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Photoionisation of Some C^{2+} Excited Terms

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Abstract Cross sections for photoionisation from the $1s^22s2p$ $^1P^0$ and $1s^22p^2$ $^1S^e$ states of C^{2+} are calculated. The close-coupling method is used to obtain wavefunctions for the initial (C^{2+}) and final (C^{3+} + e-) states. The $1s^22pn\ell$ series of autoionising terms give rise to resonances in the cross sections.

1. INTRODUCTION

Cross-sections for photoionisation from ground and excited terms of light atoms are needed in many astrophysical applications. C^{2+} for example, is an important opacity source in hot star atmosphere. Simple methods have been often used in the past to estimate cross-sections. In these methods, the dipole integrals involved in the photoionisation formula are either (i) calculated using radial wavefunctions for the bound and ejected electrons pertaining to the same central potential, or (ii) estimated from experimental data (quantum defects) by means of the method developed by Peach[1]. However, during the past decade or so great progress has been made for improving both the initial (A_i^{+m}) and final ($A_j^{+m+1} + e^-$) state wavefunctions by means of the 'close coupling' approximation[2]. As a consequence photo-excitation to (A^{+m}) autoionisation terms, as well as the possibility for the ejected electron to induce excitation of the residual ion A^{+m+1}, are taken into account in recent calculations[3,4].

In this paper, as a part of a more general research programme, we consider photoionisation from two excited terms, namely $1s^22s2p$ $^1P^0$ and $1s^22p^2$ $^1S^e$ of C^{2+} using programs developed a University College, London. We find that, for low ejected electron energies on $1s^22s$, the

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photoionisation cross-sections are strongly perturbed by the existence of several series of $1s^2 2pn\ell$ autoionising terms.

In part 2 we describe briefly the close-coupling method and the multichannel photoionisation formula. In parts 3 and 4 the initial and final states are discussed in detail. Our results are presented in section 5.

2. WAVEFUNCTIONS IN THE CLOSE COUPLING METHOD

The $(N+1)$-electron system wavefunction, either bound or free, can be expanded using the set of N-electron wavefunctions plus spherical harmonics and spin functions. With these elements a more convenient basis, the elements of which contain all variables except r_{N+1}, can be built and labelled by $i \equiv \tau LS\ell \frac{1}{2} L^T S^T$. τLS labels the N-electron terms. To each element i is therefore associated a $F_i(r_{N+1})$ radial function which has to be determined. The Kohn variational principle applied to the Schrödinger equation leads to a set of coupled integro-differential equations for defining the F_i's. Some simplifications occur: parity p, L^T and S^T split the system of equations into subgroups which are independent of M_L^T and M_S^T. Therefore for given p, L^T, S^T and if only a few τLS terms are included in the expansion, the number of channels is considerably reduced. We write the set of coupled equations for NCHF channels as follows

$$\left\{\frac{d^2}{dr_{N+1}^2} - \frac{\ell_i(\ell_i+1)}{r_{N+1}^2} + \frac{2(Z-N)}{r_{N+1}} + k_i^2\right\} F_i + \sum_{i'=1}^{\mathrm{NCHF}} U_{ii'} F_{i'} = 0 \qquad (1)$$

If the orthogonality conditions

$$(P_{n\ell}|F_i) = 0 \quad \text{if} \quad \ell_i = \ell \qquad (2)$$

are imposed on the continuum and bound state orbitals then Lagrange multiplier expressions must be introduced in eq. (1). In order to remove constraints on the total system wavefunction a suitable linear combination of $(N+1)$-electron functions will be added in the initial expansion

$$\psi = \sum_{i=1}^{NCHF} A\, \phi_i F_i(r_{N+1}) + \sum_{j=1}^{NCHB} c_j \phi_j \qquad (3)$$

A antisymmetrises $\phi_i F_i$, and the c_j are mixing coefficients that have to be determined. The set of $\phi^{pL^TS^T}$, one configuration wavefunctions (called *bound channels*) built using the $P_{n\ell}$'s of the τLS terms, can be increased to balance the truncation of the first summation in eq.(3).

The reader is referred to the articles of Seaton and co-workers for a more complete view on the coupled equation system[5,6,7]. If E is the total energy of the $(N+1)$-electron system, and E_i are the τLS term energies, we have for each channel

$$k_i^2 = E - E_i \quad \text{with E and } E_i \text{ in Rydbergs} \qquad (4)$$

The choice of E decides of the number of open channels NCHOP ($k_i^2 \geq 0$) and of the closed ones ($k_i^2 < 0$). If all $k_i^2 < 0$, these equations are used to obtain bound states. If some or all $k_i^2 \geq 0$, the total system wavefunctions are used to represent a free electron moving away and leaving the core τLS in the ground or excited states. The asymptotic form required for the open channel F_i's are

$$F_i \sim \frac{1}{2}\, k_i^{-1/2} \left(\delta_{ii'}\, e^{-ix_i} - S_{ii'}\, e^{+ix_i}\right) \qquad (5)$$

with

$$x_i = k_i r + (z/k)\ln(2k_i r) - 1/2\, \ell_i \pi + \arg\Gamma(\ell_i + 1 - iz/k_i) \qquad (6)$$

eq.(5) means that there exist NCHOP total system wavefunctions, each one for an exit channel i'. On the closed channels a decreasing asymptotic form is imposed. $\vec{S}$, the scattering matrix, is a function of E, which leads to the partial collision strengths $\Omega(\tau LS\text{-}\tau L'S')$. With these asymptotic forms, the total photoionisation cross section is given in the length formulation by

$$\sigma = \frac{4\pi\alpha a_0^2 h\nu}{3(2L+1)} \sum_{i'=1}^{NCHOP} |G_{i'}(h\nu)|^2 \qquad (7)$$

$G_{i'}$ is the reduced matrix element of the electric dipole operator

$$G_{i'} = <\psi \text{ initial} \,||\, P \,||\, \psi_{i'}> \tag{8}$$

hν is the photon energy in Rydbergs. L is the angular momentum of the initial state. The quantities under C in eq.(7) are the contributions to the total cross section from channel exit photoionisation, i.e. from these one obtains the photoionisation cross sections for the different τLS terms of the residual ion[8]. The calculations eq. (7) are repeated for the different (if any) L^T values $L^T = L \pm 1, L$. The expression of (8) is given by Jones[9]. The reader is referred to the works of Saraph[10] and Berrington *et al*[11] for details on the set of UCL programs used here to evaluate the reduced matrix elements.

3. THE INITIAL C^{2+} WAVEFUNCTIONS

Using the program of Eissner and Nussbaumer[12], the $P_{n\ell}$ radial functions 1s, 2s, 2p are determined from the minimisation of $E(1s^22s)+$ $+\,3E(1s^22p)$. We obtain the values $\lambda_s = 1.240$ and $\lambda_p = 0.876$ for the C^{3+} scaling parameters. The 2s-2p threshold energy is 0.5859 Ryd, which compares well with the experimental value 0.5883.

3.1 - $2s2p\ {}^1P^0$

Theexpansion in eq.(3) is limited to two terms: $1s^22s$ and $1s^22p$. This leads to a three channel problem ($1s^22s;kp$, $1s^22p;k's+k'd$) involving a bound channel $1s^22s2p$. We obtain -2.5637 Ryd with respect to $1s^22s$ for the $2s2p\ {}^1P^0$ energy. The experimental value is -2.586. Here, the closed channels kp, k's and k'd can be considered as acting as 2s3p, 2p3s and 2p3d configurations.

3.2 - "$2p^2$" ${}^1S^e$

Two channels $1s^22s;ks$ and $1s^22p;k'p$ plus two bound channels $1s^22s^2 + 1s^22p^2$ are present. We obtain -1.763 Ryd for the energy with respect to $1s^22s$, the experimental value beiny -1.857. "$1s^22p^2$" ${}^1S^e$ is composed of configurations $1s^22s^2 + 1s^22p^2$ plus the closed channels $1s^22s;3s$ and $1s^22p;3p$.

4. THE FINAL $C^{3+} + e^-$ WAVEFUNCTIONS

The same target are considered for different L^T, S^T and parity values. For the $^1S^e$ photoionisation ($L^T = 0$, \$ = 0, $p = 0$, only the final state $^1P^0$ ($L^T = 1$, $S^T = 0$, $p = 1$) is needed. For the $^1P^0$ initial state, three final states are needed, $L^T = 0,1,2$. Table 1 shows the free channels and bound channels occurring for all these situations.

Table 1 - Final (C^{3+} + e-) state representation. (a) free channels, (b) bound channels. $1s^22s$ and $1s^22p$ are target configurations with $\lambda = 1.240$ and $\lambda_p = 0.876$.

	$^1P^0$	$^1S^e$	$^1P^e$	$^1D^e$
(a)	$1s^22s;kp$ $1s^22p;k's + k'd$	$1s^22s;ks$ $1s^22p;k'p$	$1s^22p;k'p$	$1s^22s;kd$ $1s^22p;k'p + k'f$
(b)	$1s^22s2p$	$1s^22s^2 + 1s^22p^2$	none	$1s^22p^2$

5. PHOTOIONISATION CROSS SECTIONS

5.1 - "$2p^2$" S^e

In the ejected electron energy range (0;0.5859) Ryd a series of narrow resonances $1s^22pn\ell$ ($\ell = 0,2$) appears. The first one at $k_1^2 = 0.05$ Ryd (see fig.1), which can be noted $2p4d$ ($n^* = 4.097$), has a very high maximum, for exarnple $\sigma = 420.86$ Mb at 0.048 Ryd. The profile of this resonance indicates a large value for the q line profile index appearing in the resonance formula of Dubau and Seaton[13]

$$\sigma = \langle\sigma\rangle \frac{(1+\tau)(x+q)^2}{(1+\tau q^2)(1+x^2)} \tag{9}$$

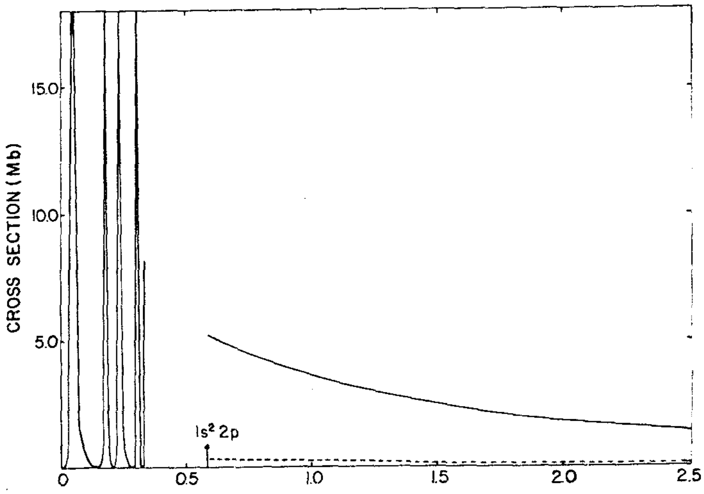

Fig. 1 - $C^{2+}1s^2 2p^{2\,1}S^e$ photoionisation cross section (Mb) as a funtions of the ejected electron energy on channel $1s^2 2s$ (Ryd). —— total cross section. --- to $1s^2 2s$ cross section.

$$x = \tan[\pi(\nu+\alpha)]/\tau \quad , \quad \tau = \tanh(\pi\beta) \quad , \quad \nu = z/k_2 \qquad (10)$$

$n^* = n-a$ is the effective quantum number for the 2p4d state, and $\tau = \tanh \pi\beta$. $<\sigma>$ is the mean value over the resonance. The full autoionisation width at half-maximum Γ is given by

$$\Gamma = 2z^2 \beta/(n-\alpha)^3 \text{ a. u.} \qquad (11)$$

We find q = 67.0, Γ = 0.00148 a.u. and $<\sigma>$ = 6.0 Mb. The second resonance at 0.18 corresponds to 2p5s (n^* = 4.708) and we find q = 15.0, Γ = 0.00520 a.u. and $<\sigma>$ = 0.8 Mb. At 0.240 and 0.345 are the 2p5d and 6d terms. At 0.310 the 2p6s term is present. Above the threshold $1s^2 2p$, we obtain the three channel contributions. Obviously photoionisation of "$2p^2$" $^1S^e$ leads mainly to $1s^2 2p$ with the largest contribution coming from the d channel (90%). Nevertheless the $1s^2 2s$

exit is, near the threshold, 7% of the total cross section. For an ejected electron energy k_0^2 = 4.0 Rydberg this latter value is 11.46%. For the two extreme k_0^2 values (0.6 and 4.0 Rydbergs) the cross section values are 5.154 and 0.606 Mb. The decrease is approximately $\nu^{-2.3}$.

5.2 - 2s2p $^1P^0$

The situation is far more complicated, the final states needed are $^1S^e$, $^1P^e$ and $^1D^e$. For $^1P^e$ only the 2p,kp channel exists, i.e. this partial photoionisation cross section appears only for $k^2 > 0.5859$ Rydbergs (fig.2). $^1S^e$ has two channels and $^1D^e$ three channels (table 1). The 2pnp resonances (fig.3) are narrow and their maximum is 0.7 Mb localised at: 0.045, 0.236, 0.342 Rydbergs.. For $^1D^e$ two series of resonances ap-

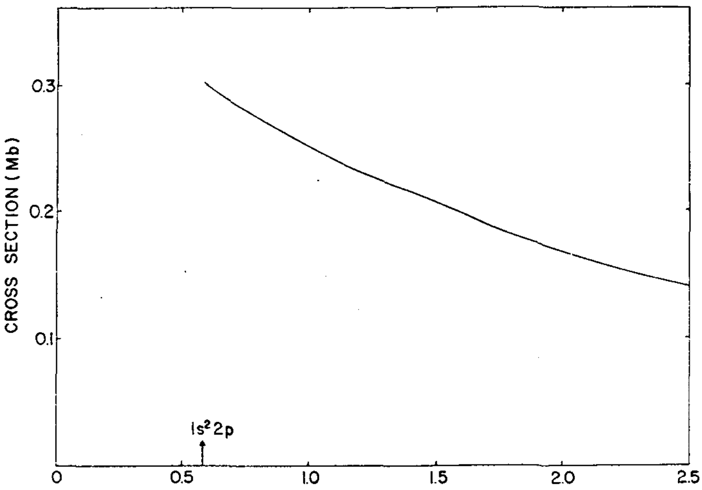

Fig.2 - C^{2+} $1s^2 2s2p$ $^1P^0$ photoionisation cross section (Mb) as function of the ejected electron energy on channel $1s^2 2s$ (Ryd). — $(C^{3+}+e^-)\,^1P^e$ contribution to the total cross section. Only photoionisation to $1s^2 2p$ is possible.

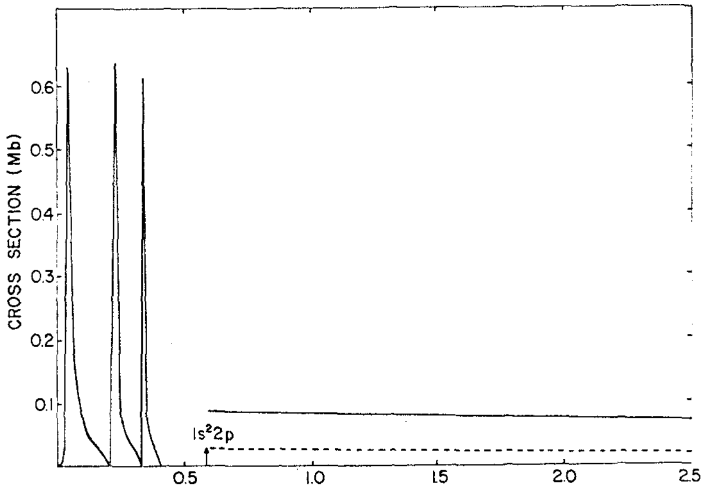

Fig.3 - $C^{2+}1s^22s2p\ ^1P^0$ photoionisation cross section (Mb) as a function of the ejected electron energy on channel $1s^22s$ (Ryd). — $(C^{3+}-e^-)\ ^1S^e$ contribution to the total cross section. --- to $1s^22s$ partial contribution. For the two first resonances we find for q, α, β, $<\sigma>$ respectively: (2.7, -0.062, 0.026, 0.115) and (2.7, -0.058, 0.027, 0.116).

pear, 2pnp and 2pnf (fig.4). The f resonances are very narrow; 2p4f appears at 0.033 Rydbergs. The p ones are larger and arise at 0.212, 0.328, 0.396. Above the 2p threshold, for k_0^2 = 0.6 Rydbergs, the contributions kd, k'f and k'p are respectively 1.038, 0.133, 0.745 (total 1.796 Mb) and for k_0^2 = 3.0 we obtain 0.190, 0.0079, 0.925 Mb. The total threshold cross section just above 2p is 2.189 Mb. It is important to note that the 2s and 2p electrons participate in the total cross section above k^2 = 0.589; this has been overlooked in the work of Sakhibullin and Willis[14].

CONCLUSION

The close coupling method allows an accurate description of the free wave functions representing the channels of the ejected electron

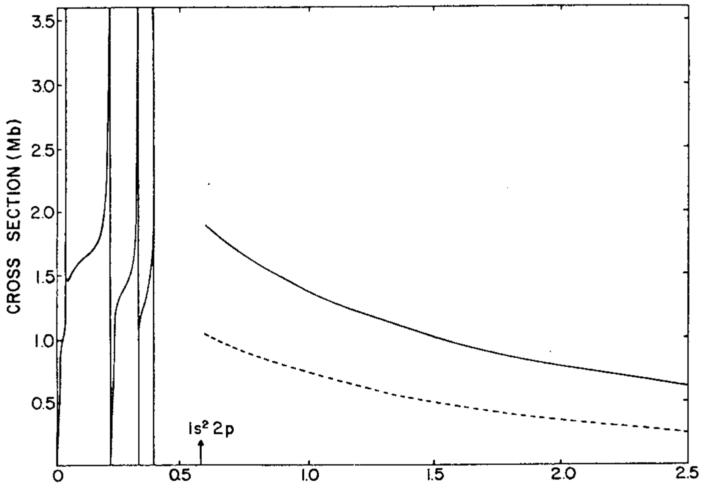

Fig.4 - $C^{2+}1s^22s2p\ ^1P^0$ photoionisation cross section (Mb) as a function of the ejected electron energy on channel $1s^22s$ (Ryd). — $(C^{3+}+e^-)\ ^1D^e$ contribution to the total cross section. --- to $1s^22s$ partial contribution.

which can leave C^{3+} either in the ground term $1s^22s$ or in the $1s^22p$ term. The core relaxation is taken into account since the initial term $^1S^e$ for example, can be written as $1s^22s^2 + 1s^22p^2$ plus closed channels $1s^22s$; vs and $1s^22p$; vp. The photoexcitation to the resonant terms $1s^22pn\ell$ followed by autoionization cannot be ignored as it increases the $1s^22s$ photoionisation. The coupling between the free final channels is taken into account and represents the C^{3+} inelastic excitation induced by the ejected electron. This latter effect is mixed with the direct ionisations, since both "$2p^2$" and 2s2p can undergo $1s^22s$ and $1s^22p$ ionisations. It would be of great interest to consider this shake-up process for the 2s photoionisation of Na and Mg, where the 3s → 3p excitation can be significant for low ejected electron energies.

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Resumo

São calculadas as secções de fotoionização dos estados $1s^22s2p\,^1P^0$ e $1s^22p^2\,^1S^e$ do C^{2+}. O método de acoplamento forte é usado para se obter as funções de onda dos estados inicial (C^{2+}) e final (C^{3+} + e-). As séries $1s^22pn\ell$ dos termos autoionizantes dão origem às ressonâncias nas secções de fotoionização.