designated by (2C), in which one can introduce (Peterkop [8]) the boundary conditions by the means of an effective charge whose value depends on the dynamics of the problem.

Another type of wave functions constructed by a correlated product of two Coulomb functions (3C) obtained by a Pluvinage [9] type approximation have been, since a long time, observed to satisfy the exact boundary conditions of the Coulomb double continuum [10,11]. Brauner *et al.* [12] have first calculated the different matrix elements obtained by using this type of wave functions to the determination of the 5DCS of $(e, 2e)$ ionisation of atomic hydrogen. The advantages of applying this type of wave functions was also demonstrated in other situations, like in the description of the electrons emerging from a photo-double-ionisation process [13], and a double ionisation by fast electron impact [14], and to the determination of the differential cross section of the $(e, 2e)$ ionisation of excited metastable $(2s)$ hydrogen by Hafid *et al.* [15] whose results were compared to those of the second Born calculations [16].

In this paper, we present the determination of the triple differential cross section (5DCS) of Na(3s) Na(3p) and Na(3d) using a model potential for the alkaline core both in the determination of the bound state wave function of the target and in the interaction potential of the incoming electron with the target. We give the M statistical population and the dicroism (Berakdar *et al.* [17]) of

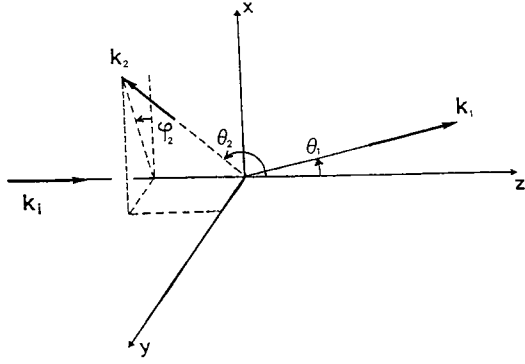a e-mail: jocelyn@ipc.sciences.univ-metz.fr

Fig. 1. Coordinates used in the text.

the 5DCS by three different descriptions of the final state to study the influence of the electron-electron correlation.

2 Theory

For given wave vectors $\mathbf{k}_i$, $\mathbf{k}_1$, $\mathbf{k}_2$ (Fig. 1) of the incident, scattered and the ejected electrons respectively, the five-fold differential cross section (5DCS) (3DCS in coplanar detection) of the $|nlm\rangle$ state of the alkaline atom will be given (in atomic units) by:

$$\sigma_{nlm}^{(5)} = \frac{d^5\sigma}{d\Omega_1 d\Omega_2 d(\frac{1}{2}k_2^2)} = \frac{(2\pi)^4 k_1 k_2}{k_i} |T_{fi}|_{nlm}^2. \quad (1)$$

Here Ω_1 and Ω_2 represent respectively the solid angles of the different wave vectors. The recoil energy of the ion being negligible, we can write:

$$\frac{k_i^2}{2} = I_{nl}^+ + \frac{k_1^2}{2} + \frac{k_2^2}{2} \quad (2)$$

where the ionisation energy $I_{3s}^+ = 5.138$ eV, $I_{3p}^+ = 3.036$ eV and $I_{3d}^+ = 1.5212$ eV. The transition amplitude is given by:

$$|T_{fi}| = \frac{1}{4}|f_{nlm} + g_{nlm}|^2 + \frac{3}{4}|f_{nlm} - g_{nlm}|^2 \quad (3)$$

with

$$f_{nlm} = \langle \Psi_f^-(\mathbf{r}_1, \mathbf{r}_2)|V|\Psi_i(\mathbf{r}_1, \mathbf{r}_2, l, m)\rangle \quad (4)$$

and

$$g_{nlm} = \langle \Psi_f^-(\mathbf{r}_2, \mathbf{r}_1)|V|\Psi_i(\mathbf{r}_1, \mathbf{r}_2, l, m)\rangle. \quad (5)$$

Ψ_f^- and Ψ_i represent the wave functions describing the whole system in its final and initial states respectively. $\mathbf{r}_1$ designates the position of the incident electron, $\mathbf{r}_2$ the bound one, and V represents the interaction between the incident electron and the target.

$$V = \frac{1}{r_1} + \frac{1}{r_{12}} + V_2 \quad (6)$$

with $r_{12} = |\mathbf{r}_1 - \mathbf{r}_2|$ and V_2, the model potential, which describes the interaction of the incident electron with the electrons of the alkaline core given by: (Klapisch [18])

$$V_2 = -\beta \exp(-\gamma r_1) - (Z-1)\frac{\exp(-\zeta r_1)}{r_1},$$

with $\beta = 23.51$, $\gamma = 2.688$, $\zeta = 7.902$ and $Z = 11$. (7)

The initial state, which takes into account the incident and the bound electrons, will be written as the product of a plane wave and the wave function of the valence electron of the alkaline atom:

$$|\Psi_i\rangle = \left| \frac{\exp(i\mathbf{k}_i \cdot \mathbf{r}_i)}{(2\pi)^{3/2}} \varphi_{nlm}(\mathbf{r}_2) \right\rangle, \quad (8)$$

the wave function $\varphi_{mlm}(\mathbf{r}_2)$ is obtained by an expansion on Slater basis

$$\varphi_{nlm} = Y_l^m(\theta, \phi) \sum_{j=0}^{n_j} C_j r^{\nu_j} \exp(-\alpha_j r) \quad (9)$$

where α_j, ν_j and n_j are empirical parameters, and the coefficients C_j are determined variationally.

The final state is approximated by a 3C type function given by:

$$\Psi_f^-(\mathbf{r}_1, \mathbf{r}_2) = M e^{i\mathbf{k}_1 \cdot \mathbf{r}_1} e^{i\mathbf{k}_2 \cdot \mathbf{r}_2} \chi(\mathbf{r}_1, \mathbf{r}_2) \quad (10)$$

with

$$\chi(\mathbf{r}_1, \mathbf{r}_2) = {}_1F_1(i\alpha_1, 1, -i(k_1 r_1 + \mathbf{k}_1 \cdot \mathbf{r}_1))$$
$$\times {}_1F_1(i\alpha_2, 1, -i(k_2 r_2 + \mathbf{k}_2 \cdot \mathbf{r}_2))$$
$$\times {}_1F_1(i\alpha_{12}, 1, -i(k_{12} r_{12} + \mathbf{k}_{12} \cdot \mathbf{r}_{12})). \quad (11)$$

The constant M is given by:

$$M = \exp[-\pi(\alpha_1 + \alpha_2 + \alpha_{12})/2]$$
$$\times \Gamma(1 - i\alpha_1)\Gamma(1 - i\alpha_2)\Gamma(1 - i\alpha_{12})/(2\pi)^3 \quad (12)$$

where

$$\alpha_1 = \frac{-1}{|\mathbf{k}_1|}, \quad \alpha_2 = \frac{-1}{|\mathbf{k}_2|}, \quad \alpha_{12} = \frac{1}{|\mathbf{k}_{12}|}, \quad (13)$$

with

$$\mathbf{k}_{12} = \frac{1}{2}[\mathbf{k}_1 - \mathbf{k}_2]. \quad (14)$$

$$W\left(\mathbf{k}_a, \mathbf{k}_b, \mathbf{k}_{ab}, \mathbf{p}_1, \mathbf{p}_2, \alpha_a, \alpha_b, \alpha_{ab}, \lambda_1, \lambda_2, \lambda_3, \boldsymbol{\eta}\right) = \int \frac{d\mathbf{r}}{r} \frac{d\mathbf{R}}{R} \, {}_1F_1(-i\alpha_a, 1, i(k_a r + \mathbf{k}_a \cdot \mathbf{r})) \exp(-i\mathbf{k}_a \cdot \mathbf{r} - i\mathbf{p}_1 \cdot \mathbf{r} - \lambda_1 r)$$
$$\times \, {}_1F_1(-i\alpha_b, 1, i(k_b R + \mathbf{k}_b \cdot \mathbf{R})) \exp(-i\mathbf{k}_b \cdot \mathbf{R} - i\mathbf{p}_1 \cdot \mathbf{R} - i\boldsymbol{\eta} \cdot \mathbf{R} - \lambda_2 R)$$
$$\times \, {}_1F_1(-i\alpha_{ab}, 1, i(k_{ab}|\mathbf{r} + \mathbf{R}| + \mathbf{k}_{ab} \cdot (\mathbf{r} + \mathbf{R}))) \exp(-\lambda_3|\mathbf{r} + \mathbf{R}|). \tag{15}$$

$$f_{nlm} = \frac{1}{\sqrt{2}(2\pi)^2} M^* \sum_{j=1}^{n_j} \lim_{\eta \to 0} \hat{D}_{nlm} \{ W(\mathbf{k}_1, -\mathbf{k}_2, \mathbf{k}_{12}, -\mathbf{k}_i, \mathbf{0}, \alpha_1, \alpha_2, \alpha_{12}, 0, \nu_j, 0, \boldsymbol{\eta})$$
$$- W(\mathbf{k}_{12}, \mathbf{k}_2, \mathbf{k}_1, \mathbf{k}_1 - \mathbf{k}_i - \mathbf{k}_{12}, \mathbf{k}_1 - \mathbf{k}_i, \alpha_{12}, \alpha_2, \alpha_1, 0, \nu_j, 0, \boldsymbol{\eta}) + \beta \frac{\delta}{\delta \nu_j} W(\mathbf{k}_1, -\mathbf{k}_2, \mathbf{k}_{12}, -\mathbf{k}_i, \mathbf{0}, \alpha_1, \alpha_2, \alpha_{12}, \gamma, \nu_j, 0, \boldsymbol{\eta})$$
$$+ (Z - 1)W(\mathbf{k}_1, -\mathbf{k}_2, \mathbf{k}_{12}, -\mathbf{k}_i, \mathbf{0}, \alpha_1, \alpha_2, \alpha_{12}, \zeta, \nu_j, 0, \boldsymbol{\eta})\}$$
$$\tag{16}$$

We define the following basic integral, which is a generalisation of the one presented in [12]:

See equation (15) above

For the m sublevel of the $|nl\rangle$ state their procedure should be extended by introducing supplementary derivations of the basic integral in terms of λ_2, η_x, η_y and η_z. The originality of our approach consists in the fact that we could perform all the derivations analytically using recursion relations developed in [19].

The direct term of the transition matrix element is given by:

See equation (16) above

The $\hat{D}_{nlm}$ are operators and their applications permits to generate the spatial and angular part of the corresponding bound state.

3 Result

We will in what follows present the variation of the five fold differential cross section (5DCS) of the $3s$, $3p$ and $3d$ levels of sodium in terms of the ejection angle for an incidence energy value of 150 eV and an ejection energy value of 50 eV. We consider two scattering angles, $0.5°$ corresponding to a situation of small momentum transfer, and $35°$ corresponding to an optimal situation in coplanar geometry giving zero recoil momentum of the ion $\mathbf{k}_{recoil} = \mathbf{K} - \mathbf{k}_2 = \mathbf{0}$ (Bethe ridge), when the ejection direction ($\mathbf{k}_2$) is parallel to the momentum transfer $\mathbf{K} = \mathbf{k}_i - \mathbf{k}_1$. On each figure we will present three curves, representing the results obtained by, the Coulomb projected Born 2C procedure [20] in dotted lines. These are realised by replacing α_{12} by zero in equation (16). This is equivalent to an independent particle description of the final state double continuum by two Coulomb wave functions. Next, the curves in full line will represent the results obtained by the 3C correlated two electron continuum wave function (Eq. (10)), which can be considered in contrast to the preceding, as a first order Born procedure with correct boundary conditions. Finally, the curves

with dashed lines will represent the results noted 2CG obtained by multiplying the 2C results by the Gamow factor $G = \dfrac{\pi \alpha_{12}}{\sinh(\pi \alpha_{12})}$, which is also present in the 3C wave function. The comparison between the 3C and the 2CG results will permit us to find out situations where the final state correlation introduced by the third hypergeometric function is important. This will show the reliability of the calculations [7, 21, 22] where the final state correlation is introduced only partially by the Gamow factor.

We consider first, in the Figures 2a and 2b the variation of the 5DCS of the ionisation of sodium for the sublevels $3p_0$ and $3p_{\pm 1}$ respectively in a coplanar geometry for an scattering angle of $0.5°$. We remark that, the 2C and 3C results differ in shape and in magnitude, specially in the forward ejection direction $\theta_2 \approx 0°$ or $360°$. In fact, the Gamow term, present in the 3C and 2CG results, hinders the ejection in this direction. On the other hand, the 3C and 2CG results are somewhat similar in shape in the $3p_0$ case but not in the $3p_{\pm 1}$ case in Figure 2b, where the maxima are translated to the forward direction.

In the case of the scattering angle of $35°$ we present in Figures 3a and 3b the 5DCS of $3p_0$ and $3p_{\pm 1}$ respectively. Here the momentum transfer direction around the ejection angle of $300°$ is an optimal direction, as in this direction the recoil momentum which is given by $\mathbf{k}_{recoil} = \mathbf{K} - \mathbf{k}_2$. Here the conclusion that we can do when comparing the different results is that the Gamow factor introduces a difference in the magnitude, as it destroys the norm of the final state wave function. More it does not contribute in any way in the modification of the general shape of the curve of 2C. One must add that, the minimum that we observe around $300°$ in Figure 3a is due to the structure of the initial state of the atom and not to the final state correlation as it exists on the three curves.

In the Figures 4a, b, 5a, b and 6a, b we present respectively for the $3s$ $3p$ and $3d$ levels for the scattering angles $0.5°$ and $35°$ by the M statistical distribution given by:

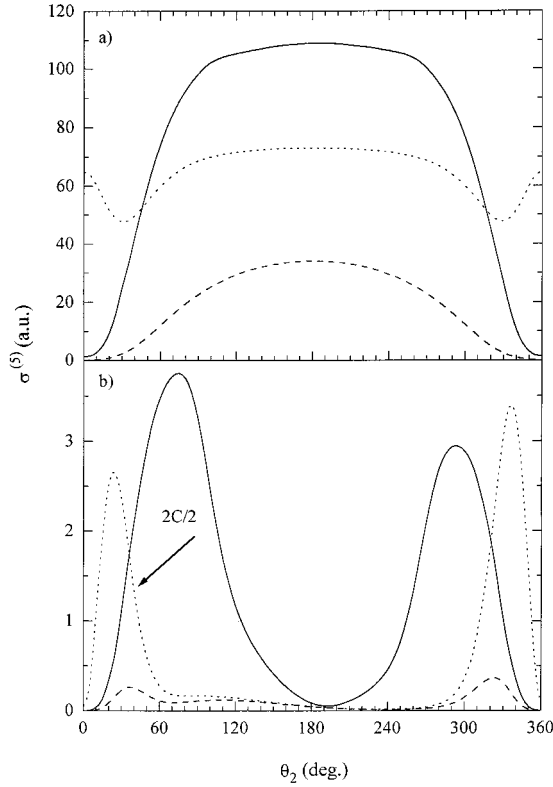$$\sigma_{nl}^{(5)} = \frac{1}{2l+1} \sum_{m=-1}^{1} \sigma_{nlm}^{(5)}. \tag{17}$$

Fig. 2. The fivefold differential cross section (5DCS) of the $(e, 2e)$ ionisation of sodium in terms of the ejection angle θ_2. The incident, ejected electron energies and the scattering angle are respectively 150 eV, 50 eV and 0.5°: (a) for the $3p_0$ level and (b) for the $3p_{\pm 1}$ level. The full curve gives the 3C results. The dotted curve gives the 2C results. The dashed curve gives the 2CG results.

Following the treatment of Berakdar *et al.* [17], we determined the tensorial parameters $\Sigma_0^{(0)}$, $\Sigma_0^{(1)}$, $\Sigma_0^{(2)}$ concerning the p sublevels with:

$$\Sigma_0^{(0)} = \frac{1}{\sqrt{3}}(\sigma_{3p_1}^{(5)} + \sigma_{3p_0}^{(5)} + \sigma_{3p_{-1}}^{(5)})$$

$$\Sigma_0^{(1)} = \frac{1}{\sqrt{2}}(\sigma_{3p_1}^{(5)} - \sigma_{3p_{-1}}^{(5)})$$

$$\Sigma_0^{(2)} = \frac{1}{\sqrt{6}}(\sigma_{3p_1}^{(5)} - 2\sigma_{3p_0}^{(5)} + \sigma_{3p_{-1}}^{(5)}). \qquad (18)$$

We give in Figure 7 their variations in terms of the azimuthal angle φ_2 of the ejected electron direction keeping $\varphi_1 = 0°$ with the spherical polar angles $\theta_1 = 35°$ and $\theta_2 = 60°$.

In Figure 7a and 7c, we present respectively the M-statistical distribution of the DCS given by $\Sigma_0^{(0)}$ and the $\Sigma_0^{(2)}$ which represents for excitation, the difference between the linearly-polarised and the unpolarised light, indeed $\Sigma_0^{(2)}$ can be written as:

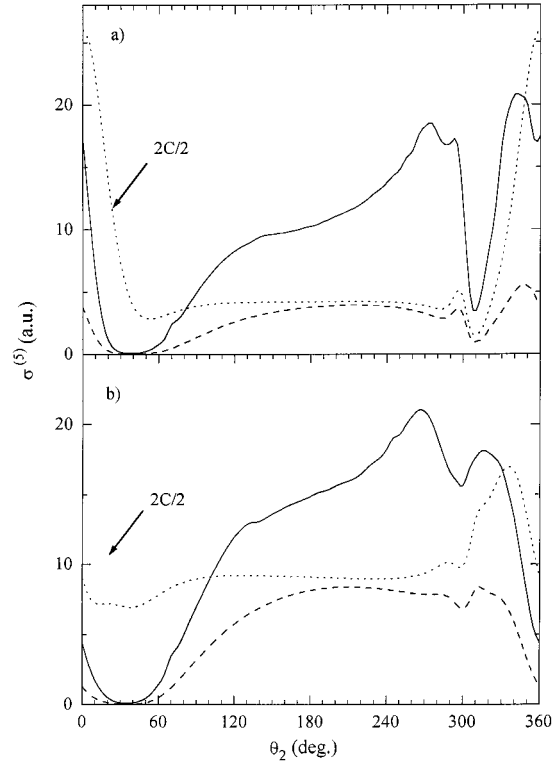$$\Sigma_0^{(2)} = \frac{1}{\sqrt{2}}(\Sigma_0^{(0)} - \sqrt{3}\sigma_{p_0}^{(5)}).$$

Fig. 3. Same as Figure 2 but for the scattering angle at 35°.
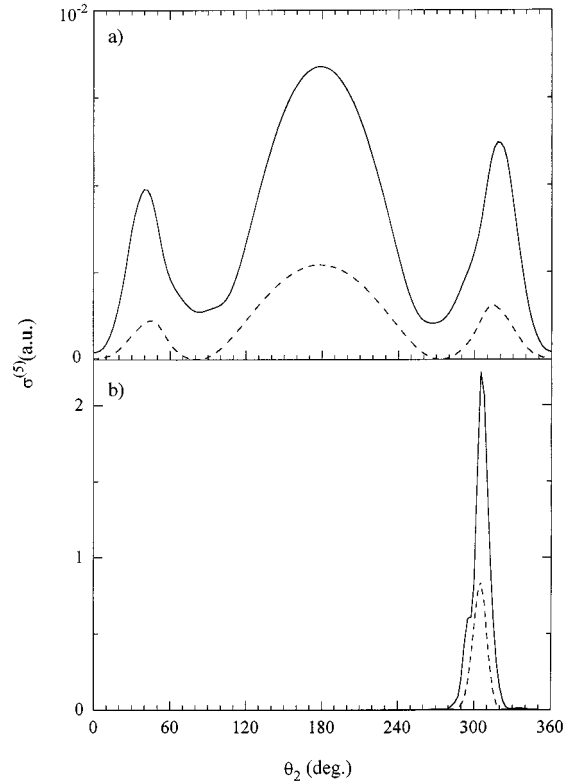

Fig. 4. The total 5DCS (Eq. (1)) for $(e, 2e)$ ionisation of sodium $3s$ in coplanar geometry for the scattering angle at: (a) 0.5° and (b) 35°.
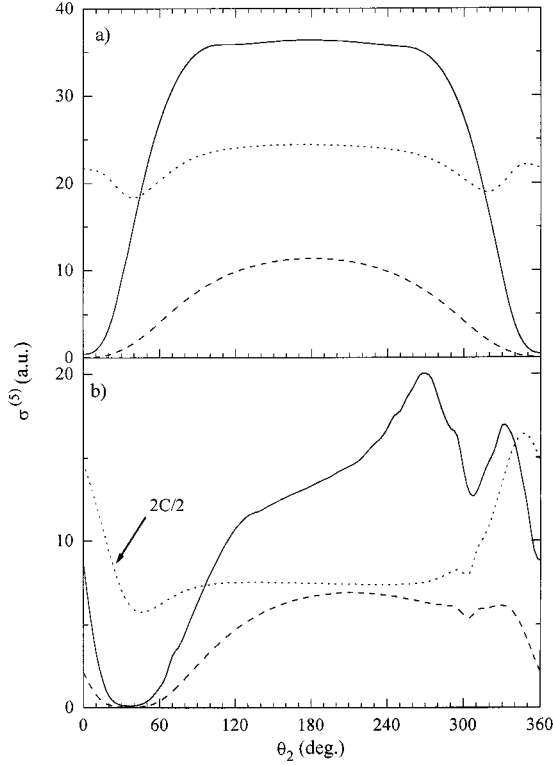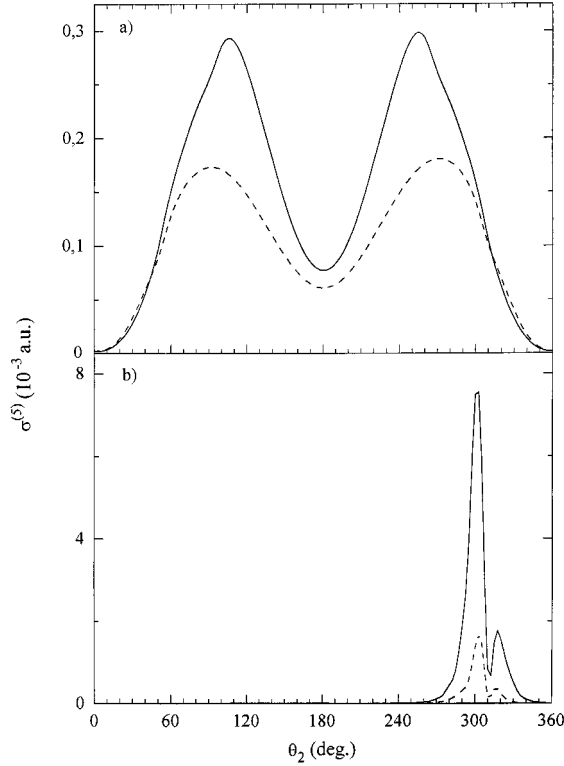
Fig. 5. Same as Figure 4 but for sodium 3*p*.

Fig. 6. Same as Figure 4 but for sodium 3*d*.
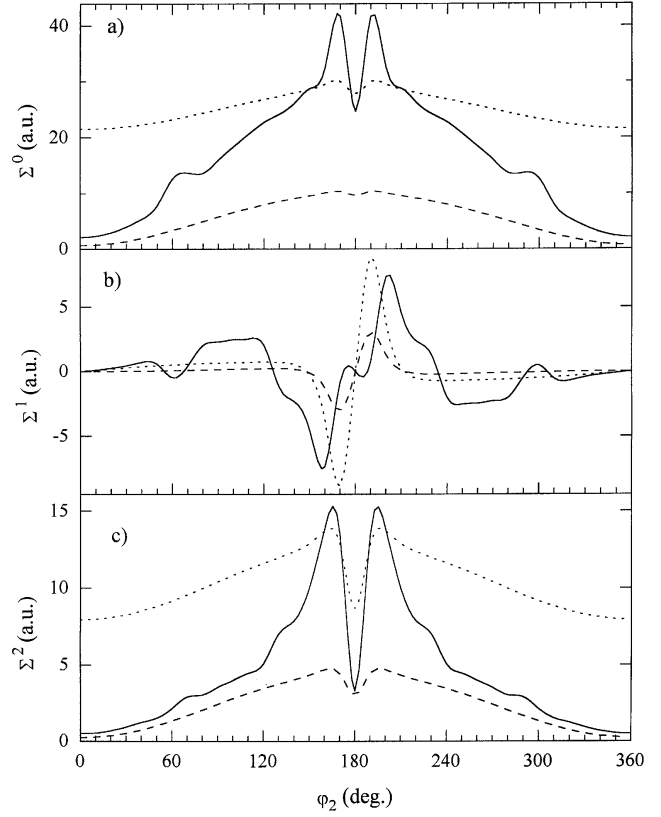

Fig. 7. The tensorial components [17] in terms of the azimutal angle φ_2 of the ejected electron. The incident, ejected electron energies, the scattering and ejection angles are respectively 150 eV, 50 eV 35° and 60°: (a) $\Sigma_0^{(0)}$, (b) $\Sigma_0^{(1)}$ and (c) $\Sigma_0^{(2)}$.

As expected, increasing φ_2 makes the recoil momentum $\mathbf{k}_{recoil} = \mathbf{K} - \mathbf{k}_2$ diminish causing the increase in the intensity, which is observed in the three curves. The direction around $\varphi_2 = 180°$ is a privileged direction (Bethe region). The minimum at $\varphi_2 = 180°$ is due to the minimum observed in Figure 3a and b around 300°. The 2C and 2CG curves have more or less the same shape which defers strongly from that of 3C. This can be explained by the fact that, as we keep the moduli of $\mathbf{k}_1$ and $\mathbf{k}_2$ fixed, $\mathbf{k}_{12}$ increases with φ_2 which is a parameter of the third hypergeometric function of the 3C, which is responsible for the final state correlation.

In Figure 7b, we present the variation of the dicroism given by:

$$\Sigma_0^{(1)} = \frac{1}{\sqrt{2}}[\sigma_{3p_1}^{(5)} - \sigma_{3p_{-1}}^{(5)}].$$

in terms of φ_2. Now as expected $\Sigma_0^{(1)}$ for $\varphi_2 = 0°$, 180°. Here also the 2CG and 2C results are in complete disagreement specially in the sensitive region around $\varphi_2 = 150°$ to 210°.

4 Conclusion

We have developed a procedure which determines the 5DCS of the $(e, 2e)$ ionisation of the different sublevels of the $n = 3$ level of sodium by applying a 3C wave function. Our results show for an unpolarized electron beam of 150 eV and an ejection energy of 50 eV the particularities of the variation of the 5DCS in terms of the ejection angle $3s$, $3p$ and $3d$ sublevels and the limitations of the application of the Gamow factor to the 2C calculations, specially in the determination of the dichroism in the $3p_{\pm 1}$.

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