J. Phys. B: At. Mol. Phys. **14** (1981) 2069–2080. Printed in Great Britain

Polarisation propagator study of the electron impact excitation of the beryllium isoelectronic sequence

A Allouche and F Marinelli

Laboratoire de Chimie Théorique, Université de Provence, 13331 Marseille Cedex 3, France

Received 12 November 1980, in final form 19 February 1981

Abstract. The second-order polarisation propagator approximation has been used to calculate the generalised oscillator strength $f(K)$ for the $^1S \rightarrow {}^1P$ transitions of B II, C III, N IV and O V. The inelastic electron scattering cross section has been deduced for incident energies from 50 to 1000 eV. The results are compared with experimental ones and other calculations.

1. Introduction

Over the past few years, some methods have been proposed for the determination of dynamical properties of atoms and molecules, for example, McKoy's method for the equation of motion (see, for example, McCurdy *et al* 1977), the time dependent Hartree–Fock method (Jamiesson 1973) and the polarisation propagator method (Oddershede 1978).

Our interest in the particle–hole Green's function lies in the great variety of physical processes that can be described: excitation energies, optical oscillator strength (OOS), radiative lifetimes, polarisabilities, inelastic electron impact cross section, generalised oscillator strength (GOS) etc.

The knowledge of the GOS $f_n(K)$ is required in diverse research fields such as plasma physics, atmospheric physics and astrophysics. In this work, the study executed on the beryllium atom (Allouche *et al* 1980) is extended to the series of its isoelectronic ions.

2. Theory

2.1. The second-order polarisation propagator approximation (SOPPA)

In the notation of the super operator formalism (Goscinsky *et al* 1970, Pickup and Goscinski 1973) the spectral representation of the polarisation propagator is

$$\langle\langle b; b^\dagger \rangle\rangle_E = (b^\dagger | (E\hat{I} - \hat{H})^{-1} | b^\dagger). \tag{1}$$

The operators $\{a_i^\dagger a_j\} = \{b_k^\dagger\} = b^\dagger$ are arranged in a spin row vector and the adjoint operators b are correspondingly arranged in a super column vector. $a_i^\dagger$ and a_j denote spin orbital creation and annihilation operators.

0022-3700/81/122069+12$01.50

An operator space X with elements $\{X_k\}$ is introduced in which the super operators $\hat{H}$ and $\hat{I}$ are defined by

$$\hat{I}X_k = X_k \tag{2}$$

$$\hat{H}X_k = [H, X_k] \tag{3}$$

and in which the scalar product is given by

$$(X_k|X_j) = \langle 0|[X_k^\dagger, X_j]|0\rangle. \tag{4}$$

Introducing the inner projection of the operator resolvent (Löwdin 1965a) $(EI-H)^{-1}$ gives

$$\langle\langle b; b^\dagger\rangle\rangle = (b|h)(h|E\hat{I}-\hat{H}|h)^{-1}(h|b) \tag{5}$$

where $|h)$ is a basis of projectors. A given order of approximation for the polarisation propagator will be obtained according to the choice of the basis $|h)$. In order to obtain the propagator consistent up to second order in electron repulsion, this basis must be

$$|h) = \{a_2|a_4\} \tag{6}$$

with

$$a_2 = a_i^\dagger a_j \tag{7a}$$

$$a_4 = a_i^\dagger a_j^\dagger a_k a_l. \tag{7b}$$

In terms of orthogonalised components, it becomes

$$|h) = \{h_2|h_4\} \tag{8a}$$

$$h_2 = a_2(a_2|a_2)^{-1/2} \tag{8b}$$

$$f_4 = a_4 - h_2(h_2|a_4) \tag{8c}$$

$$h_4 = f_4(f_4|f_4)^{-1/2}. \tag{8d}$$

The expression for the propagator is truncated to second order in electron repulsion

$$\langle\langle b; b^\dagger\rangle\rangle_E = \{(b^\dagger|h_2), (b^\dagger|h_4)\}\begin{Bmatrix} Q & R \\ T & U \end{Bmatrix}^{-1}\begin{Bmatrix} (h_2|b^\dagger) \\ (h_4|b^\dagger) \end{Bmatrix} \tag{9a}$$

with

$$Q = (h_2|E\hat{I}-\hat{H}|h_2) \tag{9b}$$

$$R = T^\dagger = (h_2|E\hat{I}-\hat{H}|h_4) \tag{9c}$$

$$U = (h_4|E\hat{I}-\hat{H}|h_4). \tag{9d}$$

The partitioning of the inverse matrix (Löwdin 1963) leads to

$$\langle\langle b; b^\dagger\rangle\rangle_E = \tilde{1}\{Q - R^\dagger U^{-1} R\}\tilde{1}. \tag{10}$$

Restricting $|b)$ to include only particle–hole-type excitations $q^\dagger$ and hole–particle-type excitations q, the propagator in components form can be written as

$$\begin{Bmatrix} \langle\langle q; q^\dagger\rangle\rangle & \langle\langle q; q\rangle\rangle \\ \langle\langle q^\dagger; q^\dagger\rangle\rangle & \langle\langle q^\dagger; q\rangle\rangle \end{Bmatrix} = \begin{Bmatrix} 1 & 0 \\ 0 & -1 \end{Bmatrix}\begin{Bmatrix} (q^\dagger|\hat{P}|q^\dagger) & (q^\dagger|\hat{P}|q) \\ (q|\hat{P}|q^\dagger) & (q|\hat{P}|q) \end{Bmatrix}^{-1}\begin{Bmatrix} 1 & 0 \\ 0 & -1 \end{Bmatrix} \tag{11}$$

where $\hat{P}$ is the super operator defined by Jorgensen (1977). Next, the inverse matrix in (11) is partitioned

$$\begin{Bmatrix} \langle\langle q; q^\dagger \rangle\rangle & \langle\langle q; q \rangle\rangle \\ \langle\langle q^\dagger; q^\dagger \rangle\rangle & \langle\langle q^\dagger; q \rangle\rangle \end{Bmatrix} = \begin{Bmatrix} E1 - A - \tilde{C}(E1-D)^{-1}C & -B \\ -B & -E1 - A - \tilde{C}(-E1-D)^{-1}C \end{Bmatrix}^{-1} \tag{12}$$

where the matrices A, B, C and D are defined as

$$A = (h_2^\dagger | \hat{H} | h_2^\dagger) \tag{13a}$$

$$B = (h_2 | \hat{H} | h_2^\dagger) \tag{13b}$$

$$C = (h_4^\dagger | \hat{V} | h_2^\dagger) \tag{13c}$$

$$D = (h_4^\dagger | \hat{H} | h_4^\dagger) \tag{13d}$$

$$\hat{V} = \tfrac{1}{4} \sum_{ijkl} (ik \| jl) a_i^\dagger a_j^\dagger a_l a_k - \sum_{\alpha ij} (\alpha\alpha \| ij) a_i^\dagger a_j. \tag{14}$$

i, j, k, l refer to unspecified spin orbitals, greek letters to spin orbitals which are occupied in the HF ground state and m, n to unoccupied HF spin orbitals

$$(ij \| kl) = (ij|kl) - (il|kj). \tag{15}$$

The ground state is described by the first-order Rayleigh–Schrödinger perturbation of the HF wavefunction (Löwdin 1965b)

$$|0\rangle = (1 + K)|\text{HF}\rangle \tag{16}$$

$$K = \sum_{\substack{\alpha\beta \\ mn}} \frac{(n\alpha|m\beta) - (n\beta|m\alpha)}{\varepsilon_m + \varepsilon_n - \varepsilon_\alpha - \varepsilon_\beta} a_n^\dagger a_m^\dagger a_\alpha a_\beta. \tag{17}$$

The A and B matrices must be calculated to second order, the C matrix to first order, and the D matrix to zero order.

The time dependent Hartree–Fock theory (TDHF) is the first-order approximation of the polarisation propagator. Hence, the ground state is merely described by the HF ground state, the projector basis $|h)$ in equation (8a) is confined to $\{h_2\}$. The A and B matrices are calculated to first order in electron repulsion and C and D vanish. The TDHF is closely related to the random phase approximation (RPA) of McKoy and co-workers (McCurdy *et al* 1977). The substitution of $(-E1-D)^{-1}$ by $(E1-D)^{-1}$ in (12) allows us to obtain the TDHF form and corresponds only to a third-order correction (Oddershede *et al* 1977). This leads to the resolution of a non-Hermitian matrix

$$\langle\langle b; b^\dagger \rangle\rangle_E = \begin{Bmatrix} E1 - A - \tilde{C}(E1-D)^{-1}C & -B \\ -B & -E1 - A - \tilde{C}(E1-D)^{-1}C \end{Bmatrix}. \tag{18}$$

The propagator is solved for different E values and gives the representation

$$\langle\langle b; b^\dagger \rangle\rangle_E = \begin{Bmatrix} Z(E) & Y(E) \\ Y(E) & Z(E) \end{Bmatrix} \begin{Bmatrix} (E1 - \omega(E))^{-1} & 0 \\ 0 & -(E1 + \omega(E))^{-1} \end{Bmatrix} \begin{Bmatrix} Z^\dagger(E) & Y^\dagger(E) \\ Y^\dagger(E) & Z^\dagger(E) \end{Bmatrix}. \tag{19}$$

$Z(E)$ and $Y(E)$ are eigenvectors of (18) while $\omega(E)$ is the vector collecting the corresponding eigenvalues.

The excitation energies are obtained at poles when $E1 = \pm\omega(E)$. The residue $\mathrm{Res}(E_n)$ for a pole is

$$\mathrm{Res}(E_n) = \begin{Bmatrix} \Gamma_n Z(E_n) Z^{\dagger}(E_n) & \Gamma_n Y(E_n) Z^{\dagger}(E_n) \\ \Gamma_n Z(E_n) Y^{\dagger}(E_n) & \Gamma_n Y(E_n) Y^{\dagger}(E_n) \end{Bmatrix} \tag{20}$$

where

$$\Gamma_n^{-1} = \left(1 - \frac{\mathrm{d}}{\mathrm{d}E}\omega_n(E)\right)_{E=E_n}. \tag{21}$$

The matrix element between an excited state $|n\rangle$ and the ground state $|0\rangle$ of a mono-electronic operator M is given as

$$|\langle 0|M|n\rangle|^2 = \sum_{\substack{i(m\gamma) \\ j(p\delta)}} \langle p|M|\delta\rangle (Z(E_n)_{jn} Z^{\dagger}(E_n)_{ni} + Y(E_n)_{jn} Y^{\dagger}(E_n)_{ni}$$
$$+ 2Z(E_n)_{jn} Y^{\dagger}(E_n)_{ni}) \langle m|M|\gamma\rangle \Gamma_n. \tag{22}$$

In practice, we proceed as follows: (i) HF calculation using a STO basis, (ii) TDHF calculation which gives a starting value of E and (iii) resolution of the SOPPA equation (18).

2.2. Inelastic scattering in the first Born approximation (FBA)

The differential Born cross section for a transfer momentum K is written in terms of the GOS $f_n(K)$ (Inokuti 1971)

$$\frac{\mathrm{d}\sigma_n}{\mathrm{d}\Omega} = \frac{2|k_f| f_n(K)}{K^2 |k_i| E_n}. \tag{23}$$

k_f and k_i are the scattered and incident electron momentum, respectively. The mathematical definition of the GOS is

$$f_n(K) = \frac{2E_n}{K^2} \left| \left\langle n \right| \sum_{j=1}^{Z} \exp(\mathrm{i}K \cdot r_j) \left| 0 \right\rangle \right|^2. \tag{24}$$

The evaluation of these integrals using Slater-type orbitals is described elsewhere (Guidotti *et al* 1979).

For $K \to 0$, the expression of $f_n(K)$ reduces to those of the OOS in its length approximation

$$F_n = \tfrac{2}{3} |\langle 0|r|n\rangle|^2 E_n. \tag{25}$$

When the FBA holds, Lassettre (1965) has shown that physically, when K approaches zero, the GOS $f_n(K)$ approaches the OOS independently calculated using formula (25).

As it is proved by Vriens and Carriere (1970) the GOS can be expanded into a K^2 polynomial

$$f_n(K) = \sum_{\nu=0}^{N} b_\nu K^{2\nu}. \tag{26}$$

This expression is well adapted to obtain the GOS limit when K tends to zero and to deduce the integrated cross section

$$\sigma_n = \frac{1}{2E_nE_i}\int_{x_-}^{x_+} f_n(x)\frac{dx}{x} \tag{27a}$$

with

$$x = K^2 \tag{27b}$$

$$x_-^+ = 2E_i[1 \pm (1 - E_n/2E_i)^{1/2}]^2. \tag{27c}$$

E_i is the kinetic energy of the incident electron.

3. Results and discussion

3.1. Transition energies and OOS

Dynamical quantities are very sensitive to correlation effects (Banyard and Taylor 1974). The SOPPA introduces them, firstly by the Rayleigh–Schrödinger correction to the Hartree–Fock wavefunction, and secondly, A and B matrices represent an interaction between excited states and C and D a perturbation caused by the $2p-2h$ terms. The HF calculations were performed using a basis of 33 s and p Slater-type orbitals.

For the poles search, we adopted an iterative procedure: the starting value of E, introduced in the $2p-2h$ part of equation (18), is taken from our TDHF calculation (table 1). Convergency is quickly reached, generally after two or three iterations. The gain in energy is 0.3–0.4 eV, with respect to the starting value. The ratio

Table 1. A comparison of present results for $2s^2\ ^1S \rightarrow 2snp\ ^1P$ excitation energies for the Be isoelectronic sequence with other theoretical and experimental values (au).

	n	SOPPA	TDHF[a]	Numerical TDHF[b]	Experimental[c]
B II					
	2	0.318 96	0.309 22	0.306 33	0.334 32
	3	0.642 12	0.628 22	0.623 51	0.656 38
	4	0.766 77	0.755 24		
C III					
	2	0.439 38	0.428 05	0.424 59	0.466 21
	3	1.190 44	1.175 48	1.141 97	1.179 43
	4	1.39? 03	1.382 62		1.468 55
N IV					
	2	0.556 10	0.543 89		0.595 32
	3	1.818 93	1.798 02		1.842 59
	4	2.277 30	2.263 59		2.309 48
O V					
	2	0.670 29	0.657 32		0.723 32
	3	2.625 64	2.602 99		2.645 66
	4	3.284 96	3.267 39		3.361 06

[a]This work.
[b]Stewart (1975).
[c]Moore (1949).

Table 2. A comparison of present values for the optical oscillator strengths F_n for the $2s^2\ ^1S \rightarrow 2snp\ ^1P$ of Be-like ions.

	n	SOPPA	Numerical TDHF[a]	IPM[b]	Restricted HF[c]	Correlated HF[d]	Experimental		
B II									
	2	1.0161	1.004	1.0166	1.495	0.9335	0.83 ± 0.09[e]	0.73 ± 0.07[f]	0.9 ± 0.2[g]
	3	0.0629	0.0908	0.1110	0.0256				
	4	0.0172	0.0390	0.0455					
C III									
	2	0.8326	0.749	0.8427	1.113	0.6974	0.65 ± 0.03[h]		
	3	0.0973	0.223	0.2127	0.166				
	4	0.0036	0.0775	0.0749					
N IV									
	2	0.6037	0.596	0.7032		0.5605			
	3	0.1743	0.323	0.3007					
	4	0.0774	0.104	0.0973					
C V									
	2	0.5144	0.495	0.5929	0.742	0.4697	0.42 ± 0.05[i]		
	3	0.3081	0.400	0.3744	0.371				
	4	0.0734	0.121	0.1144					

[a] Stewart (1975).
[b] Ganas and Green (1979).
[c] Froese (1967).
[d] Banyard and Taylor (1974).
[e] Bromander *et al* (1969).
[f] Martinson *et al* (1970).
[g] Lawrence and Savage (1966).
[h] Heroux (1969).
[i] Martinson *et al* (1971).

E_n(SOPPA)/E_n(exp) is about 95% for the 2s2p ^{1}P transition and 98% for the others except for the C III 2s3p ^{1}P transition for which the SOPPA value is less accurate than the corresponding TDHF.

The second order of approximation generally notably improves the energy as shown by the comparison with the TDHF results of Stewart (1975) and Arrighini *et al* (1973). Nevertheless this has a little repercussion on the OOS values (table 2).

The OOS values of the transition $2s^2 \rightarrow 2s2p$ are very close to the experimental results. The lack of available experimental data for the other transitions does not allow a comparison. The comparison with Froese's (1967) HF results brings out the correlation effects.

Using the OOS, we can compute the radiative lifetimes. The SOPPA does not introduce the evaluation of transition momentum between excited states, and thus only radiative lifetimes τ of the first excited state are determined

$$\tau = h^4 c^3 / 2E_n^2 F_n. \tag{28}$$

The values in table 3 have been extracted from table 2 and some others given by Hibbert (1974).

Table 3. Radiative lifetimes for the $2s^2\ ^1S \rightarrow 2s2p\ ^1P$ transitions of Be-like ions (10^{-9} s).

	SOPPA	Numerical TDHF[a]	Experimental	HF + CI[g]
B II	0.90	0.99	1.01 ± 0.12[b]	0.77
			1.14 ± 0.1[c]	
			0.93 ± 0.17[d]	
C III	0.58	0.69	0.66 ± 0.03[e]	0.52
N IV	0.40			0.41
O V	0.50		0.42 ± 0.04[f]	0.33

[a] Stewart (1975).
[b] Bromander *et al* (1969).
[c] Martinson *et al* (1970).
[d] Lawrence and Savage (1966).
[e] Heroux (1969).
[f] Martinson *et al* (1971).
[g] Hibbert (1974).

3.2. GOS and inelastic cross sections

Table 4 collects GOS for some K^2 values and 2s2p transitions. The extrapolated GOS ($K \rightarrow 0$) coincides exactly with the calculated OOS (table 2).

In their work, Banyard and Taylor (1974) have adopted besides the usual definition of $f_n(K)$ (equation (9)) two other ones denoted V1 and V2 written:

$$f_n^{V1}(K) = \frac{1}{2K^2 E_n}\left(K^2\left\langle\Psi_n\middle|\sum_{j=1}^{Z}\exp(\mathrm{i}\,Kz_j)\middle|\Psi_0\right\rangle - 2\mathrm{i}\,K\left\langle\Psi_n\middle|\sum_{j=1}^{Z}\exp(\mathrm{i}\,Kz_j)\partial/\partial z_j\middle|\Psi_0\right\rangle\right)^2 \tag{29}$$

$$f_n^{V2}(K) = -\frac{8E_n}{(2E_n + K^2)^2}\left(\left\langle\sum_{j=1}^{Z}\exp(-\mathrm{i}\,Kz_j)\partial\Psi_n/\partial z_j\middle|\Psi_0\right\rangle\right)^2. \tag{30}$$

Our table 4 can be compared with Banyard's table 1. Our values are found to be a little above his in the range of small momentum transfers. But we must notice that Banyard's results are an average over his L, V1 and V2 definitions of the GOS.

Table 4. Generalised oscillator strengths for the $2s^2\ ^1S \rightarrow 2s2p\ ^1P$ transition of Be-like ions.

K^2 (au)	B II	C III	N IV	O V
0.0	1.0161	0.8326	0.6037	0.5144
0.06	0.9335	0.7977	0.5902	0.5059
0.1	0.8831	0.7753	0.5814	0.5003
0.2	0.7608	0.7172	0.5578	0.4852
0.3	0.6760	0.6732	0.5392	0.4732
0.4	0.5949	0.6279	0.5192	0.4603
0.6	0.4654	0.5470	0.4817	0.4356
0.8	0.3684	0.4776	0.4469	0.4122
1.0	0.2946	0.4178	0.4148	0.3903
1.5	0.1746	0.3018	0.3448	0.3408
2.5	0.0685	0.1634	0.2399	0.2610
3.5	0.0296	0.0924	0.1688	0.2012
5.0	0.0095	0.0419	0.1018	0.1378
6.0	0.0047	0.0256	0.0737	0.1079
7.0	0.0024	0.0160	0.0538	0.0849
8.0	0.0012	0.0101	0.0397	0.0672
9.0	0.0006	0.0066	0.0295	0.0534
10.0	0.0003	0.0043	0.0220	0.0427
12.0	0.0001	0.0018	0.0125	0.0276

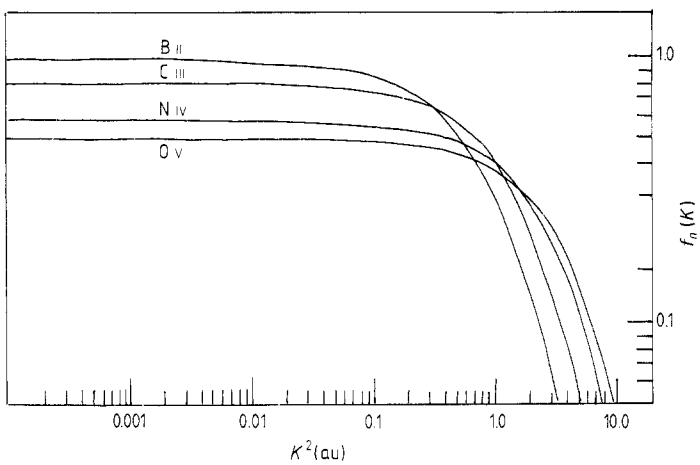

Figure 1. Generalised oscillator strengths for the $2s^2\ ^1S \rightarrow 2s2p\ ^1P$ transition of Be-like ions.

Figure 2 shows the profile of the B II GOS for three transitions studied. Similar curves have been drawn for the other ions. In the case of C III, N IV and O V, the 2s3p transition curve presents a node analogous to the B II 2s4p transition. In every event of nodal structure, the second maximum is below the first, as also occurs in Ganas and Green's (1979) work. The integrated cross section is calculated with the help of equation (27*a*) until an x value is obtained for which $f_n(x)$ reaches a non-significant level.

Figures 3 and 4 show the behaviour of the integrated cross sections. In table 5, our numerical values for the 2s2p transition are compared with those of Ganas calculated

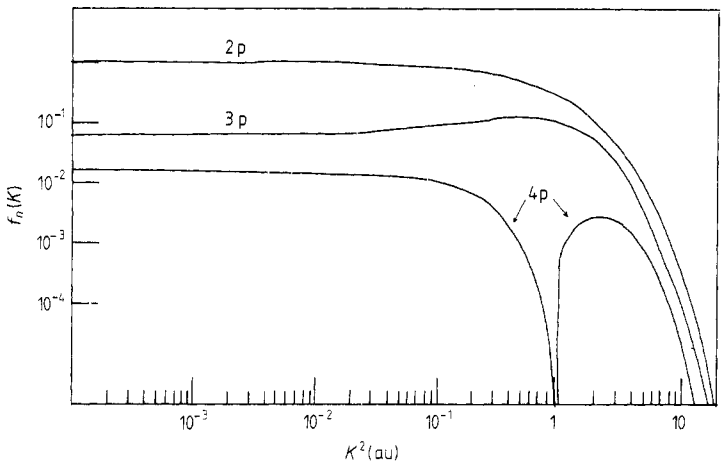

Figure 2. Generalised oscillator strengths for the $2s^2\ ^1S \rightarrow 2snp\ ^1P$ transitions of B II.

Table 5. Inelastic electron scattering cross section σ (measured in units of 10^{-16} cm^2) for the $2s^2\ ^1S \rightarrow 2s2p\ ^1P$ transition for Be-like ions.

	B II		C III		N IV		O V	
E_i (eV)	a	b	a	b	a	b	a	b
50	6.4655	6.7076	3.7482	4.0958	2.2334	2.7582	1.5435	1.9830
100	3.7803	3.8340	2.2378	2.3411	1.3182	1.5766	0.9106	1.1335
150	2.7325	2.7446	1.6206	1.6759	0.9549	1.1286	0.6639	0.8114
200	2.1636	2.1591	1.2805	1.3184	0.7549	0.8878	0.5262	0.6383
250	1.8018	1.7899	1.0673	1.0930	0.6272	0.7360	0.4379	0.5292
300	1.5531	1.5342	0.9144	0.9368	0.5391	0.6309	0.3764	0.4536
400	1.2257	1.2011	0.7212	0.7334	0.4235	0.4939	0.2958	0.3551
600	0.8697	0.8483	0.5097	0.5180	0.3005	0.3488	0.2098	0.2508
800	0.6806	0.6615	0.4034	0.4039	0.2352	0.2720	0.1643	0.1956
1000	0.5621	0.5449	0.3340	0.3327	0.1948	0.2241	0.1356	0.1611

a This work.
b Ganas and Green (1979).

Table 6. Inelastic electron scattering cross section σ (measured in units of 10^{-17} cm^2) for the $2s^2\ ^1S \rightarrow 2snp\ ^1P$ transition for Be-like ions.

E_i (eV)		B II	C III	N IV	O V
100	2s3p	1.7558	0.3585	0.2661	0.2484
	2s4p	0.1123	0.0173	0.0771	0.0427
200	2s3p	0.9715	0.2427	0.2089	0.2145
	2s4p	0.0758	0.0114	0.0629	0.0392
300	2s3p	0.6810	0.1877	0.1702	0.1798
	2s4p	0.0579	0.0086	0.0523	0.0333
600	2s3p	0.3686	0.1177	0.1117	0.1223
	2s4p	0.0352	0.0052	0.0354	0.0228
1000	2s3p	0.2337	0.0806	0.0793	0.0877
	2s4p	0.0239	0.0035	0.0025	0.0165

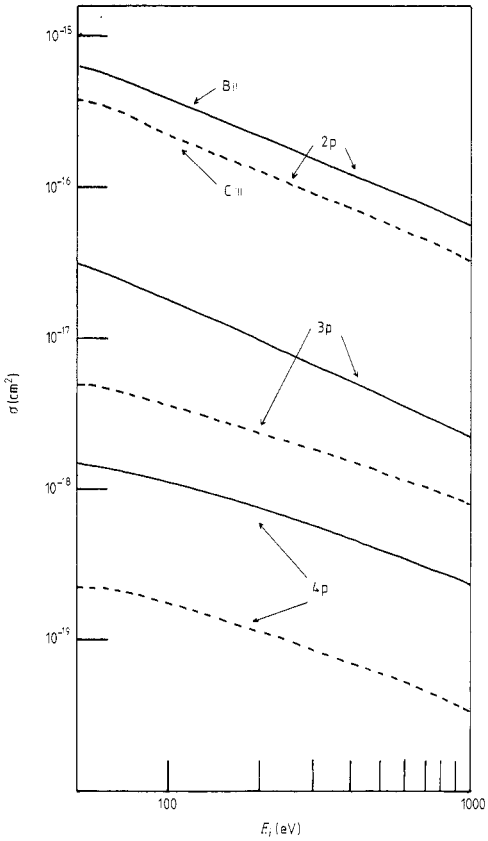

Figure 3. Integrated cross section for B II and C III.

using his formula (22). This formula is deduced from an analytical atomic independent model potential adjusted to experimental energy levels. The agreement between the two sets of results is found to be excellent.

This trend is less satisfactory concerning the other excitations. Nevertheless, according to Ganas, his formula is strictly applicable beyond 500 eV, with a precision of 10%. In fact the excitation thresholds become so large that the domain for a good application of FBA is higher in energy and consequently all these results are only indicative.

4. Conclusion

The primary purpose of this work has been to apply the polarisation propagator model to the study of the electron impact excitation of the isoelectronic sequence B II, C III, N IV, O V and its corresponding properties.

The correlation factor is found to be essential for the description of these phenomena, as indicated by the inaccuracy of the Hartree–Fock calculation. However, the polarisation propagator method improves upon the HF approach by introducing the effect of correlation in both the initial and excited states.

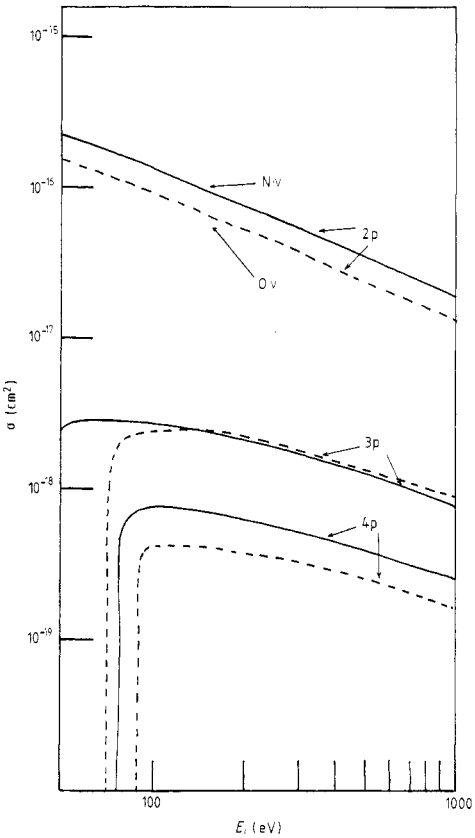

Figure 4. Integrated cross section for N IV and O V.

At the first order of approximation (TDHF) the final state is generated by single-particle excitation from the HF determinant and by de-excitation from doubly excited components. In addition to that, in the SOPPA the ground-state correlation is explicitly introduced by the Rayleigh–Schrödinger perturbation. The correlation of the excited states is better described by the contribution of the energy dependent part arising from the two-particle–two-hole components of the projector manifold $|h)$.

References

Allouche A, Marinelli F and Arrighini G P 1980 *Chem. Phys. Lett.* **76** 333–6
Andersen T, Jessen K A and Sorensen G 1969 *Phys. Rev.* **188** 76–81
Arrighini G P, Biondi F and Guidotti C 1973 *Chem. Phys.* **2** 85–94
Banyard K E and Taylor G K 1974 *Phys. Rev.* A **10** 1019–27
Bromander J, Buchta R and Lundin L 1969 *Phys. Lett.* **29A** 523–4
Froese C 1967 *J. Chem. Phys.* **47** 4010–5
Ganas P S and Green A E S 1979 *Phys. Rev.* A **19** 2197–205
Goscinski O and Lükman B 1970 *Chem. Phys. Lett.* **7** 573–6
Guidotti C, Arrighini G P and Marinelli F 1979 *Theor. Chim. Acta* **53** 165–73
Heroux L 1969 *Phys. Rev.* **188** 1–5
Hibbert A 1974 *J. Phys. B: At. Mol. Phys.* **7** 1417–34

Inokuti M 1971 *Rev. Mod. Phys.* **43** 297–345
Jamieson M J 1973 *Wave Mechanics—The First Fifty Years* ed Price, Chessick and Ravensdale (London: Butterworth)
Jorgensen P 1975 *Ann. Rev. Phys. Chem.* **26** 259–80
Lassettre E N 1965 *J. Chem. Phys.* **43** 4479–86
Lawrence G M and Savage B D 1966 *Phys. Rev.* **141** 67–70
Löwdin P O 1963 *J. Mol. Spectrosc.* **10** 12–23
—— 1965a *Phys. Rev.* **139** A537–72
—— 1965b *J. Math. Phys.* **6** 1341–53
McCurdy C W Jr, Rescigno T N, Yeager D L and McKoy V 1977 *Modern Theoretical Chemistry* vol 3, ed Miller, Schaefer, Berne and Segal (New York: Plenum)
Martinson I, Berry H G, Bickel W S and Oona H 1971 *J. Opt. Soc. Am.* **61** 519–23
Martinson I, Bickel W S and Olme A 1970 *J. Opt. Soc. Am.* **60** 1213–20
Moore C E 1949 *Atomic Energy Levels* NBS 1
Oddershede J 1978 *Adv. Quantum Chem.* **11** 275–352
Oddershede J and Jorgenson P 1977 *J. Chem. Phys.* **66** 1541–56
Oddershede J, Jorgensen P and Beebe N H F 1977 *Int. J. Quantum Chem.* **12** 655–70
Pickup B T and Goscinski O 1973 *Mol. Phys.* **26** 1013–35
Stewart R F 1975 *J. Phys. B: At. Mol. Phys.* **8** 1–10
Vriens L and Carriere J O 1970 *Physica* **49** 517–31