J. Phys. B: Atom. Molec. Phys. **13** (1980) L605–L608. Printed in Great Britain

LETTER TO THE EDITOR

Electron impact excitation of He^+

S A Wakid†§ and J Callaway‡

†Department of Computer Science, University of Pittsburgh at Johnstown, Johnstown, Pennsylvania 15904 USA

‡Department of Physics and Astronomy, Louisiana State University, Baton Rogue, Louisiana 70803 USA

Received 15 April 1980, in final form 14 July 1980

Abstract. The electron impact excitation of the $1s \rightarrow 2s$ transition in He^+ is studied in the energy range 40–102 eV using the algebraic variational method with a small pseudostate basis. Results are compared with experiment and with other calculations.

There is serious disagreement between theory and experiment with regard to the electron impact excitation of the 1s–2s transition in He^+. This problem was reviewed by Seaton (1975). The situation may be summarised as follows: this transition was investigated experimentally by Dolder and Peart (1973) whose cross section measurements are not absolute. At high energies, their results may be normalised to the results of the three-state close-coupling calculations briefly described by Seaton (1975). When this is done, there is a very serious discrepancy between the normalised experimental cross sections near threshold and the calculations of Burke and Taylor (1969). These authors used a three-state close-coupling expansion supplemented by twenty correlation terms of the Hylleraas type. Such an expansion gives good results for the excitation of hydrogen between the $n = 2$ and $n = 3$ thresholds, which is the same range of energies discussed here, and so would be expected to be rather accuracte in the present case. However, the discrepancy amounts to a factor of about 1·8. Recently Morgan (1979, 1980) has reinvestigated the energy range between the $n = 2$ and $n = 3$ thresholds using a multichannel close-coupling expansion involving thirteen states (six exact states and seven pseudostates). The computations were made using a form of the algebraic variational method (Callaway 1978). She found excitation cross sections only slightly lower than those of Burke and Taylor and still in substantial disagreement with Dolder and Peart.

At higher energies, there is a small-basis pseudostate calculation (three-state close-coupling + $\overline{3s}$ and $\overline{3p}$ pseudostates) by Henry and Matese (1976). In this work, the two pseudostates were chosen to be degenerate with a (pseudo) threshold chosen to maximise overlap with bound and continuum states of the same symmetry. They found a substantial reduction in the 2s excitation cross section below that given by three-state close coupling. Their results are shown in figure 1 (curve C). It will be noted there is an indication of an increase at low energies, indicating that their work might connect reasonably with that of Burke and Taylor (1969) at lower energies. However, they did not investigate the range near the ionisation threshold.

§Now at Computer Sciences Corporation.

0022-3700/80/190605+04$01.50

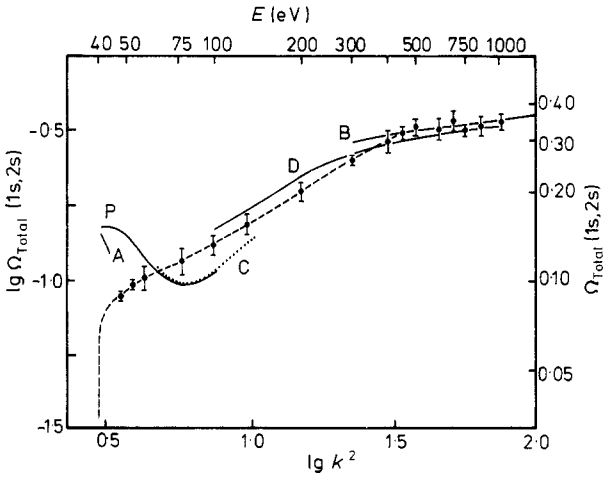

Figure 1. The logarithm (base 10) of the 1s→2s collision strength ($\Omega = 2k^2$) is plotted as a function of the logarithm of the incident energy. The broken curve with error bars shows the experimental results of Dolder and Peart (1973). Theoretical results: A, Morgan (1980) and Burke and Taylor (1969); P, present calculation; B, Seaton (1975); C, Henry and Matese (1976); D, Bransden and Noble (1976). Curves B and D include a correction for cascade, but A, P and C do not.

This letter reports the results of a small-basis pseudostate calculation (three s and three p functions) in a range from close to the excitation threshold up to 7·5 Ryd (102 eV). The results connect rather well with previous work in regions between the $n = 2$ and $n = 3$ threshold, drop significantly in the range around 5 Ryd and join smoothly on to those of Henry and Matese.

The pseudostates are expressed as

$$R_{nl}(r) = \sum_j c_{nl,j} r^{m(j)} \exp[-\zeta(j) r]. \tag{1}$$

The powers m and exponents ζ are listed in table 1. This set includes the exact 1s, 2s and 2p wavefunctions plus three pseudostates. Only a small pseudostate basis is used because otherwise the calculations become quite lengthy when many channels are open.

The calculation was made using a rather straightforward generalisation of the computer programs previously used for electron–hydrogen scattering (Callaway 1978). Thus, the basis set used to expand the scattering wavefunction was energy dependent, containing terms proportional to $\sin kr/r^2$ and $\cos kr/r^2$ at large distances (k is the channel wavenumber). Typically fifteen Slater-type orbitals for each channel were included. The only serious modifications occurred in regard to the free wavefunctions

Table 1. Pseudostate parameters (see equation (1)).

m	ζ $l=0$	E	m	ζ $l=1$	E
0	2·0	−4·0	1	2·0	−1·0
0	1·0	−1·0	1	1·6	−0·08582
1	1·0	1·24460	1	1·0	4·50225

which have specified asymptotic forms. The regular function in this case was just the regular Coulomb function but the irregular function is represented (only approximately) as a combination of regular Coulomb functions angular momenta l and $l+1$. The coefficients are chosen to give the correct asymptotic form (leading term only). The free–free integrals are computed numerically except that the leading dipole long-range contributions, when present, are evaluated analytically using relations given by Burgess *et al* (1970).

The variational calculations have so far been limited to values of the total angular momentum $L \leqslant 2$. This seems to be sufficient to give a reasonable account of the total 1s→2s cross section since (unlike, for example, 1s–2p excitation) the transition potential is of short range. Extension to higher angular momenta will be undertaken in subsequent calculations. In this work, the higher $L(L \geqslant 3)$ contribution is estimated using a unitarised Coulomb Born with exchange (UCBX) procedure (Burgess *et al* 1970), for which purpose a separate program was written. The sum over L converges rapidly for this transition and the contribution from the higher L components is not large, ranging from 2·1% of the total for $k^2 = 3{\cdot}2$ to 23% for $k^2 = 7{\cdot}5$. Consequently, although the accuracy of the UCBX procedure may not be high the potential errors are not large. In contrast, the $L \geqslant 3$ contribution to the 1s–2p excitation is already 69% at $k^2 = 5{\cdot}5$.

The small basis set used here does not permit a discussion of resonances under the $n = 3$ threshold. However, the pseudothreshold at $k^2 = 5{\cdot}24$ Ryd has a significant effect on the cross section in the neighbourhood of that energy. We do not report results close to that threshold.

Our partial and total 1s→2s excitation cross sections are given in table 2, and are shown graphically in figure 1. There are some small fluctuations in individual partial cross sections which are apparently the consequence of incomplete convergence of the expansion of the scattering wavefunction. They are too small to affect the general trend of the data. The results in the upper part of the energy range we consider agree rather well with those of Henry and Matese (1976), who used a different pseudostate set and a different computational method. In the near threshold region, our results are larger than those of Morgan (1980) and Burke and Taylor (1969). (The results of these last

Table 2. Partial (spin weighted) and total cross sections for 1s→2s excitation of He^+ at selected energies. All cross sections are in units of πa_0^2.

	$L=0$		$L=1$		$L=2$				
k^2	$S=0$	$S=1$	$S=0$	$S=1$	$S=0$	$S=1$	$L \leqslant 2$	$\sum_{L=3}^{\infty} \sigma_L$	σ_T
3·24	0·00744	0·00016	0·00332	0·00366	0·00599	0·00161	0·0222	0·0006	0·0228
3·8	0·00546	0·00021	0·00361	0·00333	0·00274	0·00201	0·0174	0·0011	0·0185
4·0	0·00423	0·00025	0·00317	0·00313	0·00177	0·00219	0·0147	0·0012	0·0160
4·2	0·00323	0·00027	0·00349	0·00305	0·00114	0·00223	0·0134	0·0013	0·0147
4·5	0·00157	0·00029	0·00364	0·00276	0·00057	0·00224	0·0111	0·0014	0·0124
5·5	0·00115	0·00028	0·00234	0·00185	0·00003	0·00198	0·00763	0·00154	0·00917
5·8	0·00096	0·00030	0·00214	0·00173	0·00001	0·00184	0·00699	0·00158	0·00857
6·0	0·00083	0·00031	0·00207	0·00169	0·00002	0·00177	0·00670	0·00161	0·00831
6·8	0·00063	0·00027	0·00201	0·00158	0·00010	0·00157	0·00618	0·00171	0·00789
7·5	0·00034	0·00027	0·00209	0·00153	0·00015	0·00149	0·00586	0·00179	0·00765

two calculations are indistinguishable on the scale of the figure.) This appears to be a consequence of the use of a small pseudobasis in the present work. The present values are, however, lower than those of the three-state close coupling by about 25%. The higher energy results of Seaton (1975) and of Bransden and Noble (1976) are also shown in the figure.

The outstanding feature of our results is a drop in the excitation cross section in the vicinity of the ionisation threshold at $k^2 = 4{\cdot}0$ Ryd. This region of decreasing σ connects the high cross sections near threshold with much lower ones at high energy. The higher energy values are below the experimental results presumably because cascade effects are not included in the calculations.

A similar decrease in the 2s excitation cross section occurs in electron–hydrogen scattering (Callaway 1978). Inspection of the partial cross sections given in table 2 reveals that the $L = 0$, $S = 0$ and $L = 2$, $S = 0$ partial waves are primarily responsible for the drop. The $L = 2$, $S = 0$ contribution to the transition matrix element evidently vanishes near an energy about 1·5 times ionisation. Similar behaviour is manifest in electron–hydrogen scattering.

The results of Morgan (1979, 1980), which cover only a limited energy range but employ a much larger basis set might be interpreted as indicating that the cross section should decrease at energies lower than predicted here. However, the extension of Morgan's calculations to higher energies would not be expected to yield monotonically descreasing results as her basis is large enough to predict complicated resonance structure below the $n = 3$ threshold, which is not contained in the present work.

We suggest that the experimental results of Dolder and Peart (1973) may be satisfactory at energies well above the ionisation threshold. The experiments need to be repeated in the 40–60 eV range.

This research was supoorted in part by the US Department of Energy under contract No EY-16-S-05-4881. I am indebted to Professor R J W Henry for many discussions on this problem and for supplying a previous version of figure 1 which we have modified for the present paper.

References

Bransden B H and Noble C J 1976 *J. Phys. B: Atom. Molec. Phys.* **9** 1507–17
Burgess A, Hummer D G and Tully J A 1970 *Phil. Trans. R. Soc.* **266** 225–79
Burke P G and Taylor A J 1969 *J. Phys. B: Atom. Molec. Phys.* **2** 44–51
Callaway J 1978 *Phys. Rep.* **45** 89–173
Dolder K T and Peart B 1973 *J. Phys. B: Atom. Molec. Phys.* **6** 2415–26
Henry R J W and Matese J J 1976 *Phys. Rev.* A **14** 1368–70
Morgan L A 1979 *J. Phys. B: Atom. Phys.* **12** L735–8
——1980 *J. Phys. B: Atom. Molec. Phys.* **13** 3703–15
Seaton M J 1975 *Advances in Atomic and Molecular Physics* ed D R Bates and B Bederson (New York: Academic) pp 83–142