J. Phys. B: At. Mol. Phys. **14** (1981) L453–L459. Printed in Great Britain

LETTER TO THE EDITOR

Electron impact excitation of helium at intermediate energies

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Received 26 March 1981

Abstract. Two recent five-state close-coupling calculations are compared with experiment for the transitions $e^- + He(1^1S) \rightarrow e^- + He\ (2^1S, 2^1P)$. It is shown that the large discrepancy between these calculations and experiment in the energy range $50 \leqslant E_i \leqslant 200$ eV is substantially reduced by adding appropriate pseudostates to the expansion. Less improvement is obtained on adding accurate $n = 3$ states.

There have been two recent five-state ($1^1S, 2^1S, 2^1P, 2^3S, 2^3P$) close-coupling calculations of electron impact excitation of helium (Bhadra *et al* 1979, Fon *et al* 1980), the first (5CCE) solving the standard integral equations by the NIEM method (see Henry 1981) and the second (5CCRE) using an R-matrix approach, which also includes some allowance for short-range correlation effects. The two groups use different approximate wavefunctions so their results differ in detail, though for the 1^1S–2^1S and 1^1S–2^1P transitions in which we are primarily interested, they are in broad agreement (figures 1 and 2). However, at impact energies below 200 eV they predict much larger cross sections than are observed experimentally, the overestimate increasing with decreasing impact energy.

This is in contrast to the results obtained by Scott and McDowell (1975, 1976) using a simple DWPO model, where close agreement was obtained with experiment for these transitions down to 30 eV. This agreement persists in the benchmark case of 1^1S–3^1S (van Zyl *et al* 1980). The DWPO approximation is not time-reversal invariant (distortion being neglected in the final channel) and from a mathematical point of view is at best a poor approximation to the five-state close-coupling models (5CCE, 5CCRE). There is, as we have shown elsewhere for e^+ excitation of 1^1S–2^1S, no question of significant numerical error in any of the calculations discussed above (Willis *et al* 1981).

The most likely source of the trouble lies in cancellation between the effects of coupling to higher states, which is totally neglected in DWPO models, and partially included in the 5CCE and 5CCRE calculations. We show in this letter that this is indeed likely to be the case, by including two additional states in the close-coupling calculations.

We calculate the two cross sections $Q_s = Q(1^1S$–$2^1S)$ and $Q_p = Q(1^1S$–$2^1P)$ in the following models:

(*a*) three-state ($1^1S, 2^1S, 2^1P$) close coupling without exchange (3CCNE);

(*b*) five-state ($1^1S, 2^1S, 2^1P, 2^3S, 2^3P$) close coupling with localised exchange, following Bransden *et al* 1978 (5CCEEP);

0022-3700/81/130453+07$01.50

(*c*) five-state (1^1S, 2^1S, 2^1P, $\overline{k^1P}$, $\overline{4^1S}$) close coupling without exchange where $\overline{k^1P}$ is a pseudostate chosen to obtain the correct ground-state static dipole polarisability and $\overline{4^1S}$ is a pseudostate with threshold just below the exact 4^1S threshold.

(*d*) five-state (1^1S, 2^1S, 2^1P, 3^1S, 3^1P) close coupling without exchange;

(*e*) seven-state (1^1S, 2^1S, 2^1P, 2^3S, 2^3P, $\overline{k^1P}$, $\overline{4^1S}$) close coupling with localised exchange.

The atomic wavefunctions used for 1^1S, 2^1S, 2^1P are given in Willis *et al* (1981). Those for the other states included in this investigation are given in the appendix.

The use of localised exchange should be a satisfactory approximation for ^1S–^1S and ^1S–^1P transitions in this energy range in view of the results of Bransden *et al* (1978). The discrepancy between our model (*b*) results (5CCEEP) and those of Fon *et al* (5CCRE) for 2^1S is of the same order as that between the 5CCRE and 5CCE calculations, while for Q_p our results are substantially closer to the 5CCRE values than are the 5CCE results (figures 1 and 2). The differences between these three sets of results is in part due to the different approximate (and inaccurate) atomic wavefunctions employed. Our oscillator strengths for several transitions are compared with the accurate values of Weiss (1967) in table A3, and with those of other workers. It is clear that those of Bhadra *et al* (1979) are anomalous. The localisation of the exchange terms follows the procedure of Bransden *et al* (1978), and these equivalent exchange potential (EEP) results will be discussed in more detail elsewhere (Willis 1981). For Q_p, all three sets of results are in poor agreement with experiment, the 5CCRE and 5CCEEP results being more than 30% higher at 80 eV, and at 50 eV (where there is no 5CCRE result) our value and that of Bhadra *et al* (1979) are more than 60% higher. For Q_s, while our results are lower than the other 5CC values above 40 eV, they are nevertheless almost a factor of two larger than experiment at 50 eV.

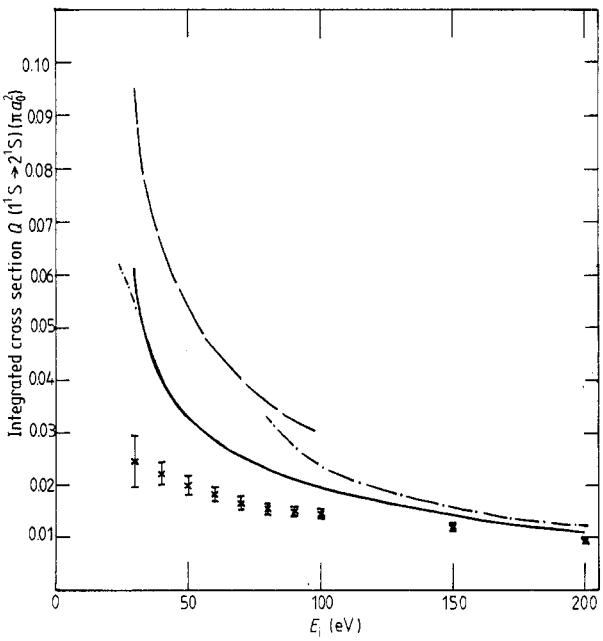

Figure 1. Calculated and experimental values for Q_s. The experimental points ‡ are those of de Heer and Jansen (1977). The theoretical curves are: – – –, 5CCE, Bhadra *et al* (1979); –·–·–, 5CCRE, Fon *et al* (1980); ——, this paper, 5CCEEP.

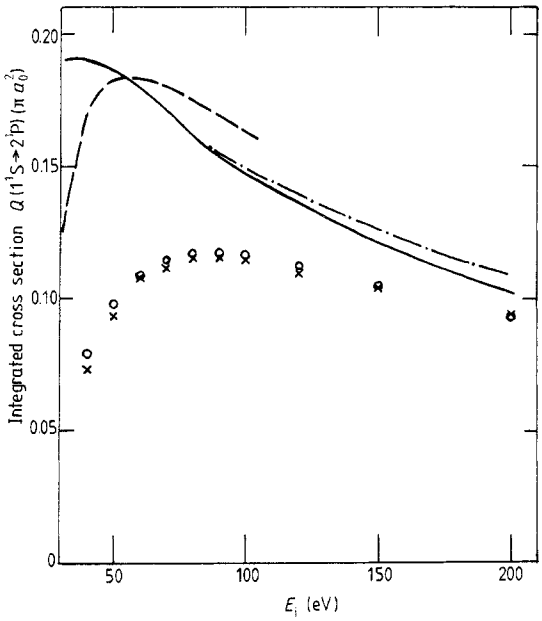

Figure 2. As figure 1, but for Q_p. The experimental points are those of Westerveld *et al* (1979) (×) and Donaldson *et al* (1972) (○).

Our model (*a*) omits 2^3S and 2^3P and the resulting values of Q_p are about 8% higher than in model (*b*): the effect of exchange is to lower the cross section. For Q_s, the effect is larger, exchange lowering the cross section by 20% at 100 eV. This is because the value of Q_p is dominated by the effect of the long-range 1^1S–2^1P dipole coupling, while such coupling is a second-order effect for Q_s (figures 3 and 4).

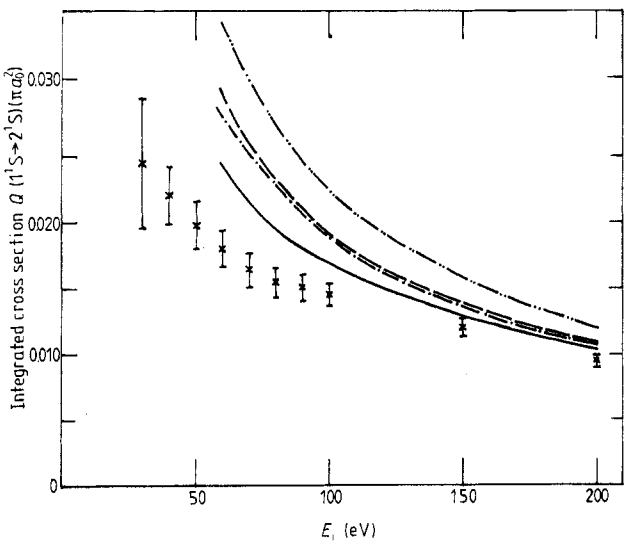

Figure 3. Calculated and experimental values of Q_s, as in figure 1, but the theoretical curves are: –·–·–, model (*a*); –––, model (*b*); – – –, model (*c*); ——, model (*e*).

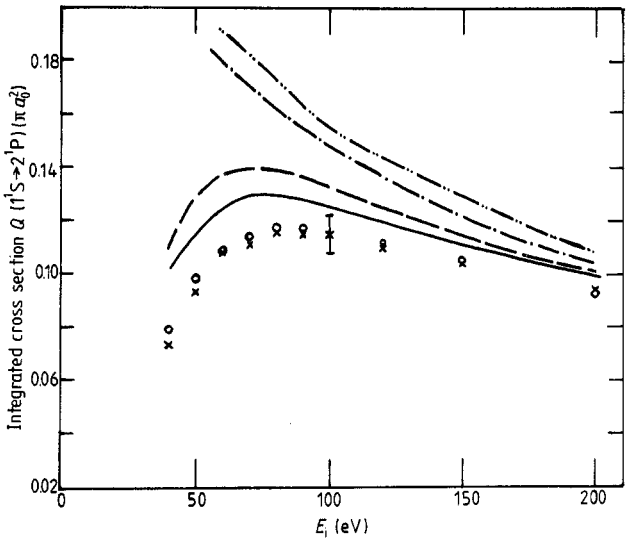

Figure 4. As for figure 3, but for Q_p. The experimental points are as in figure 2.

We now examine the effect, within models (*a*) and (*b*), of adding $\overline{4^1S}$ and $\overline{k^1P}$ pseudostates, the $\overline{k^1P}$ being chosen to give the experimental value of the static dipole polarisability for 1^1S. In model (*c*), $Q_s(c)$ is now very close to $Q_s(b)$ at all energies, while $Q_s(e)$ has reduced the overestimate of experiment to 16% at 100 eV. Again $Q_p(c)$ is considerably closer to experiment, especially at lower energies, while $Q_p(e)$ is still better, being 9% above the experimental value of Westerveld *et al* (1979) at 100 eV, and thus almost within the experimental error. At 50 eV we obtain $Q_p(e) = 1.14\ \pi a_0^2$ compared with Westerveld *et al*'s value of 0.93 ± 0.07 (assuming combined statistical and normalisation errors of 7%, which may be too large). Thus the model (*e*) calculation of Q_p gives a result which may be up to 22% higher at 50 eV. Nevertheless it is quite clear, from figure 4, that the shape of the cross section is now in satisfactory agreement with experiment.

If instead we use approximate 3^1S and 3^1P states chosen to give accurate spectroscopic energies, model (*d*), there is little improvement on the model (*a*) results (see table 1); indeed for Q_s the results are worse. However, choosing the 3^1S and 3^1P wavefunctions in this way allows us to give the 5CCNE values for 1^1S–3^1S and 1^1S–3^1P (table 2). As expected the cross sections obtained are in much worse agreement with the accurate experimental values (1^1S–3^1S, van Zyl *et al* 1980; 1^1S–3^1P, Westerveld *et al* 1979) than are the DWPO results (Scott and McDowell 1975, 1976).

To go further by including exchange, even in an approximate way, via equivalent exchange potentials, should, following our arguments for the $n = 2$ excitations, produce a marked improvement for 1^1S–3^1S, though only a modest one for 1^1S–3^1P. The addition of suitable $n = 4$ pseudostates will be necessary to produce accurate close-coupling values for these two transitions, but it is not yet clear how these pseudostates should be chosen. It would appear insufficient merely to optimise on the $n = 4$ energies. We would suggest adding the $\overline{k^1P}$ pseudostate given in the appendix to represent continuum p states, and to obtain accurate values for Q_s, Q_p, but further $\overline{^1P}$ and $\overline{^1D}$ continuum states would be necessary to obtain good 1^1S–3^1L cross sections. Before

Table 1. Calculated values of Q_s and Q_p in various models in units of πa_0^2, at energies from 60 to 200 eV, exchange omitted.

	E (eV)	(*a*)	(*c*)	(*d*)
Q_s	60	3.50, −2	2.99, −2	3.65, −2
	80	2.76, −2	2.35, −2	2.81, −2
	100	2.24, −2	1.91, −2	2.30, −2
	150	1.59, −2	1.39, −2	1.59, −2
	200	1.20, −2	1.10, −2	1.21, −2
Q_p	60	1.91, −1	1.37, −1	1.84, −1
	80	1.73, −1	1.38, −1	1.65, −1
	100	1.55, −1	1.33, −1	1.50, −1
	150	1.29, −1	1.15, −1	1.23, −1
	200	1.08, −1	1.01, −1	1.05, −1

Table 2. 5CC non-exchange cross sections for the 1^1S–3^1S, 3^1P transitions, in πa_0^2, from 40 to 200 eV, model (*d*).

E (eV)	3^1S	3^1P
40	1.52, −2	6.03, −2
50	1.08, −2	5.65, −2
60	8.58, −3	5.25, −2
80	6.25, −3	4.58, −2
100	4.99, −3	4.11, −2
150	3.35, −3	3.28, −2
200	2.54, −3	2.74, −2

returning to the e^-–He problem we intend to attempt, in collaboration with others, a converged non-exchange close-coupling calculation of all transitions in e^-–H collisions involving the $n = 1$, 2, 3 and 4 levels, in the energy range 35 to 100 eV.

Finally, we briefly discuss other observables in the 1^1S–2^1P transition at 80 eV. The detailed results will be presented elsewhere. All three (5CCE, 5CCRE, 5CCEEP) five-state calculations give poor values for the large-angle differential cross section, but adding $\overline{4^1S}$ and $\overline{k^1P}$ and using localised exchange (model (*e*)) gives agreement with the measurements of Chutjian and Srivastava (1975) out to 140°. The model (*b*) and model (*e*) results bracket the experimental values of λ (Hollywood *et al* 1979, Slevin *et al* 1980) at large angles, but while model (*b*) gives close agreement with the experimental values of $|\chi|$, this agreement disappears in model (*e*) for $\theta > 60°$.

Thus using our $\overline{4^1S}$, $\overline{k^1P}$ pseudostates and localised exchange we obtain much improved values for Q_s, Q_p and $d\sigma(1^1S–2^1P)/d\Omega$, compared with our 5CCEEP results, but little improvement, if any, for λ, and much worse agreement for $|\chi|$. It is clear that difficulties remain, though we believe these calculations represent some advance.

One of us (SLW) is indebted to the Science Research Council and the Culham Laboratory for a CASE Studentship.

Appendix

The radial parts of the wavefunctions are written

$$r_1 r_2 R(r_1, r_2) = \sum_{ij} C_{ij} \gamma_i \gamma_j r_1^{n_i+1} \exp(-\alpha_i r_1) r_2^{n_j+1} \exp(-\alpha_j r_2)$$

where $\gamma_i = [(2\alpha_i)^{2n_i+3}/(2n_i+2)!]^{1/2}$ and the coefficients for the $\overline{k^1\mathrm{P}}$ pseudostate are given in table A2.

Table A1. Basis of Slater-type orbitals $r^n e^{-\alpha r}$.

Case (*c*) (see text) basis set.

Label	Type	n	α
1	s	0	1.41
2	s	0	2.61
3	s	0	2.00
4	s	0	0.865
5	s	1	0.522
6	s	0	0.6133
7	p	1	0.485
8	p	2	0.6133

Energies: $\overline{4^1\mathrm{S}}$, −4.0735 Ryd; $\overline{k^1\mathrm{P}}$, −3.7459 Ryd.

Case (*d*) (see text) basis set (same as (*c*) with addition of three STO).

Type	n	α
s	0	0.200
p	1	0.325
p	2	0.325

Energies	(*d*)	'Exact'
$3^1\mathrm{S}$	−4.1214	−4.1223
$3^1\mathrm{P}$	−4.1095	−4.1103
$4^1\mathrm{S}$		−4.0669

Table A2. $\overline{k^1\mathrm{P}}$.

i	j	C_{ij}
1	7	−0.314 798
1	8	0.302 030
2	7	−0.078 722
2	8	0.072 006
3	7	6.049 000
3	8	−6.102 680
4	7	0.108 462
4	8	−0.116 717
5	7	0.020 020
5	8	−0.020 105
6	7	−0.037 922
6	8	0.044 817

Table A3. Oscillator strengths for some ^1S–^1P transitions, length L, velocity V.

Transition		This work	B	Bh	W
$1^1S \rightarrow 2^1P$	L	0.2875	0.2794	0.341	0.2759
	V	0.2479	0.2781	0.318	0.2761
$1^1S \rightarrow 3^1P$	L	0.0756			0.0734
	V	0.0664			0.0730
$2^1S \rightarrow 2^1P$	L	0.3867	0.3330		0.3764
	V	0.3177	0.4383		0.3774
$2^1S \rightarrow 3^1P$	L	0.1455			0.1478
	V	0.1566			0.1506
$3^1S \rightarrow 2^1P$	L	0.1423			0.1425
	V	0.1306			0.1462
$3^1S \rightarrow 3^1P$	L	0.645			0.625
	V	0.512			0.634

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Bh, Bhadra *et al* (1979).
W, Weiss (1967).

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