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Electron impact excitation of the resonance lines of Be^+, Mg^+ and Ca^+

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Abstract. The unitarised distorted-wave polarised-orbital (UDWPO) approximation is used to calculate integral cross sections for electron impact excitation of the resonance transitions of Be^+, Mg^+ and Ca^+ from threshold to 100 eV. Results are also given in a variety of simpler approximations and the cross sections are compared with other calculations and with experiment. The polarisation of the emitted Ca^+ K-line radiation is also considered and adiabatic dipole polarisabilities are calculated for the ground states of the above ions.

1. Introduction

Electron impact excitation of positive ions plays an important role in many astrophysical phenomena (Seaton 1975) and in the analysis of impurities in controlled thermonuclear devices (see e.g. McDowell 1977). In the latter case, data along an isoelectronic sequence are particularly useful and excitation cross sections are required at energies up to about twenty-five times threshold. Consequently, it is of interest to obtain results in simple approximations including the Coulomb–Born and its variants (Burgess *et al* 1970), at low and intermediate energies.

We have recently reported applications of the distorted-wave polarised-orbital (DWPO) method (McDowell *et al* 1973, 1974, 1975, Scott and McDowell 1976) to excitation of both $s \rightarrow s$ and $s \rightarrow p$ transitions in the hydrogen and helium isoelectronic sequences (McDowell *et al* 1977). The partial and total cross sections agree very well with those obtained from the distorted-wave approach of Jones (1974) at low and intermediate energies and with similar calculations by Bhatia and Temkin (1977). Where comparison is possible, they are also in good agreement with experimental data.

The modifications of the DWPO method necessary to treat alkali systems have been presented by Kennedy (1976) and applied to the resonance transitions of the alkali metals (Kennedy *et al* 1977). In this paper, we consider the resonance transitions of the positive ions Be^+, Mg^+ and Ca^+, and, following the discussions by Kennedy *et al* (1977), we present results up to about 100 eV; at higher energies the Coulomb–Born (CBI, CBII) and Coulomb–Born–Oppenheimer (CBOI, CBOII) calculations should be reasonably accurate (see §§3 and 4).

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The theoretical position up to June 1975 has been reviewed by Seaton (1975) and the experimental position by Dolder and Peart (1976). Since these reviews, further experimental work on Mg^+ and Ca^+ has been reported by Zapesochnyi *et al* (1975) and absolute measurements for the $Be^+(2p \rightarrow 2s)$ emission cross section induced by electron impact excitation of the $2s \rightarrow 2p$ transition are available from P O Taylor, L Phaneuf and G Dunn (1977 private communication). A detailed series of Coulomb–Born and close-coupling calculations have recently been presented for this ion by Hayes *et al* (1977); however, these still give a low-energy discrepancy between theory and experiment (cf He^+, Ca^+; Seaton 1975).

In §2 we review our method of obtaining the adiabatic polarisation potential between the ion and the incident electron and compare our calculated polarisabilities with those obtained by other methods. Our total cross section results for Be^+ are presented in §3, those for Ca^+ and Mg^+ in §4, and are compared with other recent theoretical models and with experiment.

2. Polarisabilities of alkali-like ions

If we consider a resonance transition $ns \rightarrow np$, then (Kennedy *et al* 1977) using Hartree–Fock orbitals as a zero-order basis we may construct a perturbed ns orbital, for the atom or ion perturbed by an external static unit charge at a distance r from the nucleus,

$$|\tilde{ns}\rangle = |ns\rangle + \beta(r)\,|np\rangle$$

where, following the approach initiated by Stone (1966) and modified by Vo Ky Lan (1972), $\beta(r)$ is determined, for fixed r, by minimising the perturbed ground-state energy with respect to this parameter. The adiabatic polarisation potential is then

$$V_{\text{pol}}(r) = \beta(r)\, V_{ns,np} \tag{1}$$

where

$$V_{ns,np} = \langle ns|\, V\, |np\rangle \tag{2}$$

and behaves asymptotically as

$$V_{\text{pol}}(r) \sim -\frac{4}{3}\frac{|C_{ns,np}|^2}{\epsilon_{np}^{(0)} - \epsilon_{ns}^{(0)}}\frac{1}{r^4} \qquad \text{(Ryd)} \tag{3}$$

in which $\epsilon_{nl}^{(0)}$ (Ryd) are the Hartree–Fock orbital energies and $C_{ns,np}$ is the overlap integral

$$C_{ns,np} = \int_0^\infty r P_{ns}(r) P_{np}(r)\, \mathrm{d}r$$

where

$$|nl\rangle = r^{-1} P_{nl}(r)\, Y_{l0}(r).$$

Thus a first estimate of the polarisability is

$$\alpha(0) = \frac{4}{3}\frac{|C_{ns,np}|^2}{\epsilon_{np}^{(0)} - \epsilon_{ns}^{(0)}} \qquad (a_0^3). \tag{4}$$

Table 1. Static dipole polarisabilities for the alkali-like ions (a_0^3).

	Be^+	Mg^+	Ca^+
n	2	3	4
Present: ns–np	23·8	35·5	78·0
continuum	0·02	0·3	0·6
core	0·05	0·5	3·3
total	23·9	36·3	81·9
Yoshimine and Hurst (1964)	16·7	37·2	96·5
Cohen and Drake (1967)	—	45·6	—
Thorhallsen *et al* (1968)	12·3	23·6	56·3
Flannery and Stewart (1963)	24.6	—	—

An improved estimate, $\alpha(1)$, may be obtained by including contributions from higher p states $|mp\rangle$, $m > n$, and adding a correction for the core polarisability (Dalgarno 1962 for Be^+; Opik 1967 for Mg^+ and Ca^+). Contributions from continuum p states may be estimated using the single-channel quantum-defect method, following Peach (1967). In the present cases this correction is less than 1%. Our values of the dipole polarisabilities are given in table 1 and compared with other theoretical results. Our results for Be^+ is in reasonable accord with the variational calculation of Flannery and Stewart (1963), while for Mg^+ and Ca^+ we agree most closely with the results of Yoshimine and Hurst (1964). The values of Thorhallson *et al* (1968) would imply anomalously low oscillator strengths for the resonance transitions in all the above cases.

Ground-state Hartree–Fock orbitals used in this work were obtained from Clementi (1965) for Ca^+ and Mg^+. For Be^+ we used $|2s\rangle$ and $|2p\rangle$ orbitals from Weiss (1963) while the excited-state orbitals for Ca^+ and Mg^+ were obtained from P G Burke (1974 private communication).

3. Excitation of the resonance transition of Be^+

All our calculations were carried out in the unitarised DWPOII approximation (UDWPOII) described by Kennedy *et al* (1977), which allows for distortion (both of the incident electron and the target state) in the initial channel only. The Weiss–Hartree–Fock wavefunctions adopted give an oscillator strength for the resonance transition of 0·5112 in the length and 0·5491 in the velocity formulation compared with the accurate configuration-interaction values of 0·5050 and 0·5205, respectively. The UDWPOII results for excitation of the resonance transition are compared with the non-unitarised values in table 2. These values were obtained by summing individual partial cross sections Q_l for each angular momentum and making the Burgess and Sheorey (1974) correction for $l \geqslant l_0$; we tested various choices of l_0 to establish the stability of our results. At $k_i^2 = 4{\cdot}0$ and $l_0 = 150$ the correction is $3 \times 10^{-5}\ \pi a_0^2$ while for $k_i^2 = 8{\cdot}0$ and $l_0 = 195$ it is $1 \times 10^{-2}\ \pi a_0^2$. We also compared our Coulomb–Born (CBI) and Coulomb–Born–Oppenheimer (CBOI) values, and their unitarised versions (CBII, CBOII), with those of Hayes *et al* (1977), who used identical wavefunctions, obtaining agreement to four figures. It is of interest to note that unitarisation reduces the cross section near threshold by about 30%, 38% and 36%, respectively, in the three approximations; CBI → CBII, CBOI → CBOII, DWPOII → UDWPOII.

Table 2. Unitarised (Q_{II}) and non-unitarised (Q_I) results (πa_0^2) in the DWPO approximation for the $2s \rightarrow 2p$ transition in Be^+.

E(eV)	Q_I	Q_{II}
4·08	38·7	24·7
6·8	26·6	20·0
13·6	16·5	14·4
27·2	10·4	9·78
54·4	6·41	6·22
108·8	3·81	3·76

In figure 1, we compare the CBI, CBOI, CBII results of Hayes *et al* (1977), the UDWPOII values and the two-state close-coupling calculations of Hayes *et al* (1977) for excitation of the resonance transition in Be^+, with the absolute experimental measurements for the resonance emission cross section of Taylor *et al* (1977). The CBI, CBOI and CBII results lie considerably too high at low energies, and the CBOII, UDWPOII and two-state close-coupling values are, respectively, 48%, 36% and 29% above the extrapolated measurement (18·2 πa_0^2) of Taylor *et al* at threshold. (The contributions of cascade from higher states in the measured 2p–2s emission cross section has been estimated by Taylor *et al* to be about 10% at low energies; hence the true discrepancies between theory and experiment at low energies may be slightly larger.) We note that the UDWPOII model does not include the effect of resonances

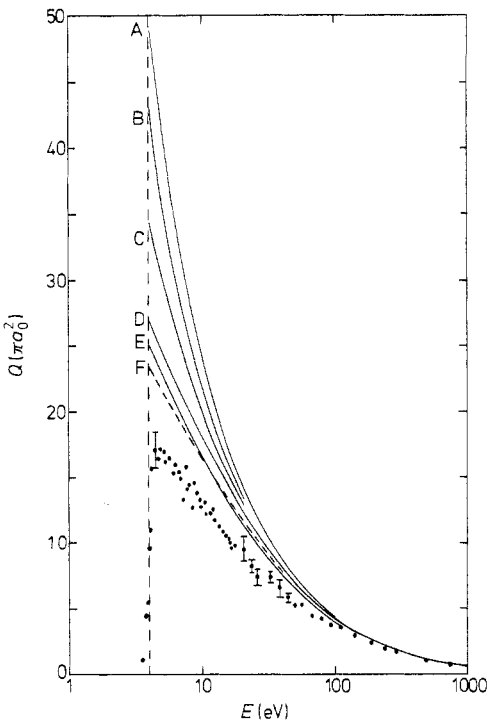

Figure 1. Integrated (total) cross section (πa_0^2) for the resonance transition of Be^+ from threshold to 1 keV. Theoretical results for excitation: A CBI; B CBOI (Hayes *et al* 1977 and this paper); C CBII; D CBOII; E UDWPOII (this paper); F two-state close-coupling (Hayes *et al* 1977). Experimental results for emission ⧫ (Taylor *et al* 1977).

below the ionisation threshold, whereas the two-state close-coupling calculations make some allowance for these. The resonances affect only the low partial waves ($L = 0, 1, 2$), whereas appreciable contributions to the cross section near threshold come from $0 \leqslant L \leqslant 6$. A five-state close-coupling calculation has recently been presented by Hayes (1976); however, this only reduces the threshold excitation cross section to 7% below the two-state value and so is still 19% above the experimental result for emission.

At higher energies, the effects of cascade in the experimental data are likely to be considerably less than 10% (Taylor *et al* 1977). At 109 eV, the CBOII and UDWPOII results are, respectively, 14% and 6% above the experimental emission value of $3{\cdot}55 \pm 0{\cdot}17\ \pi a_0^2$ at 111·7 eV. Since the DWPOII model assumes static distortion of the target, it was used only for impact energies of 100 eV or below. At 751 eV the CBOII result of $0{\cdot}855\ \pi a_0^2$ (Hayes *et al* 1977) is 2% higher than the experimental value of $0{\cdot}84 \pm 0{\cdot}05\ \pi a_0^2$ at 737 eV, while the CBOII result including the effects of cascade from the $n = 3$ and 4 states is about 7% higher. Thus it does not appear that the low-energy discrepancy between theory and experiment can be removed by any normalisation of the experimental data to the CBOII results at high energies.

4. Excitation of the resonance transitions of Mg^+ and Ca^+

4.1. Mg^+

Our results for electron impact excitation of the $3s \rightarrow 3p$ resonance transition of Mg^+ in the CBI, CBII, CBOI, CBOII, DWPOII and UDWPOII approximations are presented in table 3; in each case the Burgess and Sheorey (1974) correction has been applied for the high-l partial waves. In a similar manner to Be^+, unitarisation reduces the cross section near threshold by 34%, 42% and 41%, respectively, in the three approximations CB, CBO and DWPOII. Further, from the relatively close agreement between our CBOII and UDWPOII results at 54·4 eV, we would expect the CBOII calculations to be reliable to better than 10% for energies greater than 100 eV.

Three-state close-coupling calculations for this transition have been presented by Burke and Moores (1968) in the range 9–27 eV; their results lie about 10% lower than our UDWPOII values at the lower energies. In agreement with their calculations, we find that the dominant contributions to the total cross section come from total orbital angular momenta $L = 3$, 4 and 5. Thus the effects of resonances in the low partial waves (for which we cannot allow) are relatively unimportant. The 3s electron in Mg^+ has the maximum of its density distribution at about $2{\cdot}5\ a_0$ from the nucleus, and this suggests that low partial waves of the incident electron do not see the maximum of the target density distribution. While the contributions for $3 \leqslant L \leqslant 5$

Table 3. Cross sections (πa_0^2) for excitation of Mg^+ ($3s \rightarrow 3p$).

E(eV)	CBI	CBII	CBOI	CBOII	DWPOII	UDWPOII
4·5	55·4	36·7	46·7	27·2	37·6	22·2
6·8	41·4	30·5	35·5	25·3	29·0	21·0
13·6	26·1	21·9	23·8	20·1	20·5	17·7
27·2	16·5	15·1	15·8	14·5	14·2	13·2
54·4	10·3	9·8	10·0	9·6	9·2	8·9

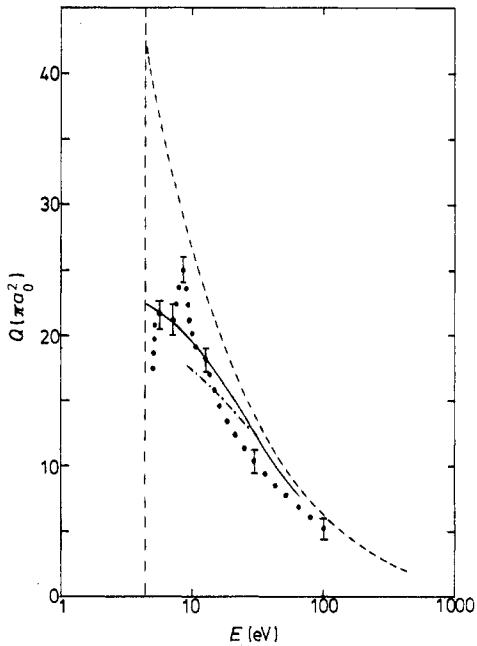

Figure 2. Integrated (total) cross section (πa_0^2) for the resonance transition of Mg^+ from threshold to 1 keV. Theoretical results: ------ CDWII (Burgess and Sheorey 1974); —— UDWPOII (this paper); -·-·-·-· three-state close-coupling (Burke and Moores 1968). Experimental results: ● (Zapesochnyi *et al* 1975). These data cannot be presented accurately due to the difficulty of retrieving the information from their original graph.

are significantly affected by distortion, higher partial-wave contributions are well described by the CBOII approximation, and this together with the small contributions from $L < 3$ accounts for its success.

Kelman *et al* (1975) and Zapesochnyi *et al* (1975) have measured the excitation cross section for the resonance transition in Mg^+, reporting a maximum of about $25\,\pi a_0^2$ at approximately 8 eV. There appears to be considerable structure in the observed data near threshold. The experimental results are compared with our UDWPOII values and the close-coupling calculations of Burke and Moores in figure 2. We also illustrate in figure 2 the results of Burgess and Sheorey (1974) using a unitarised Coulomb distorted-wave model (CDWII) but neglecting exchange and polarisation distortion; their values appear to be in good agreement with our CBOII results by 54·4 eV. The experiment, which claims to be an absolute measurement (cf Dolder and Peart 1976) may be in slightly better agreement with the UDWPOII results than the three-state close-coupling values.

4.2. Ca^+

Our results for electron impact excitation of the $4s \rightarrow 4p$ resonance transition of Ca^+ in the CBI, CBII, CBOI, CBOII, DWPOII and UDWPOII approximations are presented in table 4; in each case the Burgess–Sheorey (1974) correction has been applied for the high-l partial waves. In a similar manner to Be^+ and Mg^+, unitarisation reduces the cross section near threshold by 40%, 40% and 37%, respectively, in the three approximations CB, CBO and DWPOII. Again, we would expect CBOII calculations to be reliable to better than 10% for $E > 100$ eV.

Table 4. Cross sections (πa_0^2) for excitation of Ca^+ (4s → 4p).

E(eV)	CBI	CBII	CBOI	CBOII	DWPOII	UDWPOII
3·3	123	74·2	107	64·3	79·0	49·5
4·5	98·7	64·8	87·1	58·2	66·6	46·4
6·8	74·4	54·2	67·4	50·1	54·7	42·0
13·6	47·1	39·2	44·3	37·5	38·7	33·4
27·2	29·6	26·9	28·7	26·2	26·1	24·1
54·4	18·2	17·4	17·9	17·1	16·6	15·9
108·8	—	—	10·8	10·6	10·0	9·9

Three-state close-coupling calculations for this transition have been presented by Burke and Moores (1968) and Wells (1974). Seaton (1975) remarks that the wavefunctions used give photoionisation cross sections too large by a factor of five, and too small a calculated optical polarisation, P_K, for the K line. The total excitation cross section for the 4s → 4p transition is

$$Q = 1{\cdot}057\,[Q(\mathrm{H}) + Q(\mathrm{K})]$$

where Q(H) and Q(K) are the emission cross sections for the H and K lines of the resonance doublet and 1·057 is the inverse of the branching ratio for the 4p → 4s transition compared to 4p → 3d (Gallagher 1967). The absolute cross section for

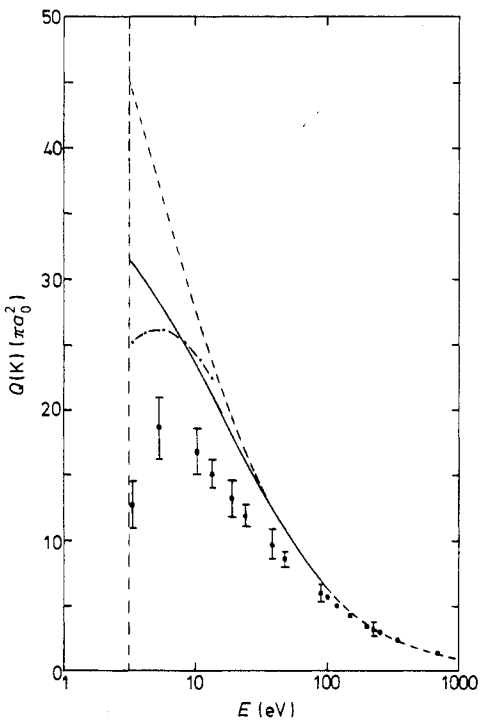

Figure 3. Emission cross section Q(K) (πa_0^2) for the K line of Ca^+ from threshold to 1 keV. Theoretical results: ----- CDWII (Burgess and Sheorey 1974); —— UDWPOII (this paper); –·–·– three-state close-coupling (Burke and Moores 1968). Experimental result: ● (Taylor and Dunn 1973).

emission of the K line has been measured by Taylor and Dunn (1973), who also confirmed that the ratio of the cross sections for K and H emission is 2·0 at all energies as expected in *LS* coupling. Taylor and Dunn further estimate that the contributions to their absolute measurements of the K-line emission due to cascade from higher states is at most $8(\pm 6)\%$.

In figure 3 we compare our UDWPOII results, the three-state close-coupling values of Burke and Moores (1968) and the CDWII calculations of Burgess and Sheorey (1974) for the emission cross section, Q(K), with the absolute experimental measurements of Taylor and Dunn. The UDWPOII results are in fair accord with the three-state close-coupling calculations, except at very low energies. However, the threshold values predicted by the UDWPOII and close-coupling models are, respectively, about 73% and 39% above the suggested experimental result of $18 \pm 2\,\pi a_0^2$ while at 13·6 eV the values from the two theoretical models are, respectively, 40% and 48% above the experimental result of $15{\cdot}1 \pm 1{\cdot}1\,\pi a_0^2$ at 13·3 eV. It does not seem likely that this low-energy discrepancy between theory and experiment can be resolved by the recent data of Zapesochnyi *et al* (1975), who present values for the K-line emission which are very similar to, though approximately 10% higher than, those of Dunn and Taylor from threshold to 100 eV.

At higher energies, the CDWII calculations of Burgess and Sheorey (1974) appear to merge smoothly into the UDWPOII results at about 50 eV and agree well with the data of Taylor and Dunn at energies greater than 200 eV. Thus, as in the case of Be^+, it does not appear that the low-energy discrepancy between theory and

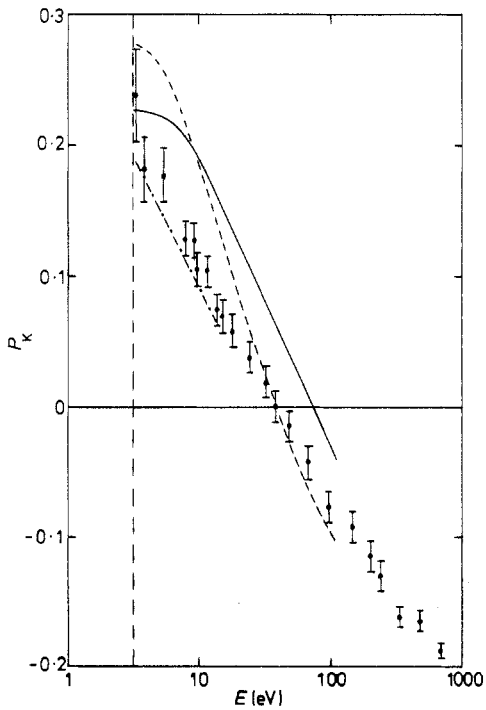

Figure 4. Polarisation fraction, P_K, for the K line of Ca^+. Theoretical results: ----- CBOII (this paper); —— UDWPOII (this paper); –·–·– three-state close-coupling (Burke and Moores 1968). Experimental results: ● (Taylor and Dunn 1973).

experiment for Ca^+ can be removed by any normalisation of the experimental data to the CDWII (or CBOII) results at high energies.

A further test is provided by Taylor and Dunn's measurement of the polarisation of the K-line emission for Ca^+ (that of the H line being zero). If $Q(M_L)$, $M_L = 0, \pm 1$, is the total (integrated) cross section for excitation of $|4pM_L\rangle$, then the polarisation fraction, P_K, of the K line at 90° to the incident beam is given by

$$P_K = \frac{3[Q(0) - Q(1)]}{5Q(0) + 7Q(1)}.$$

In figure 4, we illustrate the values obtained from Saraph (1970) using the two-state close-coupling reactance matrices of Burke and Moores (1968), together with our UDWPOII and CBOII results for P_K, and compare these with the experimental measurements of Taylor and Dunn. The close-coupling results are about 80% of those measured, while the UDWPOII values lie considerably too high at intermediate energies, though appearing to have a similar energy dependence. The CBOII results agree well with the experimental data in the region where P_K is approximately zero, but have a different energy dependence for larger and smaller values of the energy. Further work, on inclusion of higher levels and final-channel distortion, seems desirable.

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