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Electron impact excitation of the 2^1S state of helium at intermediate and high energies

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Abstract. The electron impact excitation of the 2^1S state of helium has been studied using the method of Das in the energy range 50–500 eV. The results for differential and integrated cross sections show good agreement with the experimental measurements over the entire angular scattering region.

1. Introduction

The computational method of Das (see Das *et al* 1981, Das and Biswas 1981) has been applied previously in the study of the inelastic collision of electrons with atomic hydrogen, i.e. in the study of excitation of the 2S state of hydrogen at intermediate and high energies (see Das *et al* 1982, Saha 1983). The results show good agreement with the available experimental and theoretical results. Earlier, in a series of works, Das and his associates have shown that this method works equally well in the case of the elastic collisions of electrons with atomic hydrogen as well as with atomic helium. So, here also, we expect that the same method, when applied to the inelastic collision of electrons with atomic helium, will yield good results. To confirm such an expectation, in this paper the method of Das has been applied to the very important problem of the inelastic collision of electrons with atomic helium. We undertake the study of the problem of excitation of the 2^1S state of helium by the collision of electrons in the intermediate and high energy ranges.

Since, recently, a large number of experimental measurements for differential cross sections have become available (Vriens *et al* 1968, Chamberlain *et al* 1970, Opal and Beaty 1972, Suzuki and Takayanagi 1973, Dillon and Lassettre 1975, Yagishita 1978), the accuracy of this present work can be judged to a very large extent by comparing the present result with the available experimental results.

In this context, we may recall that this excitation problem has received considerable attention during the past few years. The problem has been studied by a number of researchers by employing various important methods. Hidalgo and Geltman (1972) applied the Coulomb projected Born approximation (CPB) method, developed earlier by Geltman (1971), to calculate the direct scattering amplitude for electron impact on atomic helium. The study does not account for any exchange effect. At high energies, the modified eikonal Born series (EBS) method (Byron and Joachain 1975), the Glauber approximation method (Yates and Tenney 1972), the second-order potential method (Bransden and Winters 1975, Winters *et al* 1977) are also being applied with reasonable

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success. The five-state R-matrix calculation of Fon *et al* (1978, 1979a, b, 1980) gives fairly good results, but the calculations in this method become difficult due to the inclusion of correlation terms in the expansion of total wavefunctions. The variable-charge Coulomb projected Born (VCCPB) approximation, developed by Schaub-Shaver and Stauffer (1980), was recently applied in the excitation problem of helium by Singh *et al* (1983). The results thus obtained show a fair amount of agreement in the intermediate and high energy ranges.

We begin in § 2 by recalling the basic features of the Das method. Details of the calculations and the approximations are described in § 3. The present results are presented and compared with those of the theoretical calculations and with experiments in § 4.

2. Theory: computational method of Das

In this section, we present a brief outline of the method of Das employed in the present calculation. In this method the T-matrix element $T_{fi}(\boldsymbol{K}_f, \boldsymbol{K}_i; \varepsilon_f, \varepsilon_i)$ for the 2^1S excitation of the helium atom is obtained by solving the infinite coupled set of integral equations (see Das *et al* 1981, for details of the calculations and for terminology) for the off-shell T-matrix elements

$$T_{ni}(\boldsymbol{p}_n, \boldsymbol{p}_i; \varepsilon_n, \varepsilon_i) = T^{\mathrm{B}}_{ni}(\boldsymbol{p}_n, \boldsymbol{p}_i; \varepsilon_n, \varepsilon_i) + \sum_I \int \mathrm{d}^3 p_I \, T^{\mathrm{B}}_{nI}(\boldsymbol{p}_n, \boldsymbol{p}_I; \varepsilon_n, \varepsilon_I) \frac{1}{E - p^2_{I/2} - \varepsilon_I + \mathrm{i}\eta} T_{Ii}(\boldsymbol{p}_I, \boldsymbol{p}_i; \varepsilon_I, \varepsilon_i) \tag{1}$$

by a least-squares method introduced by Das.

Following Das, one may start the calculation by choosing a trial set of input T-matrix elements,

$$T^{(\mathrm{in})}_{ni} = (a(E) + \mathrm{i}b(E)) T^{\mathrm{B}}_{ni} \tag{2}$$

where $a(E)$ and $b(E)$ are two energy-dependent variational parameters. The corresponding output T-matrix elements, are

$$T^{(\mathrm{out})}_{ni} = T^{\mathrm{B}}_{ni} + \sum_I \int \mathrm{d}^3 p_I \, T^{\mathrm{B}}_{nI} \frac{1}{E - p^2_{I/2} - \varepsilon_I + \mathrm{i}\eta} T^{(\mathrm{in})}_{Ii}. \tag{3}$$

The parameters $a(E)$ and $b(E)$ are next obtained by minimising the quantity

$$\int |T^{(\mathrm{out})}_{fi}(\boldsymbol{K}_f, \boldsymbol{K}_i; \varepsilon_f, \varepsilon_i) - T^{(\mathrm{in})}_{fi}(\boldsymbol{K}_f, \boldsymbol{K}_i; \varepsilon_f, \varepsilon_i)|^2 \, \mathrm{d}\Omega_f \tag{4}$$

where the on-shell values are used in the above expression. The on-shell values of the relevant output amplitude with the above optimal values of $a(E)$ and $b(E)$ give the required direct scattering amplitude. This may be written as

$$f_{\mathrm{d}} = (f^{\mathrm{B}}_{fi} + a_{\min}(E) f_{\mathrm{B}_2\mathrm{R}} - b_{\min}(E) f_{\mathrm{B}_2\mathrm{I}}) + \mathrm{i}(a_{\min}(E) f_{\mathrm{B}_2\mathrm{I}} + b_{\min}(E) f_{\mathrm{B}_2\mathrm{R}}) \tag{5}$$

where f^{B}_{fi} is the first Born scattering amplitude, $f_{\mathrm{B}_2\mathrm{R}}$ and $f_{\mathrm{B}_2\mathrm{I}}$ are respectively the real and imaginary part, for the second Born amplitude. Also, $a_{\min}(E)$ and $b_{\min}(E)$ are the minimised values of the variational parameters obtained from (4).

Having obtained the direct scattering amplitude in the manner described above, the exchange effect is taken into account by utilising the Ochkur approximation (Ochkur

1964) g^{och}. Finally, the differential scattering cross section is computed by using the relation

$$\frac{d\sigma}{d\Omega} = \frac{K_f}{K_i} |f_d - g^{\text{och}}|^2 \tag{6}$$

where K_i and K_f are respectively the initial and final wavenumbers of the colliding electron. Using the conservation of energy relation one may write

$$E = \tfrac{1}{2}K_i^2 + E_0 = \tfrac{1}{2}K_f^2 + E_n \tag{7}$$

where E_0 and E_n refer to the ground state and excited state of the energies of the target atom, respectively.

3. Atomic wavefunctions and numerical computations

In our present calculation we choose for the ground (1^1S) state of helium, the Hartree–Fock wavefunction of Byron and Joachain (1966), namely,

$$\Phi_i(\boldsymbol{r}_1, \boldsymbol{r}_2) = \Phi_i(r_1, r_2) \tag{8}$$

where

$$\Phi_i(r_1, r_2) = \Phi_{1S}(r_1)\phi_{1S}(r_2) \tag{9}$$

and

$$\Phi_{1S}(r) = (4\pi)^{-1/2}[A_1 \exp(-\alpha_1 r) + A_2 \exp(-\alpha_2 r)] \tag{10}$$

where A_1, A_2, α_1 and α_2 are all parameters associated with the following set of values

$$A_1 = 2.60605 \qquad A_2 = 2.08144 \qquad \alpha_1 = 1.41 \qquad \alpha_2 = 2.61.$$

For the excited (2^1S) state of helium the wavefunction of Byron and Joachain (1975) is used, namely,

$$\Phi_{2^1S}(\boldsymbol{r}_1, \boldsymbol{r}_2) = \frac{1}{4\pi\sqrt{1+\delta^2}}[u_1(r_1)u_2(r_2) + u_1(r_2)u_2^*(r_1)] \tag{11}$$

where

$$u_1(r) = M \exp(-2r)$$

$$u_2(r) = N[\exp(-\tau_1 r) - Sr \exp(-\tau_2 r)].$$

The parameters have the values

$$M = 6.656\,854 \qquad N = 0.619\,280$$

$$\tau_1 = 0.865 \qquad \tau_2 = 0.5222$$

$$S = 0.432\,784 \qquad \delta = 0.073\,077.$$

The characteristic features of this wavefunction are that it is orthogonal to the ground-state wavefunction and also it yields an energy $E_{2^1S} = -2.14312$ au, very near to its exact non-relativistic value of $E_{2^1S}^{\text{ex}} = -2.14597$ au (Pekeris 1962).

From the computational method of Das it is clear that to determine the differential cross section following this method one has to have the second Born term in the

simplest possible form. In the present calculation of the excited collision problem, the second Born term is computed by using the simplified second Born approximation. In this computation, we have used the value of mean excitation energy $\omega = 1.5$ following Byron and Joachain (1975) and the integration over all intermediate discrete and continuum states has been performed using the closure relation.

In order to determine the value of the final wavevector using (7), we have used the ground-state energy for helium following Pekeris (1959) and the excited-state energy of Pekeris (1962).

4. Results and discussions

We have calculated the total and differential cross sections for the singlet transitions at impact energies ranging from 50 to 500 eV. Our calculated differential cross sections are displayed in table 2 and they are compared with other theoretical and experimental results in figure 1 for the impact energies 100, 150 and 200 eV. In table 1, the dependence of the minimised values of a_{min} and b_{min} on the incident energy E is displayed. The results for the angular variation of differential cross sections at 100 eV are compared with the five-state R-matrix calculations of Fon *et al* (1980), second-order potential calculations of Bransden and Winters (1975), distorted-wave potential orbital (DWPO) calculations of Scott and McDowell (1975), calculations of Winters *et al* (1977) and with the experimental results of Suzuki and Takayanagi (1973), Yagishita (1978) and Crooks (1972). The comparison shows that no theoretical model has produced results in satisfactory agreement with the experimental differential cross section results for 2^1S excitation of helium over the whole angular range. However, the present result agrees well with the experimental measurement of Crooks, although, in the intermediate angular range, it overestimates Crook's experimental measurements. The R-matrix results are slightly higher than our present result throughout the angular region except in the angular range 10°–30°. The DWPO calculations of Scott and McDowell show a sharp dip around 50° and the results, in general, are much less than other estimates except in the small angular region. The computed results of Winters *et al* agree with the experimental results of Suzuki and Takayanagi, and Yagashita below 45°, but fall well below the experimental measurements above 45°. The results of the second-order potential calculations of Bransden and Winters are in agreement with ours except at angles below 15°. At 150 eV, our results, the

Table 1. Dependence of the variational parameters a_{min} and b_{min} on energy.

E (eV)	a_{min}	b_{min}
50	0.1841	0.5008
80†	0.5762	0.5152
100	0.6395	0.4588
150	0.6911	0.3643
200	0.7111	0.3172
300	0.7374	0.2679
400	0.7567	0.2390
500	0.7719	0.2182

† Calculations at 81.63 eV.

Table 2. Differential cross sections for $1\,^1S$–$2\,^1S$ excitation (in units of $a_0^2\ sr^{-1}$) for various energies of the incident electron. The superscript denotes the power of ten by which the number should be multiplied.

Angle (deg) \ E(eV)	50	81.63	100	150	200	300	400	500
0	1.330^{-1}	2.301^{-1}	2.433^{-1}	2.515^{-1}	2.549^{-1}	2.629^{-1}	2.725^{-1}	2.827^{-1}
10	1.099^{-1}	1.532^{-1}	1.427^{-1}	1.075^{-1}	8.305^{-2}	5.549^{-2}	4.075^{-2}	3.140^{-2}
20	6.546^{-2}	6.097^{-2}	4.629^{-2}	2.274^{-2}	1.299^{-2}	5.642^{-3}	3.029^{-3}	1.846^{-3}
30	3.052^{-2}	1.932^{-2}	1.219^{-2}	4.460^{-3}	2.367^{-3}	1.145^{-3}	7.046^{-4}	4.702^{-4}
40	1.244^{-2}	6.883^{-3}	4.328^{-3}	2.014^{-3}	1.320^{-3}	6.868^{-4}	3.930^{-4}	2.416^{-4}
50	5.629^{-3}	4.153^{-3}	3.035^{-3}	1.660^{-3}	1.022^{-3}	4.483^{-4}	2.290^{-4}	1.306^{-4}
60	3.851^{-3}	3.670^{-3}	2.769^{-3}	1.377^{-3}	7.560^{-4}	2.883^{-4}	1.365^{-4}	7.418^{-5}
70	3.709^{-3}	3.456^{-3}	2.497^{-3}	1.087^{-3}	5.453^{-4}	1.890^{-4}	8.525^{-5}	4.490^{-5}
80	3.880^{-3}	3.171^{-3}	2.168^{-3}	8.418^{-4}	3.960^{-4}	1.287^{-4}	5.616^{-5}	2.896^{-5}
90	3.983^{-3}	2.837^{-3}	1.845^{-3}	6.554^{-4}	2.943^{-4}	9.146^{-5}	3.901^{-5}	1.981^{-5}
100	3.970^{-3}	2.510^{-3}	1.566^{-3}	5.194^{-4}	2.255^{-4}	6.788^{-5}	2.848^{-5}	1.431^{-5}
110	3.875^{-3}	2.219^{-3}	1.339^{-3}	4.215^{-4}	1.786^{-4}	5.253^{-5}	2.177^{-5}	1.085^{-5}
120	3.740^{-3}	1.977^{-3}	1.162^{-3}	3.513^{-4}	1.462^{-4}	4.229^{-5}	1.737^{-5}	8.600^{-6}
140	3.466^{-3}	1.635^{-3}	9.258^{-4}	2.656^{-4}	1.080^{-4}	3.059^{-5}	1.241^{-6}	6.096^{-6}
160	3.277^{-3}	1.451^{-3}	8.054^{-4}	2.248^{-4}	9.036^{-5}	2.533^{-5}	1.021^{-5}	4.996^{-6}
180	3.212^{-3}	1.393^{-3}	7.686^{-4}	2.127^{-4}	8.521^{-5}	2.380^{-5}	9.575^{-6}	4.680^{-6}

calculations of Fon *et al*, and those of Bransden and Winters are almost in close agreement with each other throughout the scattering angular region except at very small angles, where our results lie between these two calculations and slightly overestimate the experimental measurements of Yagishita. At angles above 70° the R-matrix calculation slightly overestimates, while the second-order potential calculation slightly underestimates, the experimental measurements of Suzuki and Takayanagi. At the impact energy of 200 eV, the general features are similar to those for the impact energy of 100 eV. Here, the DWPO results of Scott and McDowell no longer show a sharp dip but are still on the lower side. The R-matrix results are on the higher side compared with the experimental measurements throughout the angular region except for angles below 40°. At this energy, our results are almost coincident with the results of the modified eikonal Born series (EBS) calculations of Byron and Joachain, and are in best agreement with the experimental measurements. Around 40°, the results of Byron and Joachain produce a peculiar bend in contrast to ours which have a smooth bend there. The results of Winters *et al* show a fair amount of accuracy, almost everywhere, except at intermediate angles, where they slightly underestimate the experimental results.

Since, the experimental results for differential cross sections for impact energies above 200 eV do not exist, we have presented in table 3 the results of the present calculations which are compared with the results of the first and second Born approximations and the results of Singh *et al* (1983).

Finally, in table 4, we have presented and compared the present results of the integrated cross sections with other theoretical calculations and with the experimental estimates of de Heer and Jansen (1977). For impact energies which do not exceed 100 eV the integrated cross sections calculated by all theoretical models are much higher than the experimental results: of all the results the results of Bhadra *et al*

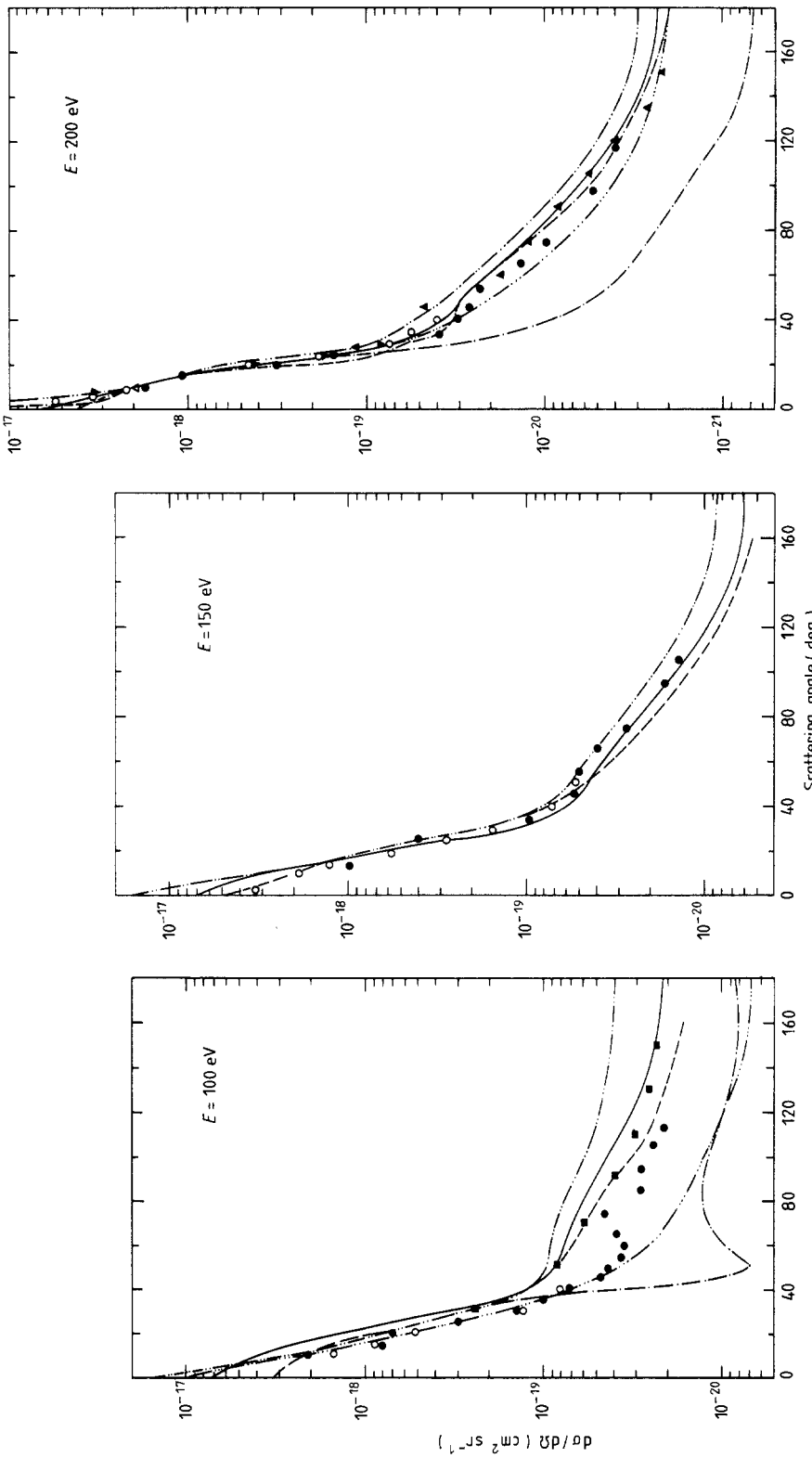

Figure 1. Differential cross sections for the process $e + He(1^1S) \rightarrow e + He(2^1S)$ at energies 100 eV, 150 eV and 200 eV. Theory: ——, present Das method of calculations; — . —, DWPO calculations of Scott and McDowell (1975); — . . —, five-state *R*-matrix calculations of Fon *et al* 1980; — . . . —, Winters *et al* (1977); — —, second-order potential calculations of Bransden and Winters (1975); – – . – –, Modified EBS calculations of Byron and Joachain (1975). Experiment: ●, Suzuki and Takayanagi; ○, Yagishita (1978); ▲, Opal and Beaty (1972); ▼, Dillon and Lassettre (1975); ■, Crooks (1972); △, Chamberlain *et al* (1970).

Table 3. Comparison of differential cross sections for 1^1S–2^1S excitation (in units of $a_0^2 S_r^{-1}$) for some energy E of the incident electrons. The superscript denotes the power of ten by which the number should be multiplied.

Energy (eV)	300				400				500			
Angle (deg)	a	b	c	d	a	b	c	d	a	b	c	d
0	2.629^{-1}	1.816^{-1}	2.165^{-1}	3.486^{-2}	2.725^{-1}	1.813^{-1}	2.295^{-1}	3.478^{-1}	2.827^{-1}	1.825^{-1}	2.411^{-1}	3.505^{-1}
30	1.145^{-3}	1.265^{-3}	1.240^{-3}	2.962^{-3}	7.046^{-4}	5.386^{-4}	4.487^{-4}	1.583^{-3}	4.702^{-4}	2.848^{-4}	1.900^{-4}	9.503^{-4}
45	5.571^{-4}	2.286^{-4}	6.558^{-5}	1.054^{-3}	2.998^{-4}	1.126^{-4}	1.817^{-5}	5.207^{-4}	1.768^{-4}	6.328^{-6}	6.366^{-6}	2.911^{-4}
60	2.883^{-4}	1.003^{-4}	5.987^{-6}	4.796^{-4}	1.365^{-4}	4.790^{-5}	1.434^{-6}	2.186^{-4}	7.418^{-5}	2.529^{-6}	4.549^{-7}	1.155^{-4}
90	9.146^{-5}	3.596^{-5}	1.876^{-7}	1.445^{-4}	3.901^{-5}	1.264^{-5}	3.907^{-8}	6.059^{-5}	1.981^{-5}	6.245^{-6}	1.130^{-8}	3.025^{-5}
120	4.229^{-5}	1.657^{-5}	2.146^{-8}	6.651^{-5}	1.737^{-5}	5.214^{-6}	4.214^{-9}	2.693^{-5}	8.600^{-6}	2.419^{-6}	1.174^{-9}	1.313^{-5}
150	2.739^{-5}	9.240^{-6}	6.457^{-9}	4.536^{-5}	1.107^{-5}	3.639^{-6}	1.237^{-9}	1.718^{-5}	5.424^{-6}	1.352^{-6}	3.392^{-10}	8.289^{-6}
180	2.380^{-5}	1.355^{-6}	4.392^{-9}	3.749^{-5}	9.575^{-6}	7.959^{-6}	8.352^{-10}	1.487^{-5}	4.680^{-6}	2.240^{-7}	2.281^{-10}	7.156^{-6}

[a] Present Das method of calculations.
[b] VCCPB calculations of Singh *et al* (1983).
[c] First Born calculations.
[d] Second Born calculations.

Table 4. Integral cross sections for 2^1S excitation in units of πa_0^2

E (eV)	a	b	c	d	e
50	0.036 6	—	—	—	0.019 9
80†	0.031 7	0.032 6	0.036 2	0.024 23	0.015 5
100	0.024 6	0.023 6	0.030 2	0.020 11	0.014 6
150	0.014 3	0.016 0	—	0.013 88	0.012 1
200	0.009 97	0.012 5	—	0.010 53	0.009 55
300	0.006 24	—	—	0.007 08	0.007 19
400	0.004 57	—	—	0.005 33	0.005 57
500	0.003 63	—	—	0.004 27	0.004 81

† Present calculations and five-state R-matrix calculations at 81.63 eV.
[a] Present Das method of calculation.
[b] Five-state R-matrix calculations (Fon *et al* 1980).
[c] Five-state close coupling calculations (Bhadra *et al* 1979).
[d] VCCPB calculations (Singh *et al* 1983).
[e] 2^1S experimental values estimated by de Heer and Jansen (1977).

(1979) are greatest. At 150 and 200 eV our results together with the results of Singh *et al* are in close agreement with the experimental measurement of Jansen. For energies above 200 eV, we have presented our results together with the results of Singh *et al.*

5. Conclusion

We observe that, in general, the Das computational method provides a fairly accurate description of both the differential cross sections and the integrated cross sections for the electron–helium (1^1S–2^1S) excitation problem at intermediate and high energies. We expect that the same method may be successfully applied in other electron–atom excited collision problems in the intermediate and high energy ranges. The method may also be suitable to describe the triplet transitions in the electron–helium excited collision problem. In any event works on triplet transition, and on still higher excited states are in progress, and are expected to be communicated in future publications.

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