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Electron impact optical excitation of helium-like ions in Coulomb-Glauber approximation

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Abstract. The Coulomb-Glauber approximation is applied to evaluate the electron-impact excitation integrated cross sections for $1^1S - n^1P$ ($n = 2, 3$) transitions in helium-like ions, C^{4+}, N^{5+}, O^{6+} and Ne^{8+}. The results are presented in terms of scaled collision strength $n^3Z^2k_i^2\sigma$ and scaled integrated cross-section $Z^4\sigma$. Our values when compared with other available theoretical results are found to be larger than the Coulomb-Born and distorted wave polarised orbital (DWPO) values.

Keywords. Electron impact excitation; helium-like ions; Coulomb-Glauber approximation.

1. Introduction

Electron-impact excitation of positive ions has been currently receiving considerable attention, as the excitation cross-sections for this process are of fundamental importance in astrophysics and plasma physics. Recently Seaton (1975) reviewed the various approaches used for a theoretical study of the electron-impact excitation. Dolder and Peart (1976) have reviewed the experimental situation. However, hardly any measured cross-sections are available for electron-impact excitation of any helium-like ion. Tully (1974) has calculated collision strengths for electron-impact excitation of Li^+, Be^{2+} and O^{6+} from their ground states to n^1S and n^1P ($n \leqslant 6$) levels at impact electron energies $X = 1$, 2 and 3 threshold units using the Coulomb-Born (CB) method. Tully and Serrao (1974) have calculated the collisional strengths for $2^1S - n^1P$ and $2^3S - n^3P$ ($n \leqslant 6$) transitions for the same ions using the CB approach at $X = 1$, 2, 4 and 8. Vainshtein (1975) has calculated the cross sections for 1^1S—n^1P ($n = 2, 3$) excitation by slow electrons in Coulomb-Born-Oppenheimer (CBO) approximation and found that exchange contribution has considerable effect on excitation cross-sections for allowed transitions near the threshold. Nakazaki (1976) has used CB approximation for calculating electron-impact excitation cross-sections for C^{4+}, N^{5+}, O^{6+} and Ne^{8+} at incident energies from threshold to 20 keV for $1^1S - n^1P$ ($n =$ 2, 3) transitions to 1 keV for 2^3S—2^3P and to 2 keV for 2^3P—3^3P and 2^3P—3^3S transitions. Bhatia and Temkin (1977) have calculated the integrated cross-sections for electron ion impact excitation ($1^1S - 2^1S$, 2^1P, 2^3S, 2^3P) of two electron ions using distorted wave method. McDowell *et al* (1977) have applied the distorted wave polarised orbital (DWPO) model for evaluating the electron impact excitation cross-sections for one-electron positive ions and for helium-like ions ($3 \leqslant Z \leqslant 10$ and Si^{12+},

Ca^{18+} and Fe^{24+}). Very recently Tully (1978) has calculated the integrated cross-section for collisional excitation of 1^1S-2^3S transition in helium-like ions with atomic number $2 \leqslant Z \leqslant 8$ using a modified form of the Oppenheimer approximation. Das *et al* (1978) have studied the excitation of helium-like ions by electron-impact in CBO approximation. Van Wyngaarden *et al* (1979) have calculated the collisional strengths for excitation of Li^+, C^{4+}, O^{6+} and Si^{12+} from their ground states to the $n = 2$ states (2^3S, 2^1S, 2^3P and 2^1P) in the energy range from near threshold to five times the threshold energy solving five-state close-coupling equations. Recently Thomas and Franco (1976), Thomas (1978), Narumi and Tsuji (1975) and Ishihara and Chen (1975) have extended the Glauber approximation to collisions of charged particles with ions. The Coulomb-Glauber (CG) scattering amplitudes obtained by these authors are essentially identical to each other though they have used somewhat different methods. The CG predictions for e^-— He^+ ($1s-2p$) integrated excitation cross-section are found to be reasonably reliable in the intermediate and high energy region when compared with experiment (Dashchenko *et al* 1975). Singh *et al* (1979) have studied electron-impact excitation of hydrogenic ions in a modified Coulomb-Glauber (MCG) approximation. It was found that the MCG approximation affects the differential cross-sections in comparison with the Coulomb-Glauber approximation in the large scattering-angle region only, but not the integrated cross-section. In the present paper we, therefore, use the CG approximation to study the integrated cross-sections for the electron-impact excitation of C^{4+}, N^{5+}, O^{6+} and Ne^{8+} for 1^1S-n^1P ($n = 2, 3$) transitions. Our aim is to investigate the scaled behaviour and the limiting form of the Coulomb-Glauber results in relation to other approaches.

In the next section, we outline the procedure. § 3 contains details of the calculation. The results are given and discussed in § 4.

2. Procedure

The Glauber amplitude F_{fi} ($\mathbf{q}$, k_i) for the inelastic scattering of a particle of charge Z_i scattered by a positive ion having a nuclear charge Z_n and N bound electrons is given by (Thomas and Franco 1976)

$$F_{fi}(\mathbf{q}, k_i) = \frac{ik_i}{2\pi} \int d^2b d\mathbf{x} \exp(i\mathbf{q}\cdot\mathbf{b})\, b^{-2i\Lambda_n}\, \phi_f^*(\mathbf{x})\,(1 - \exp(i\chi_a))\, \phi_i(\mathbf{x}) \quad (1)$$

where $\mathbf{k}_i$ is the incident wave vector, $\mathbf{q}$ is the momentum transfer, $\mathbf{r} = \mathbf{b} + \mathbf{z}$ is the position vector of the incident particle and $\mathbf{x}$ denotes the coordinates of the target electrons, $\phi_i(\mathbf{x})$ and $\phi_f(\mathbf{x})$ are respectively the initial and final state wavefunctions of the target ion,

$$\chi_a = \sum_{j=1}^{N} 2\eta \ln\left(\frac{\mathbf{b} - \mathbf{s}_j}{b}\right) \quad (2)$$

with $\eta = -Z_i/k_i$, $\mathbf{s}_j$ is the projection of $\mathbf{x}_j$ onto the plane containing $\mathbf{q}$ and $\mathbf{b}$,

$$\Lambda_n = -Z_i(Z_n - N)/k_i. \quad (3)$$

Equation (1) is similar to the conventional form of Glauber scattering amplitude for scattering from a neutral atom except for the difference that it contains an additional b dependent phase factor $\mathbf{b}^{-2i\Lambda_n}$.

We assume that the wavefunctions ϕ_i and ϕ_f are such that the product of $\phi_f^* \phi_i$ may be written as

$$\phi_f^* \phi_i = \prod_{j=1}^{N} \left(\sum_{k=1}^{N_j} C_{k,j}\, x_j^{n_{k,j}} \exp(-\alpha_{k,j}\, x_j) \right) Y_{l_j m_j}(\theta_j, \phi_j)\, Y^*_{l'_j m'_j}(\theta_j, \phi_j). \tag{4}$$

For $1\,{}^1S$–$n\,{}^1P$ ($n = 2, 3$) transitions in the two-electron ion, we have

$$\begin{aligned} &l_1 = l_2 = m_1 = m_2 = 0, \\ &l'_1 = m'_1 = 0, \\ &l'_2 = 1,\ m'_2 = 0, \pm 1, \end{aligned} \tag{5}$$

and $\phi_f^* \phi_i$ may be written as

$$\phi_f^* \phi_i = \prod_{j=1}^{2} P_j,$$

where

$$P_j = a_j \left(\sum_{k=1}^{N_j} C_{k,j}\, x_j^{n_{k,j}} \exp(-\alpha_{k,j}\, x_j) \right) \tag{6}$$

$$a_1 = \frac{1}{4\pi} \text{ and } a_2 = Y^*_{\mathrm{l}m'_2}(\theta_2, \phi_2) \,/\, \sqrt{4\pi}. \tag{7}$$

Using (6) and (7) in (1) we get

$$F_{fi}(\mathbf{q}, k_i) = -\frac{ik_i}{2\pi} \int d^2 b \exp(i\mathbf{q}\cdot\mathbf{b})\, b^{-2i\Lambda_n} \prod_{j=1}^{2} \int P_j \left[\frac{|\mathbf{b}-\mathbf{s}_j|}{b} \right]^{2i\eta} d\mathbf{x}_j. \tag{8}$$

Integration over $d\mathbf{x}_j$ can now be carried out in the standard way (Franco 1971; Thomas and Gerjuoy 1971; Kumar and Srivastava 1975, 1976) to give

$$\int P_1 \left[\frac{|\mathbf{b}-\mathbf{s}_1|}{b} \right]^{2i\eta} d\mathbf{x}_1 = \frac{1}{4\pi} \sum_{k=1}^{N_1} C_{k,1} (-1)^{1+n_{k,1}} \times \left(\frac{\partial}{\partial \alpha_{k,1}} \right)^{1+n_{k,1}} I(\alpha_{k,1}, b) \tag{9}$$

$$= \frac{1}{4\pi} T_1(b) \tag{10}$$

where $$I(a_{k,1}, b) = 2b^2 E(\eta) \int_0^\infty dt\, t^{-2i\eta} \frac{d}{dt}\left(\frac{J_0(t)}{t^2 + (a_{k,1} b)^2}\right), \tag{11}$$

$$E(\eta) = -\pi\, 2^{1+2i\eta} \frac{\Gamma(1+i\eta)}{\Gamma(1-i\eta)}, \tag{12}$$

and $$\int P_2 \left[\frac{|\mathbf{b}-\mathbf{s}_2|}{b}\right]^{2i\eta} d\mathbf{x}_2 = \mp \frac{\sqrt{6}}{8\pi} \exp(\mp i\phi_b) \left[8i\,\eta E(\eta)\, b^3 \sum_{k=1}^{N_2} C_{k,2} (-1)^{n_{k,2}} \left(\frac{\partial}{\partial a_{k,2}}\right)^{n_{k,2}} H(a_{k,2} b)\right]$$

$$= \mp \frac{\sqrt{6}}{8\pi} \exp(\mp i\phi_b)\, T_2(b) \tag{13}$$

where $$H(a_{k,2} b) = \int_0^\infty \frac{J_1(t)\, t^{-2i\eta}}{(t^2 + a_{k,2}^2 b^2)^2} dt. \tag{14}$$

Putting (9) and (13) in equation (8) and carrying out integration with respect to ϕ_b finally yields

$$F_{fi}(\mathbf{q}, k_i; m_2' = \pm 1) = \pm \frac{\sqrt{6}\, k_i}{32\pi^2} \exp(\mp i\phi_q) \times \int_0^\infty db\, b\, J_1(qb) b^{-2i\Lambda_n} T_1(b)\, T_2(b). \tag{15}$$

The differential and integrated cross-sections are given by

$$\frac{d\sigma(q)}{d\Omega} = \frac{k_f}{k_i} [|F_{fi}(\mathbf{q}, k_i; m_2' = 1)|^2 + |F_{fi}(\mathbf{q}, k_i; m_2' = -1)|^2] \tag{16}$$

and $$\sigma(k_i) = \frac{2\pi}{k_i k_f} \int_{k_i-k_f}^{k_i+k_f} \frac{d\sigma}{d\Omega} q\, dq. \tag{17}$$

3. Calculation

For ground state of the two-electron ions considered here we have chosen variational wavefunctions of Green *et al* (1954) having the analytic form

$$\phi_i(\mathbf{x}_1, \mathbf{x}_2) = u(\mathbf{x}_1)\, u(\mathbf{x}_2), \tag{18}$$

with $$u(\mathbf{x}) = N[\exp(-px) + \lambda \exp(-qx)]\ Y_{oo}(\theta, \phi). \quad (19)$$

For excited state we use the wavefunctions of Nakazaki (1976) which are of the form

$$\phi_f(\mathbf{x}_1, \mathbf{x}_2) = u_1(\mathbf{x}_1)\, u_2(\mathbf{x}_2) + u_1(\mathbf{x}_2)\, u_2(\mathbf{x}_1). \quad (20)$$

The orbital u_1 in this case has the form

$$u_1(\mathbf{x}) = N \exp(-\alpha x)\ Y_{oo}(\theta, \phi), \quad (21)$$

while the orbital u_2 is of the form

$$u_2(\mathbf{x}) = Nx \exp(-px)\ Y_{lm}(\theta, \phi) \quad (22)$$

for $2^1\,P$ states and

$$u_2(\mathbf{x}) = N\,[x \exp(-px) + \lambda x^2 \exp(-qx)]\ Y_{lm}(\theta, \phi) \quad (23)$$

for 3^1P states.

4. Results and discussion

The integrated cross-sections for the dipole-allowed transitions ($1^1S - 2^1P$ and $1^1S - 3^1P$) in helium-like ions are calculated by using eqs (15) to (17). The wave-functions for the ground state of the ions, used in the present calculation are identical to those used by McDowell *et al* (1977) (for C^{4+}) and Nakazaki (1976). For N^{5+}, O^{6+} and Ne^{8+} McDowell *et al* have used wave-functions of Morse *et al* (1935). For excited states McDowell *et al* have taken the frozen-core Hartree-Fock (FCHF) wave-functions of Cohen and McEachran (1967a, b) and McEachran and Cohen (1969). These wave-functions are represented as a product of the core-orbital and the valence-orbital. The core-orbital has the hydrogenic form while the valence-orbital is expressed as a series of associated Laguerre functions. The appearance of Laguerre functions in the target wave-functions makes the Glauber calculations unnecessarily complicated. We have therefore used Nakazaki's wave-functions which have simple analytic form and predict for O^{6+} the oscillator strength and the Coulomb-Born cross-section (within 2% accuracy) results of Tully (1974) who has used the FCHF wave-functions of Cohen and McEachran for both the initial and final states of the ion.

The results can be expressed either as scaled cross-sections $Z^4\sigma$ against scaled energy E_Z or following Tully (1973), as scaled collision strength $\Omega' = n^3 Z^2 k_i^2 \sigma$ for a mutual comparison of results in any isoelectronic sequence. It is known (Seaton 1975) that $Z^4 E_Z \sigma$, where $E_Z = k_i^2/Z^2$, tends to a definite limit as Z tends to infinity for fixed k_i^2 for any isoelectronic sequence. In table 1, we have presented the scaled collision strengths for $1^1S - 2^1P$ transitions along with those obtained from DWPO results of McDowell *et al* (1977) and CB results of Tully (1974), where available. Table 2 gives the scaled collision strengths for $1^1S - 3^1P$ transitions. To have an overall comparative view of the various results we have plotted in figure 1, the scaled

Table 1. Scaled collision strengths $\Omega' = n^3 Z^2 k_i^2 \sigma$ for $1^1S - n^1P$ ($n = 2$) transitions of helium-like ions.

X		Ions			
		C^{4+}	N^{5+}	O^{6+}	Ne^{8+}
1·5	P	27·7	29·9	31·6	33·9
2	P	37·5	39·8	42·0	44·3
	MC	25·29	25·07	25.96	—
	T	—	—	37·4	—
3	P	49·03	51·3	53·3	54·9
	MC	38·13	37·11	38·23	39·66
	T	—	—	47·8	—
4	P	57·0	60·0	62·8	61·5
	MC	47·45	45·96	47·22	48·98
5	P	63·9	63·2	69·2	71·3
	MC	54·75	52·86	54·28	56·08
10	P	81·5	83·3	85·4	85·2
	MC	73·0	74·70	76·40	79·11

$X = E/\Delta E$ (incident energy in threshold units); P, present results; MC, results of McDowell *et al.* (1977); T, results of Tully (1974).

Table 2. Scaled collision strengths $\Omega' = n^3 Z^2 k_i^2 \sigma$ for $1^1S - n^1P$ ($n = 3$) transitions of helium-like ions. $X = E/\Delta E$ (incident energy in threshold units)

X	Ions			
	C^{4+}	N^{5+}	O^{6+}	Ne^{8+}
1·5	20·66	21·97	22·82	23·79
2·0	27·71	28·96	29·67	30·65
3·0	36·18	36·96	37·02	38·51
4·0	41·82	42·29	42·86	42·59
5·0	45·56	46·44	45·66	47·59
10·0	57·58	63·69	60·99	62·17

cross-sections $Z^4\sigma$ against $E/25Z^2$. We have also shown the scaled cross-sections obtained from DWPO results of McDowell *et al* (1977), the CB results of Nakazaki (1976), and the CB and DW results of Bhatia and Temkin (1977). Scaled cross-sections for C^{4+} and O^{6+} obtained from five-state close-coupling results of van Wyngaarden *et al* (1979) are also shown. They have used configuration-interaction functions for initial and final states using $1s$, $2s$ and $2p$ Slater type orbitals. For O^{6+} the scaled cross-sections obtained from Tully's CB results (1974) and from Bhatia and Temkin's results (1977) of the University College, London (UCL) distorted wave code are also shown. Our scaled cross-sections lie above all the other results, but approach the CB values of Nakazaki, as the incident energy increases. The CB results of Bhatia and Temkin (1977) who have used simpler ground state and excited state wavefunctions (Morse *et al* 1935) are nearly identical with those of Nakazaki in the case of N^{5+} and Ne^{8+},

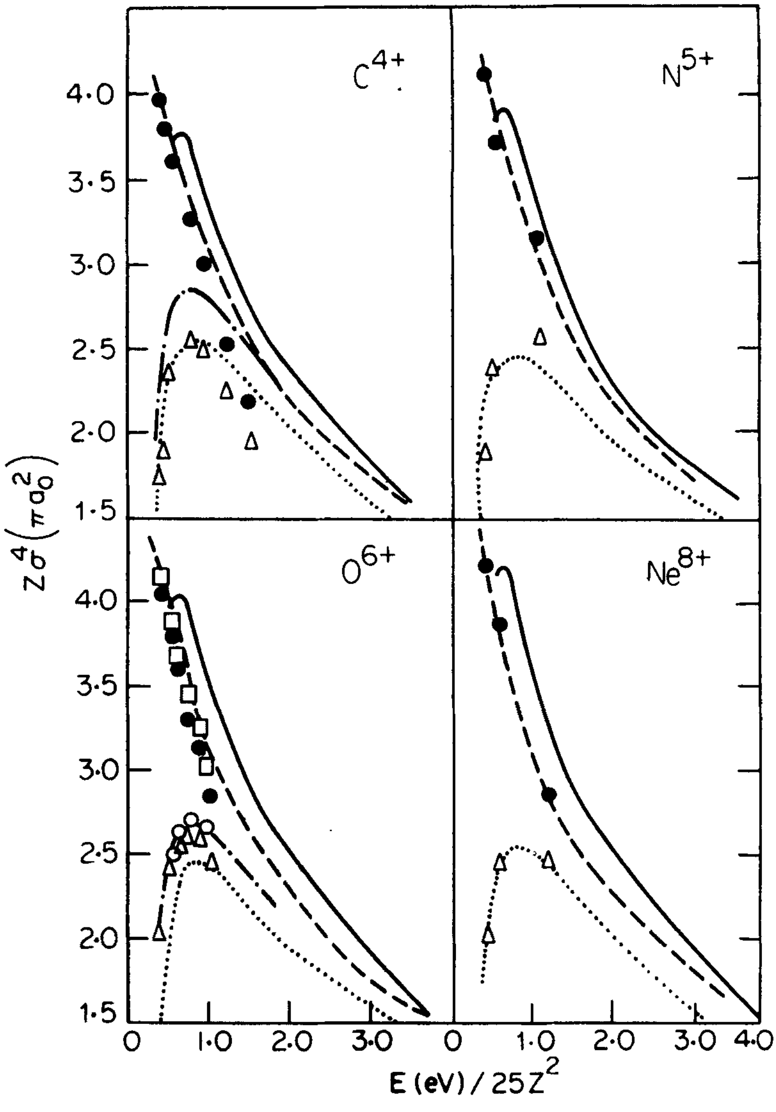

Figure 1. Scaled integrated cross-sections $Z^4\sigma$ in units of πa_0^2 for $1^1S - 2^1P$ excitation of C^{4+}, N^{5+}, O^{6+} and Ne^{8+} plotted against $E(eV)/25Z^2$.—, present results; ———, results of Nakazaki (1976); ......, DWPO results of McDowell *et al* (1977); ●, CB results; △, DW results of Bhatia and Temkin (1977); □, CB results of Tully (1974); ○, results of UCL distorted-wave code (Bhatia and Temkin 1977); —. —. —, results of van Wyngaarden *et al* (1979).

but for C^{4+} and O^{6+}, they differ from it and the difference increases with the increase of energy. In the case of O^{6+}, where the CB results of Tully (1974) are available, the results of Nakazaki and Tully are practically the same. The difference in the various CB calculations is perhaps due to the different choice of target wavefunctions. The DWPO results of McDowell *et al* and the DW results of Bhatia and Temkin are comparatively closer to each other, but they are much lower than the CB results. The results of van Wyngaarden *et al* (1979) are in good agreement with those of the DWPO results of McDowell *et al* (1977) and the DW results of Bhatia and Temkin (1977) at lower energies. The UCL distorted wave code results of Bhatia and Temkin (1977) are in excellent agreement with those of van Wyngaarden *et al* throughout the entire energy range, where they are available. However, for C^{4+}, the results of van Wyngaarden approach the CB results at higher energies. In figure 2 we have shown our scaled cross-sections for 1^1S — 3^1P transitions along with the CB results of Nakazaki. In this case also our results stand higher than those of Nakazaki. A similar feature is observed by Thomas (1978) and Singh *et al* (1979) in the case of 1*s* — 2*p* scaled excitation cross-sections for electron impact excitation of hydrogenic ions. The scaled CG excitation cross-sections increase with ionic nuclear charge and overtake the CB results. In the case of 1*s* — 2*s* excitation also, the scaled cross-sections increase with the ionic nuclear charge but are not able to overtake the CB results. The result is that the CB limit for 1*s* — 2*s* excitation lies above the CG results. For 1*s* — 2*p* excitation the reverse is true. The relative magnitude of limiting values of CB and CG results really depends on the convergence of Coulomb-Born series since the CG results contain contributions coming from higher order Born terms.

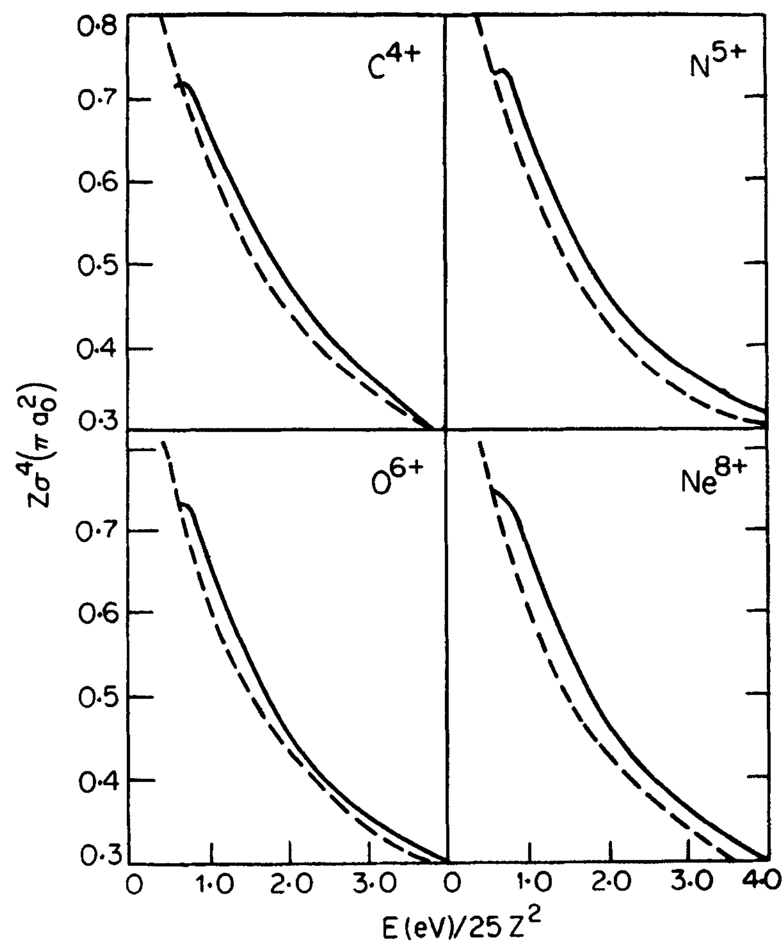

Figure 2. Scaled integrated cross-section $Z^4\sigma$ in units of πa_0^2 for 1^1S — 3^1P excitation of C^{4+}, N^{5+}, O^{6+} and Ne^{8+} plotted against E(eV)/25Z^2. —, present results; — — —, results of Nakazaki (1976).

To summarize, the present CG results stand higher but exhibit the same general trend of variation with energy as the CB results. Neither of them could be used near the threshold where the DWPO results of McDowell *et al* (1977), the DW results of Bhatia and Temkin (1977) and the close-coupling results of van Wyngaarden appear certainly superior. The exchange contribution has been ignored. It would mainly affect the present results near the threshold region where these Coulomb-Glauber predictions in any case fail as expected on general theoretical grounds. In the intermediate and high energy region, looking at the results of the inelastic scattering of electrons by neutral atoms and He^+, one expects CG predictions to be better than those of CB. In the absence of any experimental data it is difficult to draw any definite conclusions.

References

Bhatia A K and Temkin A 1977 *J. Phys.* **B10** 2893
Cohen M and McEachran R P 1967a *Proc. Phys. Soc.* **92** 37
Cohen M and McEachran R P 1967b *Proc. Phys. Soc.* **92** 539
Das A K, Maiti N and Sil N C 1978 *Indian J. Phys.* **B52** 83
Dashchenko A I, Zapesochnyi I P, Imre A I, Bukstick V S, Danch F F and Kelman V A 1975 *Sov. Phys. JETP* **40** 249
Dolder K T and Peart B 1976 *Rep. Prog. Phys.* **39** 693
Franco V 1971 *Phys. Rev. Lett.* **26** 1088
Green L C, Mulder M M, Lewis M N and Woll J W 1954 *Phys. Rev.* **93** 757
Ishihara T and Chen J C Y 1975 *J. Phys.* **B8** L417
Kumar S and Srivastava M K 1975 *Phys. Rev.* **A12** 801
Kumar S and Srivastava M K 1976 *Phys. Rev.* **A13** 1307
McDowell M R C, Morgan L A, Myerscough V P and Scott T 1977 *J. Phys.* **B10** 2727
McEachran R P and Cohen M 1969 *J. Phys.* **B2** 1271
Morse P M, Young L A and Haurwitz E S 1935 *Phys. Rev.* **48** 948
Nakazaki S 1976 *J. Phys. Soc. Jpn* **41** 2084
Narumi H and Tsuji A 1975 *Prog. Theor. Phys.* **53** 671
Seaton M J 1975 *Advances in atomic and molecular physics*, ed D R Bates and B Bederson (New York: Academic Press) Vol. II, pp. 83
Singh S N, Kumar S and Srivastava M K 1979, *J. Phys.* **B12** 2351
Thomas B K 1978 *Phys. Rev.* **A18** 452
Thomas B K and Franco V 1976 *Phys. Rev.* **A13** 2004
Thomas B K and Gerjuoy E 1971 *J. Math. Phys.* **12** 1567
Tully J A 1973 *Can J. Phys.* **51** 2047
Tully J A 1974 *J. Phys.* **B7** 386
Tully J A 1978 *J. Phys.* **B11** 2923
Tully J A and Serrao J M P 1974 *Astr. Astrophys.* **23** 15
Vainshtein L A 1975 *Soviet Phys. JETP* **40** 32
van Wyngaarden W L, Bhadra K and Henry R J W 1979 *Phys. Rev.* **A20** 1409