Electron-impact excitation of the beryllium isoelectronic sequence

P. S. Ganas* and A. E. S. Green
University of Florida, Gainesville, Florida 32611
(Received 11 October 1978)

An analytic atomic independent-particle model potential adjusted to experimental energy levels is used to generate wave functions for the excited states of Be I, B II, C III, N IV, and O V. Using these wave functions in conjunction with the Born approximation and the *LS*-coupling scheme, the authors calculate optical oscillator strengths, generalized oscillator strengths, and total cross sections for excitations from the $2s^2(^1S_0)$ ground state. The results are compared with experimental ones and other calculations. Regularities and systematic trends along the isoelectronic sequence are discussed.

I. INTRODUCTION

Atomic oscillator strengths of highly ionized atoms have many important applications. Recent advances in fusion research with magnetically confined plasmas have made possible detailed spectral observations of the plasmas.[1] These investigations have revealed the presence of highly ionized atoms which affect the behavior of the plasma. In astrophysics, the interpretation of the physical conditions in quasars and other nebulae depends on knowledge of the excitation cross sections of various lines. Emission lines corresponding to the resonance transition $2s^2(^1S_0) - 2s2p(^1P_1)$ in the isoelectronic ions C III, N IV, O V have been identified in some stellar objects.[2] Unfortunately there is little experimental information available on important cross sections.

From a theoretical viewpoint the ions of the beryllium sequence plus the incident electron constitute a five-electron system. Techniques for treating many-electron systems rigorously in a systematic fashion have not yet been reduced to practice. For this reason the present theoretical approach exploits a realistic independent-particle-model (IPM) description for arriving at approximate electron-impact cross sections in the Born-Bethe approximation.

In comparison to Hartree-Fock-Slater (HFS) calculations and to experiment, a simple two-parameter IPM potential has been found to provide a good representation of atoms[3-8] and molecules.[9,10]

II. IPM POTENTIALS

The potential for an electron in an atom or ion with nuclear charge Z and number of electrons N is, in atomic units,

$$V(r) = -(2/r)[(Z-\eta)\Omega(r) + \eta], \tag{1}$$

where $\Omega(r)$ is the screening function

$$\Omega(r) = [H(e^{r/d} - 1) + 1]^{-1} \tag{2}$$

and $\eta = Z - N + 1$. The parameters d, H may be adjusted to a selected body of experimental data. This potential is inserted into the radial Schrödinger equation

$$\left(\frac{d^2}{dr^2} - \frac{l(l+1)}{r^2} - V(r) + E_{nl}\right)P_{nl}(r) = 0 \tag{3}$$

to obtain the energy eigenvalues E_{nl} and wave functions $P_{nl}(r)/r$. The parameters d, H are determined by requiring the energy eigenvalues to agree with the experimental energy levels which are obtained from the tables of Moore.[11] The ground state of the Be sequence being a singlet state: $1s^22s^2(^1S_0)$, only singlet states can be reached with a direct interaction. Accordingly we confine our attention to the singlet states of Be I, B II, C III, N IV, O V. By searching over the excited state energies and the 2*s* ground state energy we obtain the parameter values given in Table I. To initiate the search we take as the initial parameter estimates the values obtained by Green, Garvey, and Jackman[8] (GGJ) from the *ab initio* procedure of total-energy minimization. The GGJ parameters are included in Table I for comparison. For all the levels included in the search, the IPM values agree with the experimental values to within 5% in 85% of cases, and to within 2% in 50% of cases. The experimental levels which we have used to determine the potential parameters are the s, p, d, f states having principal quantum number $n \leq 7$, wherever data for such states exist. However, there is a considerable variation in the quantity of experimental data available from one ion to the next. Thus for Be I, B II, C III, N IV, O V the total number of states which we have considered is 14, 8, 18, 9, 16, respectively. We may extend the levels in a given series by using the formula[12]

 ©1979 The American Physical Society

TABLE I. IPM potential parameters.

Atom/ion		This work	GGJ
Be I	d	0.3854	0.7690
	H	0.2396	1.4457
B II	d	0.1967	0.4900
	H	0.1159	1.1824
C III	d	0.1321	0.3600
	H	0.0735	1.0674
N IV	d	0.0994	0.2957
	H	0.0521	1.0394
O V	d	0.0797	0.2454
	H	0.0392	0.9998

$$E_{nl} = -[(Z - s_l)/(n - \delta_l)]^2 \tag{4}$$

where s_l is the screening constant and δ_l is the quantum defect. We find that for a given value of l, all the excited states within the isoelectronic sequence are accurately reproduced by Eq. (4) if the screening constants and quantum defects are chosen as in Table II where it becomes obvious that the screening constant varies only slightly. Therefore it is not unreasonable to define a universal screening constant for the Be sequence. By choosing $s_l = 2.87$ for all l, the "chi squares" of the various fits are not appreciably altered (see Table III). The "chi square" is a measure of the goodness of a fit, and is defined as

$$\chi^2 = \sum_i [w(y - y_c)^2]_i \,. \tag{5}$$

Here y is the experimental or given value, y_c is the calculated value, and w is the weight. We use Poisson weighting $w = y^{-1}$ in all of our searches.

We have found a systematic trend in the behavior of the potential parameters along the isoelectronic sequence. We find that the quantities d^{-1} and H/d have a linear dependence on η. (η is the degree of ionization plus one.) Since $N = 4$, this translates into a linear dependence on Z. These linear dependences may be expressed as

$$d^{-1} = 0.1068 + 2.4885\eta \tag{6a}$$

$$= -7.3587 + 2.4885Z \,, \tag{6b}$$

TABLE II. Screening constants and quantum defects for s, p, d, f excited states of the Be sequence, to be used in Eq. (4).

States	s_l	δ_l	χ^2 ($\times 100$)
s	2.8119	0.1303	1.19
p	2.9241	0.0810	1.19
d	3.0342	0.0337	0.123
f	2.9532	−0.0904	0.473

TABLE III. Quantum defects for s, p, d, f excited states of the Be sequence, to be used in Eq. (4) with a screening constant $s_l = 2.87$ for all l.

States	δ_l	χ^2 ($\times 100$)
s	0.1779	1.53
p	0.0486	1.84
d	−0.1254	3.07
f	−0.1843	0.56

$$H/d = 0.6543 - 0.0326\eta \tag{6c}$$

$$= 0.7521 - 0.0326Z \,. \tag{6d}$$

Similar linear dependences on η have been observed by GGJ for all atoms and ions with $Z \leq 36$.

From the early work of Layzer[13] it is expected that for a fixed transition within an isoelectronic sequence, the transition energies x_t may be expanded as

$$x_t = a_0 Z^2 + a_1 Z + a_2 \,. \tag{7}$$

The coefficient a_0 is zero for "in-shell" transitions (i.e., no change in the principal quantum number.) We have verified that the IPM transition energies conform to Eq. (7). For the principal resonance transition $2s$-$2p$, we set $a_0 = 0$ and vary the two coefficients a_1, a_2 so as to obtain the best fit to the IPM $2s$-$2p$ transition energies along the sequence. For the other transitions $2s$-nl we vary all three coefficients a_0, a_1, a_2. The coefficients which reproduce the transition energies best are given in Table IV.

III. GENERALIZED OSCILLATOR STRENGTHS FORMULATION

We give a brief presentation of the general formulas used in this work. Derivations of these formulas may be found in Ref. 5. We consider the transition of an atom or ion from its ground state to an excited state with momentum transfer $\vec{K}$. We define $x = K^2 a_0^2$, where a_0 is the

TABLE IV. Coefficients a_0, a_1, a_2 to be used in Eq. (7).

$2s$ to	a_0	a_1	a_2	χ^2 ($\times 10^4$)
$2p$	0	0.2321	−0.6587	2.34
$3s$	0.1555	−0.7381	0.9230	1.02
$3p$	0.1553	−0.6744	0.7199	1.22
$3d$	0.1602	−0.6800	0.6990	1.27
$4s$	0.2070	−0.9974	1.2375	0.70
$4p$	0.2039	−0.9359	1.0608	0.094
$4d$	0.2091	−0.9739	1.1408	1.10

Bohr radius and $x_t = W/R$, where W is the transition energy in eV and R is the Rydberg energy. In our discussions of generalized oscillator strengths (GOS) considerable use will be made of the reduced or scaled quantity $\xi = x/x_t$. We suppose that the atom or ion is initially in a state which has quantum numbers L_i, S_i, J_i, M_i. After the active electron has been promoted from a $n_0 l_0$ orbital to a nl orbital, the atom or ion is in a final state which has quantum numbers L_f, S_f, J_f, M_f. Only transitions with $S_f = S_i$ are considered.

By using the first Born approximation and assuming the Russell-Saunders LS-coupling scheme for the initial and final states, it can be shown that the GOS is given by

$$f(x) = \sum_L C_L (2l_0+1)(2l+1)(2L+1)\begin{pmatrix} l_0 & l & L \\ 0 & 0 & 0 \end{pmatrix}^2 S_L^2 , \tag{8}$$

where

$$S_L = \xi^{-1/2} \int_0^\infty P_{n_0 l_0}(r) j_L(Kr) P_{nl}(r)\, dr \tag{9}$$

and

$$C_L = N_0 F^2 (2L_i+1)(2L_f+1)(2J_f+1) \times \begin{Bmatrix} L_f & L & L_i \\ l_0 & L_c & l \end{Bmatrix}^2 \begin{Bmatrix} J_i & L & J_f \\ L_f & S_i & L_i \end{Bmatrix} . \tag{10}$$

The array in the large parentheses in Eq. (8) is a $3j$ symbol, and the arrays in large curly brackets in Eq. (10) are $6j$ symbols.[14] The quantities $P_{n_0 l_0}(r)/r$ and $P_{nl}(r)/r$ are the bound-state radial wave functions for the single-particle excitations, and $j_L(Kr)$ is a spherical Bessel function. The quantity N_0 in Eq. (10) is the number of electrons in the active subshell, and F is the coefficient of fractional parentage[15] for constructing the initial state $(n_0 l_0)^{N_0} S_i L_i$ from the core state $(n_0 l_0)^{N_0 - 1} S_c L_c$ and an $n_0 l_0$ electron.

In the limit as $K \to 0$ the GOS becomes the optical oscillator strength (OOS). The OOS is calculated from[16]

$$f_0 = \tfrac{1}{3} C (2l_0+1)(2l+1)\begin{pmatrix} l_0 & l & 1 \\ 0 & 0 & 0 \end{pmatrix}^2 T^2 , \tag{11}$$

where T is a radial dipole matrix element

$$T = x_t^{1/2} \int_0^\infty P_{n_0 l_0}(r) r P_{nl}(r)\, dr \tag{12}$$

and C is a coefficient

$$C = N_0 F^2 (2L_i+1)(2L_f+1)(2J_f+1) \times \begin{Bmatrix} L_f & 1 & L_i \\ l_0 & L_c & l \end{Bmatrix}^2 \begin{Bmatrix} J_i & 1 & J_f \\ L_f & S_i & L_i \end{Bmatrix}^2 . \tag{13}$$

For the Be sequence we have the assignments $L_i = S_i = J_i = L_c = l_0 = 0, N_0 F^2 = 2$. The $6j$ symbols in Eq. (13) vanish unless the triads $(L_f\ 1\ L_i) = (L_f\ 1\ 0)$ and $(l_0\ 1\ l) = (0\ 1\ l)$ satisfy a triangle condition. This requires that $L_f = l = 1$. Hence the OOS vanishes unless the final atomic state is $2s\,np(^1P_1)$, $n = 2, 3, 4, \ldots$.

IV. RESULTS FOR OOS

The OOS for the Be sequence have been intensively studied theoretically and experimentally, especially the resonance transition $2s^2(^1S_0)$

TABLE V. Comparison between IPM, experimental, HFS, TDHF, and other calculations of OOS for the principal resonance transition $2s^2(^1S_0) \to 2s\,2p(^1P_1)$ of the Be isoelectronic sequence.

Atom/ion	IPM	Expt	HFS	TDHF	Other works
Be I	1.1240	1.21 ± 0.03 [a]	1.317 [b]	1.378 [c]	1.256 [d]
		1.08 ± 0.05 [e]			1.4 [f]
		1.34 ± 0.05 [g]			
B II	1.0166	0.83 ± 0.09 [h]		1.004 [c]	0.94 [f]
		0.73 ± 0.07 [i]			0.985 ± 0.015 [j]
		0.9 ± 0.2 [k]			
C III	0.8427	0.65 ± 0.03 [l]		0.749 [c]	0.73 [f]
N IV	0.7032		0.573 [m]	0.596 [c]	0.61 [f]
O V	0.5929	0.42 ± 0.05 [n]	0.480 [m]	0.495 [c]	0.52 [f]

[a] Reference 17.
[b] Reference 25.
[c] Reference 27.
[d] Reference 28.
[e] Reference 18.
[f] Reference 29.
[g] Reference 19.
[h] Reference 20.
[i] Reference 21.
[j] Reference 30.
[k] Reference 22.
[l] Reference 23.
[m] Reference 26.
[n] Reference 24.

TABLE VI. Results of IPM, HFS, and TDHF calculations of OOS for the transitions $2s^2(^1S_0) \rightarrow 2s\,np\ (^1P_1)$, $3 \leq n \leq 7$, of the Be sequence.

Atom/ion	2s to	IPM	HFS	TDHF
Be I	3p	0.022 0	0.0041 [a]	0.022 7 [b]
	4p	0.013 1	0.0050 [a]	0.001 02 [b]
	5p	0.007 0		
	6p	0.004 05		
	7p	0.002 53		
B II	3p	0.111 0		0.090 8 [b]
	4p	0.045 5		0.039 0 [b]
	5p	0.022 1		
	6p	0.012 3		
	7p	0.007 56		
C III	3p	0.212 7		0.223 [b]
	4p	0.074 9		0.077 5 [b]
	5p	0.034 6		
	6p	0.018 9		
	7p	0.011 5		
N IV	3p	0.300 7	0.547 [c]	0.323 [b]
	4p	0.097 3	0.150 [c]	0.104 [b]
	5p	0.043 8	0.059 [c]	
	6p	0.023 6		
	7p	0.014 3		
O V	3p	0.374 4	0.588 [c]	0.400 [b]
	4p	0.114 4	0.158 [c]	0.121 [b]
	5p	0.050 6	0.062 [c]	
	6p	0.027 1	0.030 [c]	
	7p	0.016 2	0.017 [c]	

[a] Reference 25.
[b] Reference 26.
[c] Reference 27.

$\rightarrow 2s\,2p(^1P_1)$. The computed OOS based on Eqs. (11)–(13) are presented in Tables V and VI. In Table V we compare the IPM OOS for the resonance transition $2s^2(^1S_0) \rightarrow 2s\,2p(^1P_1)$ to the experimental values,[17-24] Hartree-Fock-Slater (HFS) results,[25,26] time-dependent Hartree-Fock (TDHF) results,[27] and other results.[28-30] We see that the IPM values are in reasonable agreement with all the other values. In Table VI we present the IPM OOS for the transitions $2s^2(^1S_0) \rightarrow 2s\,np(^1P_1)$, $3 \leq n \leq 7$, and compare them with HFS and TDHF results where possible. For the cases of N IV and O V we have computed the HFS values from Kelly's formula[26]:

$$f_0 = (0.333\Delta E) S(M) S(L) \sigma^2 / w\,, \tag{14}$$

where ΔE is the transition energy, w is the statistical weight of the ground state, and σ^2 is the square of the radial dipole matrix element. The quantities $S(M)$, $S(L)$ are the relative multiplet strength and relative line strength, respectively, and are evaluated using general formulas given by Rohrlich.[31] Extensive tabulations of σ^2 using HFS wave functions have been given by Kelly for the various species of oxygen and nitrogen. The small differences between corresponding results in the various calculations may be a reflection of the sensitivity of OOS to fine details of the potential and the radial wave functions, particularly near the valence orbit.[16,32]

TABLE VII. Coefficients a_0, a_1, a_2 to be used in Eq. (15).

2s to	a_0	a_1	a_2	χ^2 ($\times 10^4$)
2p	0	5.3818	−2.9364	74.3
3p	1.1602	−7.9873	13.736	0.51
4p	0.2824	−1.5962	2.0757	0.31
5p	0.1132	−0.5712	0.5852	0.11
6p	0.0578	−0.2739	0.2351	0.05
7p	0.0333	−0.1486	0.1017	0.05

We have found that the OOS exhibit systematic trends along the isoelectronic sequence. From several discussions[1,29,33,34] it is expected that for a fixed transition within an isoelectronic sequence, the OOS may be expanded in inverse powers of the nuclear charge:

$$f_0 = a_0 + a_1/Z + a_2/Z^2\,. \tag{15}$$

The coefficient a_0 is zero for in-shell transitions. We have verified that the IPM OOS conform to Eq. (15). For the principal resonance transition $2s$-$2p$, we set $a_0 = 0$ and vary the two coefficients a_1, a_2 so as to obtain the best fit to the IPM $2s$-$2p$ OOS along the sequence. For the other transitions $2s$-nl, we vary all three coefficients a_0, a_1, a_2. The coefficients which reproduce the OOS best are given in Table VII.

V. RESULTS FOR GOS AND INTEGRATED CROSS SECTIONS

For Be I, B II, C III, N IV, O V we have computed the GOS for a variety of excitations from the $2s$ ground state and for a range of ξ from 10^{-2} to 10^3. We find that the GOS exhibit a striking nodal structure which becomes more complex as ξ gets large. These features are illustrated in Fig. 1 which displays our results for B II. The results for the other ions have the same general characteristics.

To expedite use in applications, we have parametrized all the GOS with simple analytic forms. For optically allowed transitions such as $2s$-$2p$, $2s$-$3p$, etc., we use the form

$$f(\xi) = A(e^{-\alpha\xi} + \beta\xi e^{-\gamma\xi})^2\,; \tag{16}$$

and for optically forbidden transitions such as $2s$-$3s$, $2s$-$3d$, etc., we use

$$f(\xi) = \xi A(e^{-\alpha\xi} + \beta\xi e^{-\gamma\xi})^2\,. \tag{17}$$

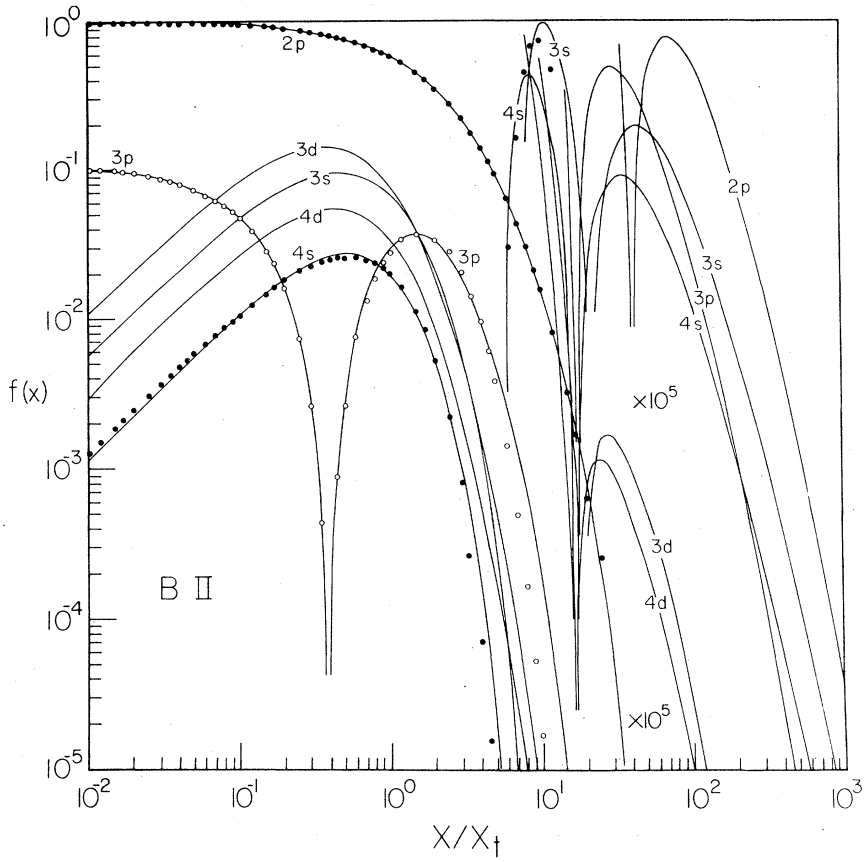

FIG. 1. Solid curves are the GOS results for B II generated numerically from Eq. (8). The solid dots and open circles give representative fits using Eqs. (16) or (17) with parameter values in Table VIII.

We only attempt to fit the GOS up to the second node. This is a reasonable approximation in view of the rapid decline of the GOS beyond the second node. In Eqs. (16) and (17) the quantities A, α, β, γ are adjustable parameters. For optically allowed transitions A may be identified as the OOS. Accordingly, for optically allowed transitions we set $A = f_0$ and vary the three parameters α, β, γ so as to obtain the best fit to the GOS (up to the second node). For optically forbidden transitions we vary the four parameters A, α, β, γ. The best values of the parameters are given in Table VIII. Thus all our GOS results can be reproduced by means of Eqs. (16) and (17) with parameter values taken from Table VIII, and with an accuracy comparable to the fits shown in Fig. 1. It may be noted that for the optically forbidden transitions, the second maximum is much weaker than the first maximum, by at least four orders. Thus, even with Poisson weighting, the second maximum was not in general reproduced by Eq. (17).

Apart from providing a compact representation of a large body of numerical results, the analytic forms (16) and (17) also lead to an integrated cross section which is expressible in closed form. The integrated cross section is defined by

$$\sigma = \frac{q_0}{WE} \int_{\xi_l}^{\xi_u} \frac{f(\xi)}{\xi} d\xi \,, \tag{18}$$

where W is the transition energy in eV, E is the incident electron energy in eV, $q_0 = 6.514 \times 10^{-14}$ cm^2 eV^2, and

$$\xi_{u,l} = (2E/W)[1 \pm (1 - W/E)^{1/2} - W/2E] \,. \tag{19}$$

The weighting of $f(\xi)$ by ξ^{-1} in Eq. (18) combined with the rapid decline of $f(\xi)$ beyond the second node minimizes the errors associated with our approximate analytic representations (16) and (17). Equations (16) and (17) correspond, respectively, to the first three terms and the first four terms of the general form[35]

$$f(\xi) = \sum_{s=0}^{\infty} f_s \xi^s \exp(-\alpha_s \xi) \,. \tag{20}$$

On substituting Eq. (20) into Eq. (18), the integrated cross section is obtained in closed form

$$\sigma(E) = \frac{q_0}{WE} \left(f_0 [E_1(\alpha_0 \xi_l) - E_1(\alpha_0 \xi_u)] + \sum_{s=1}^{\infty} \frac{f_s}{\alpha_s^s} [\gamma(s, \alpha_s \xi_u) - \gamma(s, \alpha_s \xi_l)] \right) . \tag{21}$$

TABLE VIII. Values of parameters to be used in Eqs. (16) and (17).

Atom/ion	2s to	A	α	β	γ	χ^2 ($\times 10^3$)
Be I	3s	0.4043	1.2950	0.2056	0.7870	0.06
	4s	0.0890	0.6533	−0.2287	0.7866	0.33
	5s	0.0351	0.5335	−0.3044	0.6588	0.30
	3d	0.4174	1.8864	0.2050	1.0145	0.19
	4d	0.1681	1.5908	0.1140	0.8557	0.02
	5d	0.0830	1.4761	0.0775	0.7683	0.01
	2p	1.1240	0.4298	0.0868	0.2205	1.03
	3p	0.0220	4.2231	−2.3455	0.6719	8.66
	4p	0.0131	2.8393	−1.6658	0.6670	2.05
B II	3s	0.5839	1.5001	0.3269	1.0323	0.08
	4s	0.1274	0.4281	−0.4673	0.6013	0.98
	3d	1.1129	1.6637	0.1943	0.9550	0.28
	4d	0.3286	1.1733	0.0239	0.5625	0.50
	2p	1.0166	0.3492	0.0707	0.2039	0.18
	3p	0.1110	2.8814	−1.0927	0.6786	3.19
C III	3s	0.6647	1.6806	0.4543	1.1924	0.17
	4s	0.1664	0.7249	−0.2962	0.8213	4.90
	5s	0.0602	0.4147	−0.5005	0.5921	1.53
	3d	1.4733	1.5741	0.1915	0.9307	0.27
	4d	0.3694	1.0289	0.0053	0.4312	2.43
	5d	0.1515	0.7548	−0.1621	0.7498	3.25
	2p	0.8427	0.2866	0.0621	0.1795	0.04
	3p	0.2127	2.4829	−0.7569	0.6735	1.37
	4p	0.0749	1.3631	−1.1895	0.8364	2.70
	5p	0.0346	0.4972	−1.8594	0.8036	2.33
N IV	3s	0.7132	1.8214	0.5633	1.2987	0.26
	3d	1.6820	1.5219	0.1904	0.9163	0.24
	4d	0.3765	0.8618	−0.0848	0.8704	5.33
	2p	0.7032	0.1355	−0.0509	0.2241	0.01
	3p	0.3007	2.2883	−0.6155	0.6703	0.68
	4p	0.0973	0.7851	−1.4881	0.8678	3.15
	5p	0.0438	0.3673	−1.8033	0.7481	4.18
O V	3s	0.7497	1.1024	−0.1814	2.0519	0.22
	4s	0.1701	0.4866	−0.5140	0.6711	1.92
	3d	1.8229	1.4851	0.1896	0.9058	0.22
	4d	0.3709	0.4939	−0.3804	0.6384	7.76
	5d	0.1437	0.3762	−0.4051	0.5171	9.51
	2p	0.5929	0.2099	0.0525	0.1410	0.01
	3p	0.3744	2.1701	−0.5361	0.6674	0.35
	4p	0.1144	0.4862	−1.6466	0.7989	4.69
	5p	0.0506	0.3617	−1.6373	0.7230	5.09

Here E_1 is the first exponential integral function[36] and $\gamma(s,y)$ is the incomplete gamma function.[36] The first term in this series which is dominant at high energies leads to the familiar $E^{-1}\ln E$ dependence usually associated with the Born approximation.

For Be I, B II, C III, N IV, O V we have computed the integrated cross sections for a variety of excitations from the 2s ground state, and for incident electron energies ranging from threshold to 1 keV. The results are displayed in Figs. 2–6. We see that the 2s-2p cross sections dominate strongly throughout the sequence. Unfortunately there is little information available with which to compare our results. Almost the only results available are the calculated 2s-2p integrated cross sections for BeI based upon the non-closed-shell many-electron theory (NCMET) of Sinanoglu *et al.*[28] We are gratified by the harmony between the IPM and NCMET results, especially in light of the rigorous nature of the NCMET calculations which take full account of all correlation effects.

We have investigated the existence of regularities and systematic trends in the cross sections along the isoelectronic sequence. We have found that for a given energy in the range 300 to 1000 eV, the 2s-2p cross sections along the isoelectronic sequence conform very accurately to the formula

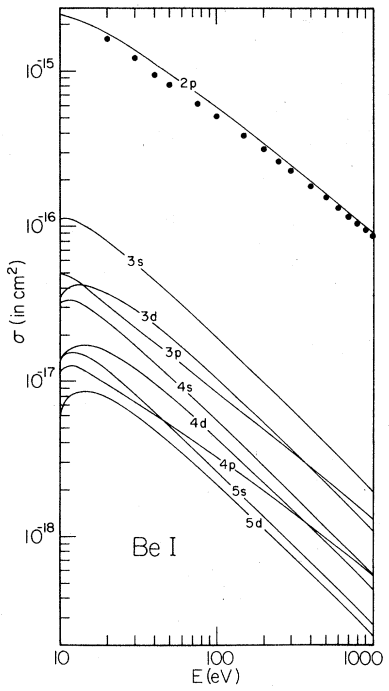

FIG. 2. Integrated cross sections for BeI. The solid dots are the NCMET results of Sinanoğlu and Davis (Ref. 28).

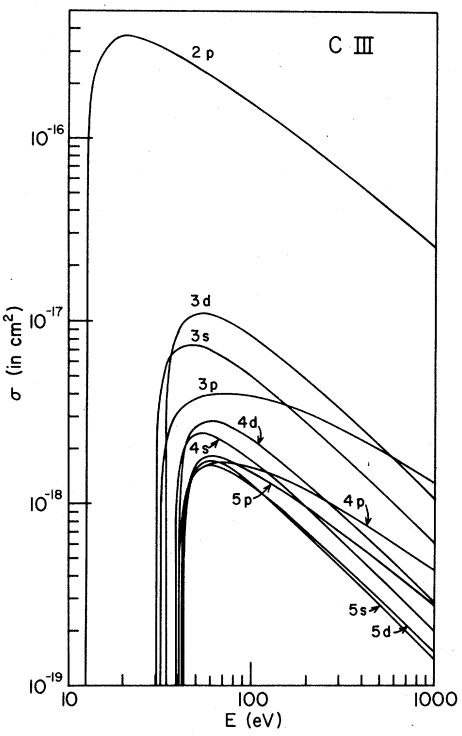

FIG. 4. Integrated cross sections for C III.

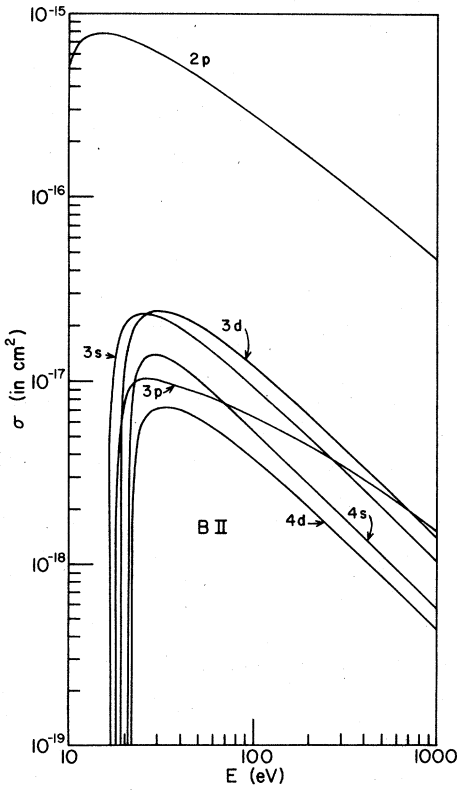

FIG. 3. Integrated cross sections for BII.

$$\sigma(2s\text{-}2p) = \sigma_0 \frac{K}{(n-\delta)^3 (Z-a)^2 E} \ln\left(\frac{E}{bE} + e\right), \quad n = 2, \tag{22}$$

where $\sigma_0 = 10^{-16}$ cm^2, $K = 7205$ eV, $\delta = 0$, $a = 1.425$, $b = 0.4388$ eV, and e is the base of natural logar-

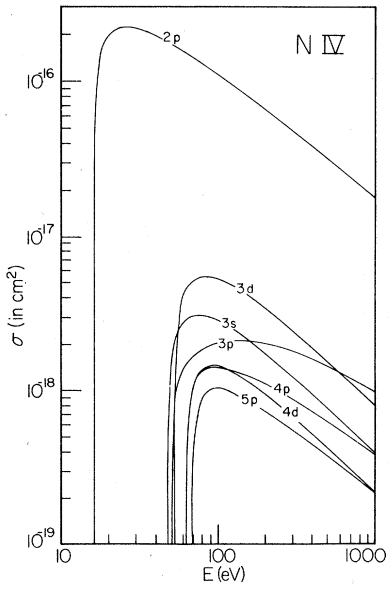

FIG. 5. Integrated cross sections for NIV.

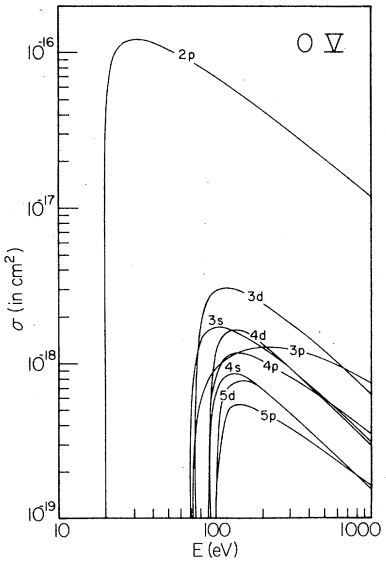

FIG. 6. Integrated cross sections for O V.

ithms. The cross sections computed using this formula are not shown since they fit the corresponding curves in Figs. 2–6 within the line width. It is interesting to note that Eq. (22) accounts approximately for the success of the scaling factor $(Z-1.35)^2$ employed by Watson, Dalgarno, and Stewart[37] for scaling photoionization cross sections of the Be sequence. An explicit formula for the major resonance transition is, of course, more convenient in applications.

We have also examined the applicability of Eq. (22) to all members of the $2s$-np isoelectronic series. If we set $K=132\,35$ eV, $\delta=0.015$, $a=-10.8$, and $b=0.455$ eV, we achieve 10% level agreement with the $3p$, $4p$, and $5p$ results above 500 eV in Figs. 2–6. However, the fits are not of high calibre and more work needs to be carried out should these small cross sections be significant in experimental situations. One problem which arises is that the threshold (transition) energies become so large that the domain of the Born approximation moves to higher energies. In earlier work Green and Dutta[35] empirically modified Born cross sections by using a cofactor of the form $[1-(x_t/E)]^\nu$ which reduces to the Born cross section as $E\to x_t$, the transition energy. It is not unreasonable to use a similar cofactor for isoelectronic sequences but it would take experimental measurements or distorted wave calculations to fix the parameter ν.

For excitations $2s$-ns and $2s$-nd our theoretical results display approximately the behavior

$$\sigma(2s\text{-}nl)=\sigma_0 K/(n-\delta)^3(Z-a)^p E\,, \tag{23}$$

where for ns states $K=29409$, $\delta=0.569$, $a=-0.811$, and $p=3$ and for nd states $K=872.1$, $\delta=0.606$, $a=-0.968$, and $p=1$. Again one would have to fix a cofactor $[1-(x_t/E)]^\nu$ to establish precisely the overall magnitude of K.

VI. SUMMARY AND CONCLUSION

The isoelectronic ions of the beryllium sequence play important roles in a number of phenomena in plasma physics and astrophysics, as indicated in the introduction to this work. The primary purpose of this work has been to apply a realistic independent particle model to the programmatic generation of optical oscillator strengths, generalized oscillator strengths, and electron-impact cross sections for a variety of excitations from the $2s$ valence shell of the isoelectronic sequence Be I, B II, C III, N IV, O V. From our results we have obtained several phenomenological relationships representing the systematic behavior of potential parameters, transition energies, oscillator strengths and cross sections, along the sequence. Such relationships are important since they facilitate the evaluation of data and make possible the acquisition of new data simply by interpolation or extrapolation.

The substantial differences in Table I between the screening function parameters found in the present work and those found by GGJ are a matter of physical interest. Recall that we have adjusted d and H to yield eigenvalues to be in best agreement with the experimental valence and excited energy levels whereas GGJ following Bass *et al.*[38] adjust these parameters to minimize the total energy. Since the GGJ screening functions are expected to closely simulate an average Hartree-Fock screening function, to the extent that our screening function departs from GGJ, probably represents its departure from the effective average Hartree-Fock screening function. We have examined the systematics of these differences and in general find that $\Omega-\Omega_{GGJ}$ is positive at small r but negative at large r with the sign change occurring at $r\simeq 1.5$ in Be I, $r\simeq 0.5$ in C III, and $r\simeq 0.3$ in O V. This implies that our Be isoelectronic potentials are systematically more repulsive outside these radii than are the GGJ potentials. Green and Kutcher[39] have previously found potential differences between excited state adjusted potentials and energy minimized adjusted potentials which vary in an apparently unsystematic manner from atom to atom. The present work suggests a systematic trend at least for an isoelectronic series. The study of Green and Kutcher suggests that these potential differences might represent non-IPM

effects such as residual electron-electron interactions, polarization contributions, and rearrangement effects. A more-detailed study of differences in IPM potentials obtained in various ways is now underway.

Returning to our results here we should note that they are in reasonable agreement with experiment and at the same time in approximate conformity with results based upon the Hartree-Fock method. The fact that we tune the two parameters in our analytic model to experimental energy-level data appears to ensure that our model provides a realistic single-particle description of what is actually a complex many-body problem. The compatibility which we have found to exist between the IPM and NCMET results (see Fig. 2) strongly suggests that our potentials empirically embody effects not included in the Hartree-Fock model or in various *ab initio* IPM approximations to it.

In final summary, we emphasize that the analytic independent particle model is addressed towards practical applications of atomic theory. Its convenience in applications as illustrated by the systematic regularities in various properties we have derived from it are important assets. Other important assets are the computational simplicity and the orthogonality and closure properties, which are particularly helpful in calculations of the properties of excited states which are needed in numerous applications.

ACKNOWLEDGMENT

This work was supported by the Division of Biomedical and Environmental Research of the U. S. Department of Energy.

---

*Permanent address: California State University at Los Angeles, Los Angeles, Calif. 90032.

[1]W. L. Wiese and S. M. Younger, Beam-Foil Spectrosc. 2, 951 (1976).
[2]G. Burbidge and M. Burbidge, *Quasi-Stellar Objects* (Freeman, San Francisco, 1967).
[3]A. E. S. Green, D. L. Sellin, and A. S. Zachor, Phys. Rev. 184, 1 (1969).
[4]P. S. Ganas and A. E. S. Green, Phys. Rev. A 4, 182 (1971).
[5]P. A. Kazaks, P. S. Ganas, and A. E. S. Green, Phys. Rev. A 6, 2169 (1972).
[6]T. Sawada and P. S. Ganas, Phys. Rev. A 7, 617 (1973).
[7]P. P. Szydlik and A. E. S. Green, Phys. Rev. A 9, 1885 (1974).
[8]A. E. S. Green, R. G. Garvey, and C. H. Jackman, Int. J. Quantum Chem. Symp. 9, 43 (1975).
[9]T. Sawada, P. S. Ganas, and A. E. S. Green, Phys. Rev. A 9, 1130 (1974).
[10]K. J. Miller and A. E. S. Green, J. Chem. Phys. 60, 2617 (1974).
[11]C. E. Moore, *Atomic Energy Levels*, Natl. Bur. Stand. (U. S.) Circ. No. 467 (U. S. GPO, Washington, D. C., 1958), Vols. I–III.
[12]A. E. S. Green and P. J. Wyatt, *Atomic and Space Physics* (Addison-Wesley, Reading, Mass., 1965).
[13]D. Layzer, Ann. Phys. (N. Y.) 8, 271 (1959).
[14]A. R. Edmonds, *Angular Momentum in Quantum Mechanics* (Princeton University, Princeton, N.J., 1957).
[15]B. W. Shore and D. H. Menzel, *Principles of Atomic Spectra* (Wiley, New York, 1968).
[16]P. S. Ganas and A. E. S. Green, J. Quant. Spectrosc. Radiat. Transfer 13, 1171 (1973).
[17]I. Bergstrom, J. Bromander, R. Buchta, L. Lundin, and I. Martinson, Phys. Lett. 28A, 721 (1969).
[18]T. Andersen, K. A. Jessen, and G. Sorensen, Phys. Rev. 188, 76 (1969).
[19]I. Martinson, A. Gaupp, and L. J. Curtis, J. Phys. B 7, L463 (1974).
[20]A. Bromander, R. Buchta, and L. Lundin, Phys. Lett. A29, 523 (1969).
[21]I. Martinson, W. S. Bickel, and A. Ölme, J. Opt. Soc. Am. 60, 1213 (1970).
[22]G. M. Lawrence and B. O. Savage, Phys. Rev. 141, 67 (1966).
[23]L. Heroux, Phys. Rev. 180, 1 (1969).
[24]I. Martinson, H. G. Berry, W. S. Bickel, and H. Oona, J. Opt. Soc. Am. 61, 519 (1971).
[25]E. J. McGuire, Sandia Labs. Research Rept. No. SC-RR-70-406, 1971 (unpublished).
[26]P. S. Kelly, J. Quant. Spectrosc. Radiat. Transfer 4, 117 (1964).
[27]R. F. Stewart, J. Phys. B 8, 1 (1975).
[28]O. Sinanoğlu and S. L. Davis, Chem. Phys. Lett. 32, 449 (1975).
[29]M. W. Smith and W. L. Wiese, Astrophys. J. Suppl. 23, 103 (1971).
[30]O. W. Day and E. G. Larson, J. Quant. Spectrosc. Radiat. Transfer 17, 613 (1977).
[31]F. Rohrlich, Astrophys. J. 129, 441 (1959).
[32]D. D. Doda, R. H. Garvey, and A. E. S. Green, Phys. Rev. A 12, 712 (1975).
[33]M. W. Smith, G. A. Martin and W. L. Wiese, Nucl. Instrum. Methods 110, 219 (1973).
[34]G. A. Martin and W. L. Wiese, Phys. Rev. A 13, 699 (1976).
[35]A. E. S. Green and S. K. Dutta, J. Geophys. Res. 72, 3933 (1967).
[36]W. Gautschi and W. F. Cahill, in *Handbook of Mathematical Functions*, edited by M. Abramowitz and I. A. Stegun, Appl. Math. Series No. 55 (U. S. GPO, Washington, D. C., 1964), Chap. 5.
[37]D. K. Watson, A. Dalgarno, and R. F. Stewart, Phys. Rev. A 17, 1928 (1978).
[38]J. N. Bass, A. E. S. Green, and J. H. Wood, Adv. Quantum Chem. 7, 263 (1973).
[39]A. E. S. Green and G. J. Kutcher, Int. J. Quantum Chem. Symp. No. 10, 135 (1976).