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Two-electron excitation in helium-like ions by electron impact

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Abstract. Calculation of cross-sections for the two-electron excitation in helium-like ions by electron impact employing Coulomb-Born-Oppenheimer (CBO) approximation is presented. Analytical expressions for the differential and total scattering cross-sections without using partial wave expansion of the wavefunction reported earlier have been used. The total and differential scattering cross-sections for each of the excitations $1s^2\,{}^1S^e \rightarrow 2s^2\,{}^1S^e, 2s2p\,{}^{1,3}P^0, 2p^2\,{}^1S^e, {}^3P^e, {}^1D^e$ in Be^{2+} and B^{3+} are computed. Results for Li^+ reported earlier are also included for comparison.

Keywords. Two-electron excitation cross-section; electron impact; Coulomb-Born-Oppenheimer approximation.

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1. Introduction

Excited states involving simultaneous excitation of two electrons in atoms have gained interest recently (Fano 1983; Rau 1984). Such states not only in neutral species, but also of ions have been identified as important in astrophysics, atomospheric and laboratory plasma physics (Drawin 1981). The production of such states in neutral species by electron impact has been investigated theoretically (Massey and Mohr 1935; Becker and Dahler 1963, 1964; Fano 1964; Kulander and Dahler 1972; Roy and Sil 1976; Srivastava and Rai 1977; Hickerson *et al* 1978a, b; Mohan and Vidhani 1977; Williamson *et al* 1982; Ellis *et al* 1982; Srivastava and Kumar 1985; Srivastava and Williamson 1987; Padhy *et al* 1987) as well as experimentally (Burrow 1970; Westerveld *et al* 1979) in a few cases. It is seen that the simple Born-Oppenheimer (BO) approximation does provide a reasonable estimate for the total cross-sections (Becker and Dahler 1964; Kulander and Dahler 1972; Roy and Sil 1976; Hickerson *et al* 1978a; Srivastava and Rai 1977; Padhy *et al* 1987). No experimental measurement of cross-sections for electron-impact double excitation in any ionic species has been reported so far; but encouraged by the success of the BO approximation we performed (Padhy *et al* 1983a, b) recently a CBO calculation for the total cross-section for electron impact excitation of Li^+ from its ground state to each of the six low-lying doubly-excited states ($2s^2\,{}^1S^e; 2s2p\,{}^{1,3}P^0; 2p^2\,{}^1S^e, {}^3P^e, {}^1D^e$). Recently, a similar calculation employing the distorted wave (DW) method has been reported by Srivastava and Katiyar (1986).

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In this paper we have extended our previous investigation (Padhy *et al* 1983a, b) to the double excitations in Be^{2+} and B^{3+} and have also calculated the differential cross-sections. A comparative discussion of our earlier Li^+ result, vis-a-vis the more recent DW calculation (Srivastava and Katiyar 1986), is also included. The various excitation energy values for Li^+ have been obtained from the experimental results of Bruch *et al* (1975), while for Be^{2+} and B^{3+} these energies are obtained from the theoretical calculations due to Lipsky *et al* (1977). The experimental values for various ionization potentials of Li^+, Be^{2+} and B^{3+} have been taken from the compilation of Moore (1971). The details of the analytical work relating to closed-form expressions for the differential and total scattering cross-sections have been given in our earlier papers (Padhy *et al* 1983a, b).

2. Results and discussion

In figures 1–3 we graphically display the total cross-sections for electron impact double excitation in Li^+, Be^{2+} and B^{3+}, respectively, as a function of the incident electron energy. We have also displayed the DW results of Srivastava and Katiyar (1986) in figure 1 for comparison. The differential scattering cross-sections for excitation in Li^+ are plotted in figure 4 as a function of the angle of scattering (θ) for a typical impact energy, 200 eV. In figure 5 the corresponding differential cross-sections for Be^{2+} have been displayed as a function of θ for 300 eV impact energy while the values for B^{3+} at an impact energy of 500 eV are given in figure 6 as a function of θ.

2.1 *Total cross-section*

The computed total cross-sections show a rapid increase in magnitude close to the energy threshold so as to reach a peak magnitude within approximately 15–20 eV of this threshold. A more gradual decrease of the cross-sections with the incident energy is then observed. In figures 1–3, the energy scale is such that this rise in cross-sections near threshold is difficult to visualize and we only see the higher energy decrease of the cross-sections. However, in each of the curves labelled *A*, *B* and *C* in figure 1 (corresponding to excitations to $2p^2\,{}^1S^e, {}^1D^e, {}^3P^e$ states, respectively) one does see a flat maximum quite close to the threshold.

The total cross-sections for the three states arising from the $2p^2$ configuration, i.e., $2p^2\,{}^1S^e, 2p^2\,{}^1D^e$ and $2p^2\,{}^3P^e$ are in the order $\sigma_{^3P^e} > \sigma_{^1D^e} > \sigma_{^1S^e}$ which is in the inverse sequence to the excitation energies. Similar is the case for the two states ${}^1P^0$ and ${}^3P^0$ arising from the configuration $2s2p$. The cross-section for the state with the lowest excitation energy is the largest and there seems a inverse monotonic relation between σ and ΔE_{ex}. The ${}^1S^e$ state arising from the configuration $2s^2$ is an exception as this has a cross-section which is smaller in magnitude than for the $2s2p\ {}^3P^0$ state. This general feature of the calculated cross-section holds also for Be^{2+} and B^{3+}.

The total cross-section for the excitation of all of these six doubly-excited states in the three ions seems to vary in the same manner as a function of incident electron energy when the incident energy minus the threshold energy is more than 2/3 times the threshold energy. This variation is qualitatively of the type $\sigma \sim A\exp(-bE)$ where *A* and *b* are positive constants. Comparison of the cross-section curves for Li^+, Be^{2+}

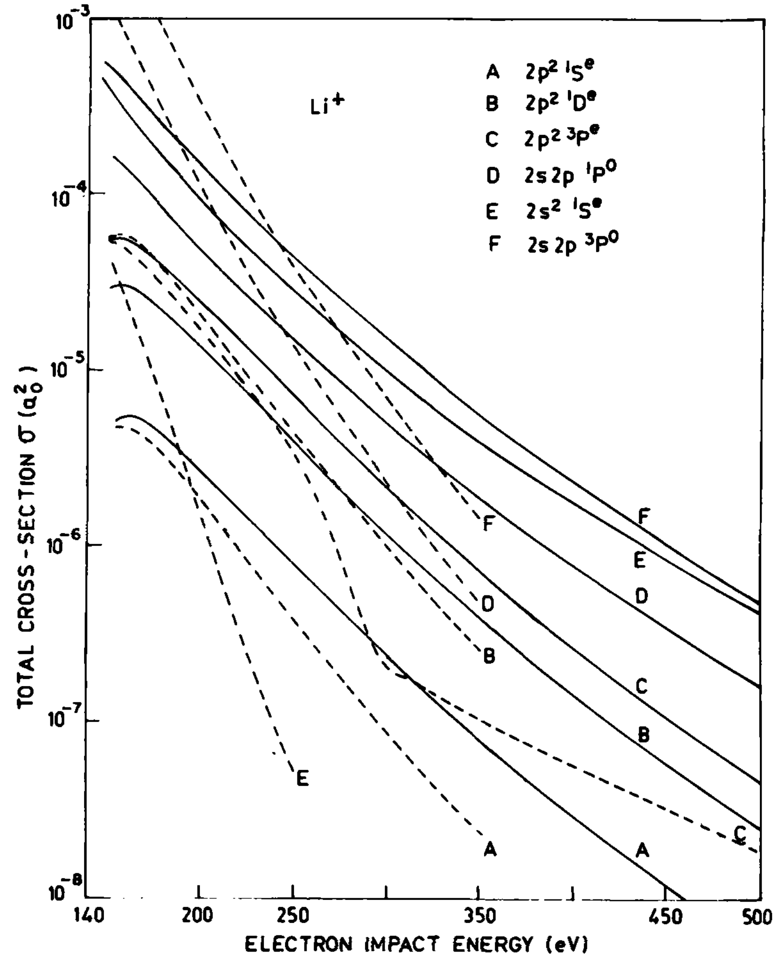

Figure 1. Total electron-impact excitation cross-sections for the first six low-lying doubly-excited states of Li^+ plotted against impact energy: (——) present CBO results, (....) DW results of Srivastava and Katiyar (1986).

and B^{3+} indicates that the value of the constant b tends to decrease slightly as the net charge on the ion increases.

Comparison with DW results for Li^+: Results of a recent study of the electron impact excitation of these six doubly-excited states in Li^+ using the distorted wave (DW) method by Srivastava and Katiyar (1986), are plotted in figure 1. It is observed that the two sets of calculations (the present one and that of Srivastava and Katiyar) show great divergence. Thus, while the cross-sections for excitation to the $2s2p\ {}^1P^0$ and the $2s2p\ {}^3P^0$ states are the largest in the DW method in the whole energy range, the cross-section for the $2s^2\ {}^1S^e$ state is the lowest. Similarly, for the three states ${}^3P^e$, ${}^1D^e$ and ${}^1S^e$ arising from the configuration $2p^2$, the DW cross-section for the ${}^1S^e$ state is the lowest in agreement with the fact that it has the highest excitation threshold, the

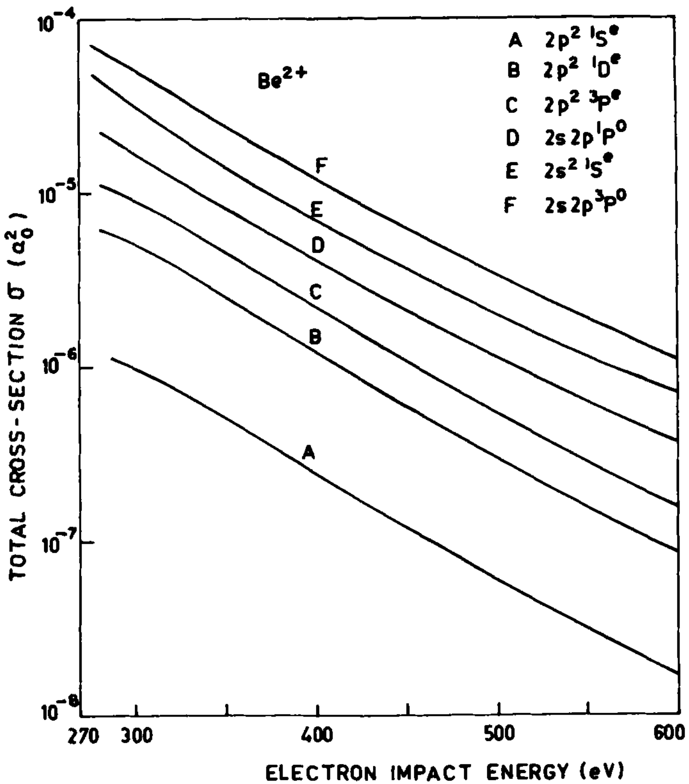

Figure 2. Total electron-impact excitation cross-sections for the first six low-lying doubly-excited states of Be^{1+} plotted against impact energy.

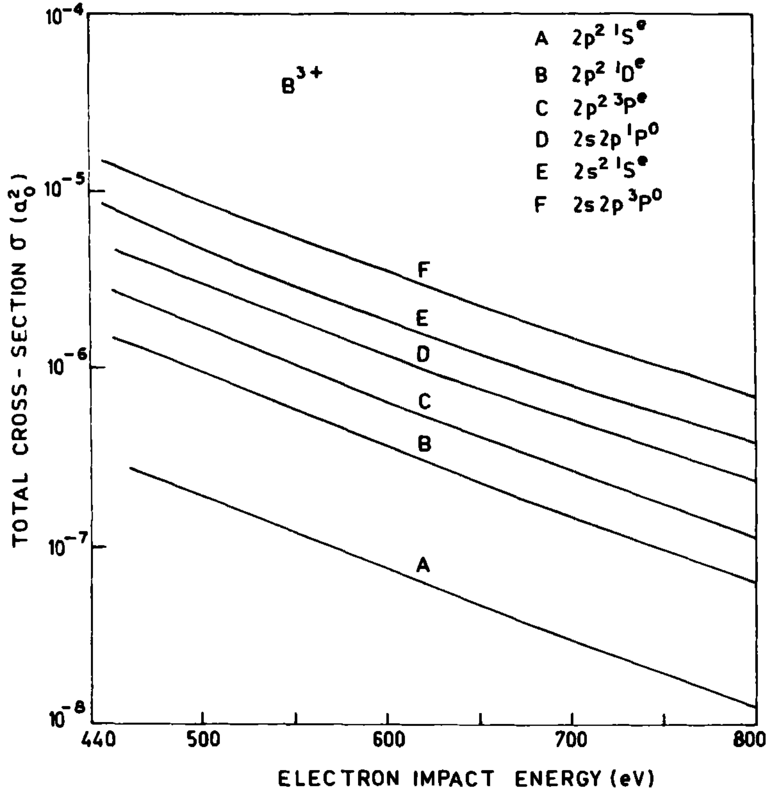

Figure 3. Total electron-impact excitation cross-sections for the first six low-lying doubly-excited states B^{3+} plotted against impact energy.

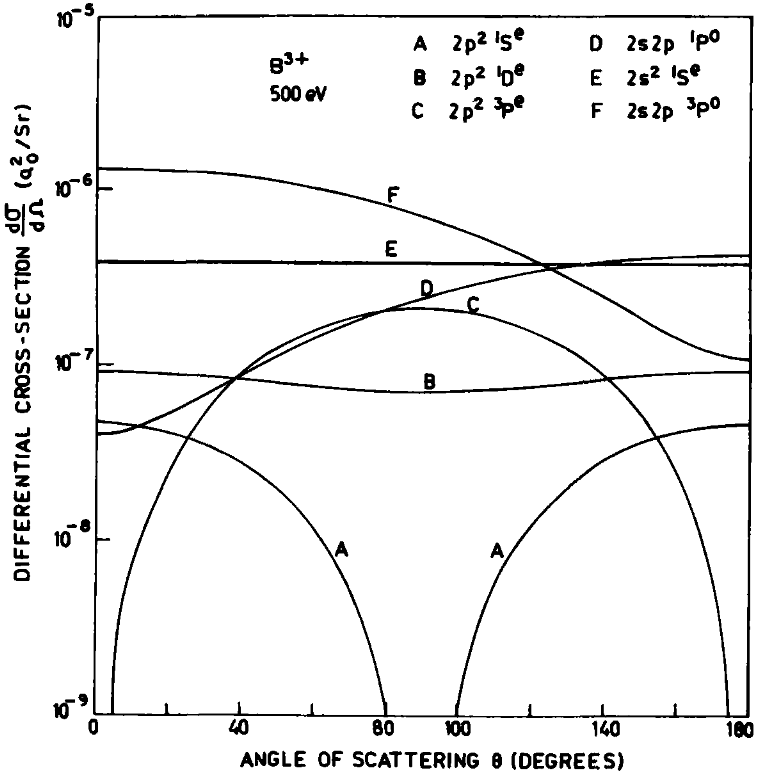

Figure 4. Electron-impact excitation (differential) cross-sections for the first six low-lying doubly-excited states of B^{3+} against angle of scattering at 500 eV impact energy.

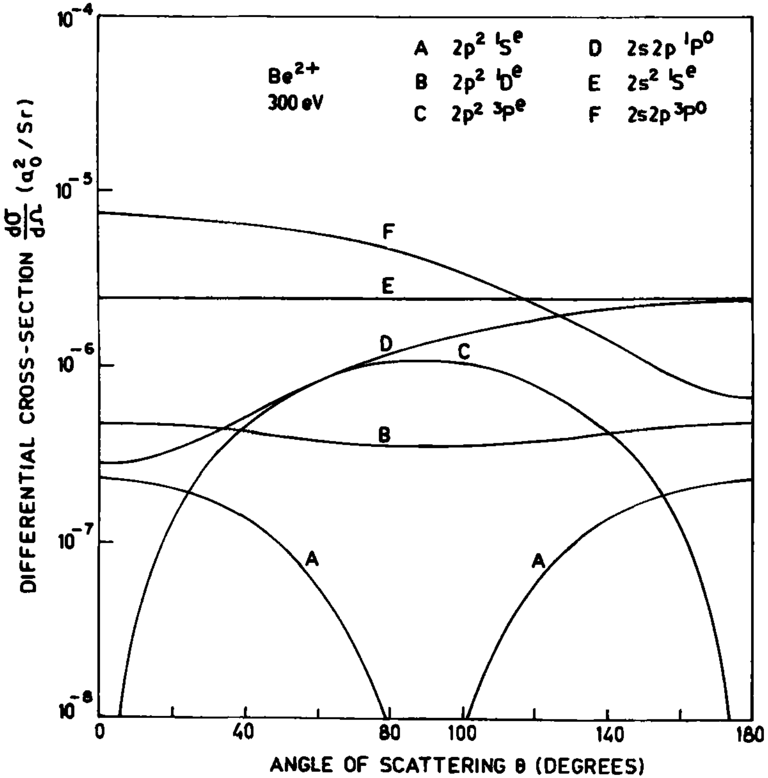

Figure 5. Electron-impact excitation (differential) cross-sections for the first six low-lying doubly-excited states of Be^{2+} against angle of scattering at 300 eV impact energy.

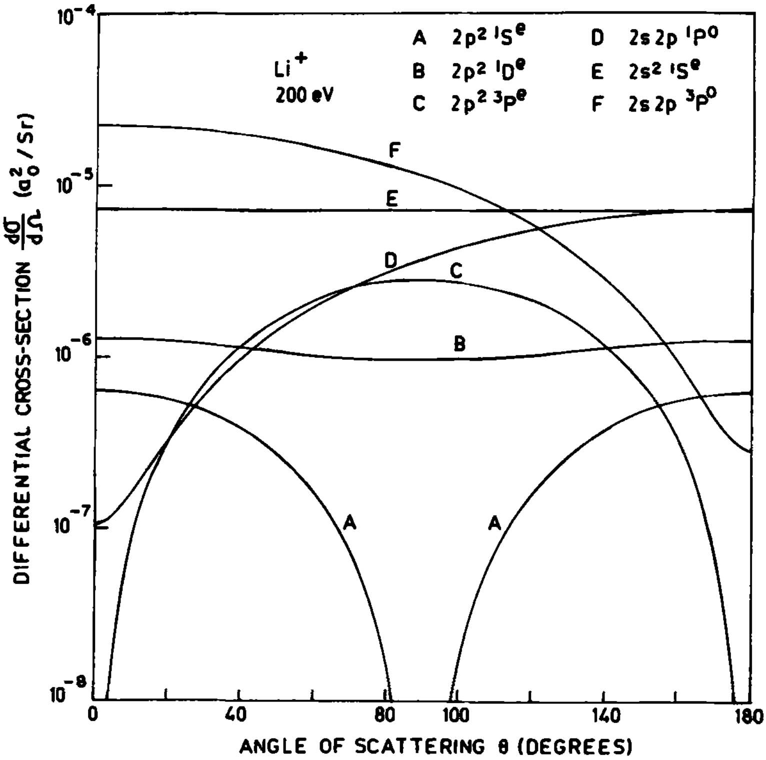

Figure 6. Electron-impact excitation (differential) cross-sections for the first six low-lying doubly-excited states of Li^+ against angle of scattering at 200 eV impact energy.

DW cross-section for the $^3P^e$ state is smaller than for the $^1D^e$ state while their excitation energies are in the order $E(^3P^e) < E(^1D^e)$. Further, while the DW cross-section curves for all the other states show a monotonic decrease with increasing incident energy, the $^3P^e$ state shows a change of shape near 300 eV. No explanation of this feature is available. Another intriguing feature that emerges from a comparison of the DW and CBO results is that whereas for the $2p^2\,{}^3P^e$ and $2p^2\,{}^1S^e$ states the two results are quite close to one another near the peak of the cross-section curve, the DW result for the $2p^2\,{}^1D^e$ state is much larger than the CBO result near the peak. Again, for the $2s^2\,{}^1S^e$ state the DW result is much lower than the corresponding CBO result whereas for the $2s2p\,{}^1P^0$ and $2s2p\,{}^3P^0$ states the DW result is much larger in the low impact energy region. At higher incident energies, the DW results are almost always much lower than the CBO results.

2.2 *Differential cross-section*

From figures 4–6 we observe that the shape of the differential scattering cross-section versus angle of scattering (θ) curve for excitation to a particular doubly-excited state remains unchanged with change in nuclear charge. This is not surprising since the variation is largely determined by the angular symmetries of the wavefunctions for the initial and the final target states. Thus for excitation to the $2s^2\,{}^1S^e$ state the differential cross-section is independent of the scattering angle, a result which is a reflection of the spherical symmetry of the orbitals involved. The curve corresponding to $2p^2\,{}^3P^e$ excitation clearly shows a $\sin^2\theta$ dependence in agreement with the general result obtained by Fano (1964) and the observation of Becker and Dahler (1963, 1964), since of all the doubly-excited states considered presently, the $2p^2\,{}^3P^e$ state is the only one which cannot autoionize and $1s^2\,{}^1S^e \rightarrow 2p^2\,{}^3P^e$ is a parity unfavoured transition. The two segments for the $2p^2\,{}^1S^e$ curve indicate that the differential cross-section tends to zero as $\theta \rightarrow \pi/2$ and has a maximum for $\theta = 0$ or π. This behaviour is clearly reflected in the analytical expression in which we find that $2p^2\,{}^1S^e$ cross-section is proportional to $\cos^2\theta$. The differential scattering cross-section for excitation to the $2p^2\,{}^1D^e$ state attains the same maximum value in the forward as well as the backward direction, falls very slowly with an increase in the scattering angle, and becomes minimum at $\theta = \pi/2$. The curve is symmetric about $\theta = \pi/2$. These observations for the $2p^2\,{}^1S^e$ and ${}^1D^e$ case can be traced back to the fact that (if one considers the atomic states arising from the p^2 configuration) the ${}^1S^e$ state arises from the $2p_0$ components, while the ${}^1D^e$ state involves the $2p_{\pm 1}$ as well as the $2p_0$ states.

The $2s2p\,{}^1P^0$ curve shows that the differential cross-section is minimum in the forward direction, slowly increases with the angle of scattering and attains a maximum value in the backward direction. This maximum value is almost equal to the $2s^2\,{}^1S^e$ cross-section. The differential cross-section for exciting the $2s2p\,{}^3P^0$ state is maximum in the forward direction, falls slowly with the increase in the angle of scattering and attains a minimum value in the backward direction. In the approximate description of the excited states used in the present work, the states $2s2p\,{}^1P^e$ and $2s2p\,{}^3P^0$ have spatial wavefunctions of the type $2s(1)2p(2) \pm 2s(2)2p(1)$, respectively. One would, therefore, expect the differential cross-sections for the two states to show a nearly complementary behavior, in agreement with what is observed. One must, however, keep in mind that the inclusions of angular and radial correlations between the two excited electrons may have very significant consequences, and the above qualitative considerations may need revision [see Greene and Rau 1983].

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