J. Phys. B: At. Mol. Phys. **16** (1983) 2399–2404. Printed in Great Britain

Angular distribution of electrons scattered by He^+

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Received 31 January 1983

Abstract. Theoretical results are given for the angular distribution of low-energy electrons scattered in collisions with He^+ in which the 1s state is excited to the 2s state. The distribution was calculated using T matrices obtained from R-matrix calculations with three states 1s, 2s, 2p and also with six states 1s, 2s, 2p, $\overline{3}$s, $\overline{3}$p, $\overline{3}$d. In both approximations for low electron energies the differential cross section is largest for backward scattering with a maximum at approximately 90°. This disagrees with early calculations of the differential cross section obtained using the distorted-wave approximation.

1. Introduction

The electron excitation of He^+ from the 1s to the 2s state

$$e + He^+(1s) \rightarrow e + He^+(2s) \tag{1}$$

is the simplest electron–ion excitation process. It has been the subject of much theoretical and experimental research (Dance *et al* 1966, Burke and Taylor 1969, Dolder and Peart 1973, McDowell *et al* 1973, 1974, Weatherford 1976, Morgan 1979). Dolder and Peart (1973) obtained relative values of the cross sections for electron energies from threshold to 1000 eV. At high electron energies these measurements were normalised to the PWB approximation results of Massey (1956) and the Coulomb–Born distorted-wave results of Vainshtein (1965). At low impact energies these normalised measured cross sections are in quite good agreement with distorted-wave calculations (Weatherford 1976) and modified distorted-wave results (McDowell *et al* 1973, 1974). However, the measurements are a factor of two lower than the very sophisticated calculations of Burke and Taylor (1969), who used a three target state and twenty correlation term model for their calculations. The results of Burke and Taylor have recently been confirmed by accurate algebraic variational calculations by Morgan (1979).

A critical review of this major disagreement between theory and experiment has been given by Seaton (1975) but he was unable to reconcile theory and measurements. In order to provide more detail about the scattering process we present here low-energy differential cross sections for the excitation of the 2s state of He^+. It is hoped that this information may assist in the design of a new experiment to resolve the disagreement between theory and experiment.

2. Theory

The angular distributions given in this paper were calculated using a new computer code (Salvini 1982) which employs the angular momentum transfer formalism (Fano and Dill 1972). This consists essentially in recoupling the orbital angular momenta of the target and the incoming electron to provide an expansion of the differential cross sections in terms of the angular momentum transfer j_t, i.e. the angular momentum transferred from the incident electron to the target during the collision, subject to the constraints on the total angular momentum:

$$\boldsymbol{j}_t = \boldsymbol{l}' - \boldsymbol{l} = \boldsymbol{L}_N - \boldsymbol{L}_{N'} \tag{2}$$

where $\boldsymbol{l}$, $\boldsymbol{l}'$ are the initial and final angular momentum of the incoming electron respectively, and $\boldsymbol{L}_N$, $\boldsymbol{L}_{N'}$ those of the target.

The differential cross section at an angle θ for inelastic scattering from an initial state N to a final state N' can then be written as

$$\frac{\mathrm{d}\sigma}{\mathrm{d}\Omega}(N \to N' | \theta) = \sum_{\lambda} A_\lambda(N \to N') P_\lambda(\cos\theta) \tag{3}$$

where

$$\begin{aligned} A_\lambda(N \to N') = {} & \frac{1}{8k_N^2[L_N][S_N]} \sum_{\substack{ll'l_1l_1' \\ Sj_t}} \mathrm{i}^{l-l'+l_1'-l_1} \exp[\mathrm{i}(\rho_l + \rho_{l'} - \rho_{l_1} - \rho_{l_1'})] \\ & \times (-1)^{j_t+\lambda}[j_t]\langle ll_1 00 | \lambda 0\rangle\langle \lambda 0 | l'l_1' 00\rangle W(ll'l_1l_1'; j_t\lambda) \\ & \times M^{Sj_t*}_{l_1l_1'}(N \to N') M^{Sj_t}_{ll'}(N \to N') \end{aligned} \tag{4}$$

and

$$M^{Sj_t}_{ll'}(N \to N') = ([l][l'][S])^{1/2} \sum_{L\pi} (-1)^L [L] W(lL_N l' L_{N'}; Lj_t) T^{LS\pi}_{ll'}(N \to N'). \tag{5}$$

Throughout the above we used the following notation: l, l', l_1, l_1' represent the angular momenta of the free electron; L_N, $L_{N'}$ of the target states N, N'; S_N, S the spin of the target and the total spin respectively; π the parity of the target + incoming electron system; L the total orbital angular momentum; $[L] = (2L+1)$; k_N^2 the energy (in Ryd) of the electron incident on the target in the state N; ρ_l the Coulomb phaseshift:

$$\rho_l = \arg\Gamma(l+1+\mathrm{i}\alpha)$$

where $\alpha = z/k_N$ with z being the residual charge of the ion. P and W represent the Legendre polynomial and Racah coefficient respectively.

To evaluate (5) we obtained T matrices from the R-matrix program (Berrington *et al* 1978) with two different target-state expansions. In one calculation we used the 1s, 2s and 2p states of He^+ as target states and in the other calculation we used six target states: the 1s, 2s, 2p states with three $\overline{3}$s, $\overline{3}$p and $\overline{3}$d pseudo-states, which were included in the target-state expansion to make some allowance for the higher excited-states which are neglected in the three-state calculation. The $\overline{3}$s, $\overline{3}$p and $\overline{3}$d radial orbitals were chosen to be of similar range to the 2s and 2p orbitals (i.e. to lie within the R-matrix boundary of 15 au). They were also chosen to make the $\overline{3}$s, $\overline{3}$p and $\overline{3}$d states degenerate. The pseudo-state threshold was at 3.9123 Ryd. These orbitals and states were the same as those used by Berrington *et al* (1982), who examined the complementary process of photoionisation of helium.

T matrices were obtained for $L = 0$ to $L = 5$, singlet and triplet symmetries. To check the convergence of the partial-wave expansion, the three-state calculation was extended to $L = 12$. For the energies considered here T matrices up to $L = 5$ were sufficient to give reliable differential cross sections at all angles of scattering.

3. Results

The total cross section for electron excitation of $He^+(2s)$ calculated using the R-matrix method with three and with six target states is given in figure 1. The results are compared with other theoretical calculations (Burke and Taylor 1969, McDowell *et al* 1973, 1974, Weatherford 1976, Morgan 1979) and with the normalised measurements of Dolder and Peart (1973). Our three-state results are about 25% larger than our six-state results, but our six-state results are in good agreement with the very accurate theoretical results of Burke and Taylor (1969) and the results of Morgan (1979). The normalised measurements of Dolder and Peart (1973) are a factor of two lower than these calculations, but they are in good agreement with the distorted-wave calculations of Weatherford (1976) and they lie above the modified distorted-wave calculations of McDowell *et al* (1973, 1974).

A more detailed comparison of our six state results and the calculations of Burke and Taylor (1969) is given in table 1 where we compare the partial and total cross sections for the two calculations. In general the two calculations give results which agree to better than 10%.

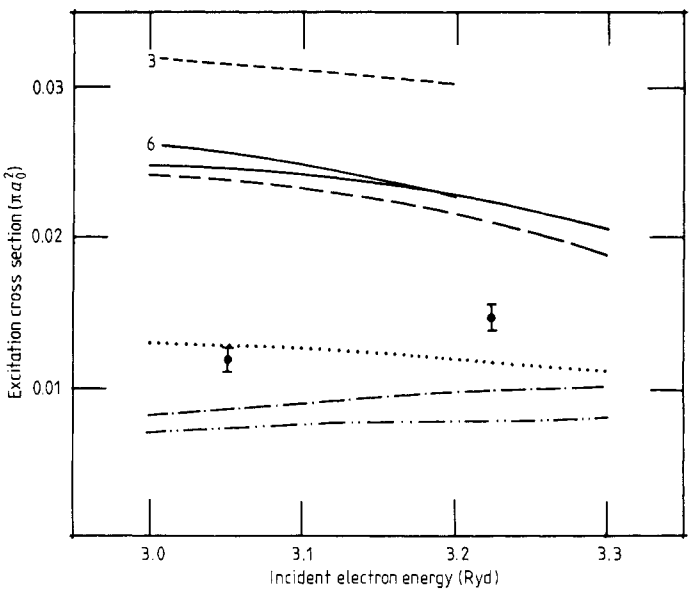

Figure 1. Total cross section (πa_0^2) for excitation of $1s \rightarrow 2s$ in He^+. Normalised measured cross section: Dolder and Peart (1973), ●. Theoretical cross sections: present six-state results, 6——; present three-state results, 3— —; close-coupling plus correlation term results, Burke and Taylor (1969), ——; algabraic variational results, Morgan (1979), – – –; distorted-wave results, Weatherford (1976), · · · · · ; DWPO results, McDowell *et al* (1973), — · —; DWPO with coupling, McDowell *et al* (1974), — · · —.

Figures 2(*a*), (*b*) and (*c*) give our differential cross sections for the excitation of the 2s state of He^+ using both three states and six states in the R-matrix method. Although the two calculations have the same shape, the more reliable six-state

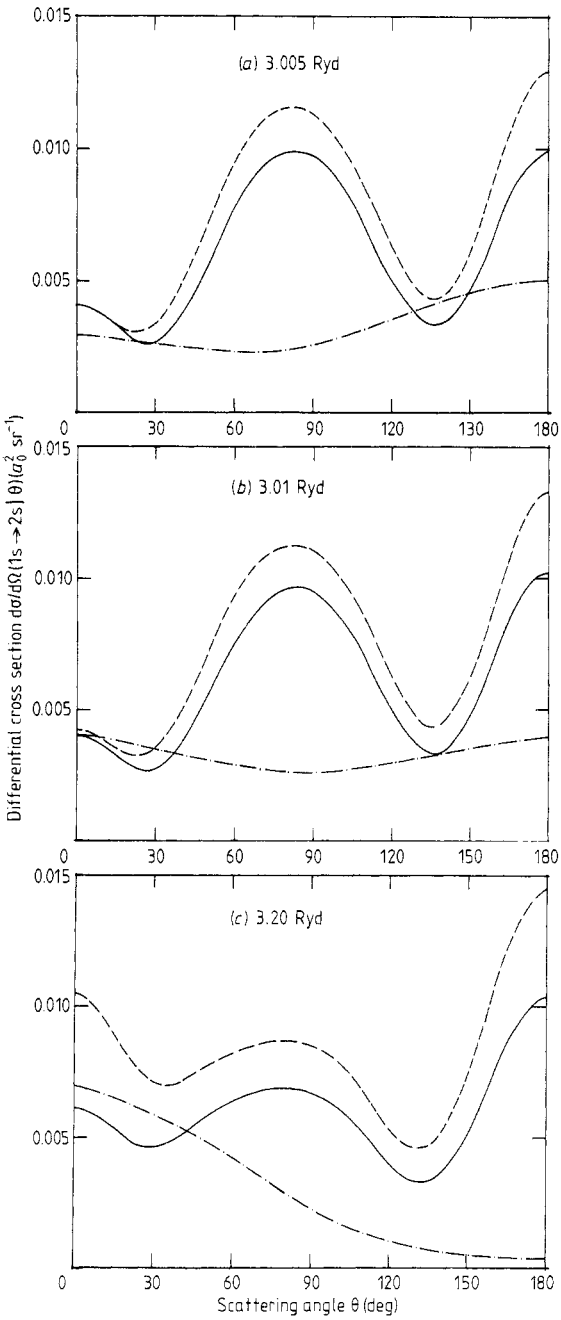

Figure 2. Differential cross section $d\sigma/d\Omega$ (a_0^2 sr^{-1}) for excitation 1s→2s in He^+. Present six-state results, ——; present three-state results — —; distorted-wave results, Weatherford (1976), — · —. incident electron energies: (*a*) 3.005 Ryd; (*b*) 3.01 Ryd; (*c*) 3.2 Ryd.

Table 1. Partial cross sections for e^-–He^+ 1s–2s (in units of πa_0^2).

	$k^2 = 3.005$ Ryd		$k^2 = 3.2$ Ryd	
πLS	R matrix (six state)	Burke and Taylor (1969)†	R matrix (six state)	Burke and Taylor (1969)
^1S	0.008 49	0.007 80	0.006 84	0.006 16
^3S	0.000 16	—	0.000 17	—
^1P	0.002 38	0.002 42	0.003 41	0.003 72
^3P	0.003 91	0.004 00	0.003 94	0.003 41
^1D	0.009 00	0.008 41	0.005 74	0.005 18
^3D	0.001 11	0.001 01	0.001 45	0.001 33
^1F	0.000 20	0.000 20	0.000 42	0.000 49
^3F	0.000 97	0.000 90	0.000 48	0.000 44
Total	0.026 24	0.024 86	0.022 54	0.022 68

† Extrapolated values at 3.0 Ryd.

calculations are up to 25% lower than the three-state calculations. At all three energies the differential cross section has two minima, one at about 30° and the other at about 140°. There is a large maximum at about 90°, but the differential cross section is largest in the backward scattering direction and in the energy range considered here this maximum increases with increasing energy. This complex behaviour of the differential cross section may be attributed to the part that the S, P and D waves all contribute significantly to the differential cross section (see table 1).

Our differential cross sections differ significantly from the earlier distorted-wave results of Weatherford (1976) which are also given in figures 2(*a*), (*b*) and (*c*). The major difference occurs at 90° where the distorted-wave results fail to give the pronounced maximum which we obtained at all three energies considered. At the lowest energy considered Weatherford obtained a maximum in the backward direction which is in qualitative agreement with our results, but as the energy increases his results soon give a maximum in the forward scattering direction. The difference between our calculations and those of Weatherford can be attributed to his neglect of the D waves.

Acknowledgments

We wish to thank Professor P G Burke for his continued support and advice and to thank Mr M F A Harrison for useful discussions on the experiments. One of us (SAS) thanks the SERC for a research grant. Most of the computing for this work was carried out on the SERC Daresbury Laboratory computers using a workstation provided by the SERC.

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