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LETTER TO THE EDITOR

Electron impact on H and He^+
II Coupling effect in the distorted wave polarized orbital approximation

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Abstract. Coupling terms which were previously omitted are retained in a distorted wave polarized orbital calculation of electron impact excitation of the $1s \rightarrow 2s$ transition in H and He^+. The results for H are in very good agreement with the best close coupling results at low energies. For He^+ the previous results are reduced by 18% at threshold, and fall 50% below experiment there.

In an earlier paper, I (McDowell *et al* 1973) we applied the distorted wave polarized orbital (DWPO) approximation of Lloyd and McDowell (1969) to the electron impact excitation of $1s \rightarrow ns$ transitions in H and He^+.

The matrix element for the transition was taken to be (equation (19) of I)

$$T_{if}^{\pm}(1) = \langle \psi_f | V_f | (1 \pm P_{12}) \phi_i(1) F^{\pm}(2) \rangle \tag{1}$$

in our earlier notation, terms explicitly involving the polarized orbital $\phi_{pol}(1,2)$ having been neglected. The scattering function $F^{\pm}(2)$ was obtained in the exchange-adiabatic model (cf Drachman and Temkin 1972) which allows for direct polarization but neglects exchange polarization and other non-adiabatic effects. It is therefore consistent with this model to retain direct polarization terms in (1). That is, the T-matrix element $T_{if}^{\pm}(1)$ of (I) should be replaced by

$$T_{if}^{\pm} = T_{if}^{\pm}(1) + \langle \psi_f | V_f | \phi_{pol}(1,2) F^{\pm}(2) \rangle. \tag{2}$$

The Callaway–Temkin potential (I(13)) is obtained if $\phi_{pol}(1,2)$ is taken to be:

$$\phi_{pol}(1,2) = -\frac{\epsilon(r_1,r_2)}{r_2^2} \frac{U_{1s \rightarrow p}(r_1)}{r_1} \frac{P_1(\cos\theta_{12})}{\sqrt{\pi}} \tag{3}$$

where $U_{1s \rightarrow p}(r)$ satisfies Sternheimer's equation

$$\left[-\frac{d^2}{dr^2} + \frac{P_{1s}''(r)}{P_{1s}(r)} + \frac{2}{r^2} \right] U_{1s \rightarrow p}(r) = r P_{1s}(r) \tag{4}$$

and $P_{1s}(r)$ is the r-multiplied hydrogenic radial function for the ground state. The step function $\epsilon(r_1,r_2)$ cuts off the perturbation at $r_1 = r_2$.

The effect of $\phi_{\rm pol}(1,2)$ is to directly couple s and p states as required by the physics of the problems (degenerate nl states). The Sternheimer function may be obtained in closed form as

$$U_{1s\to p}(r) = f(z,r)P_{1s}(r) \tag{5}$$

with

$$f(z,r) = \frac{1}{2z^3}(x+\tfrac{1}{2}x^2) \qquad x = zr. \tag{6}$$

With this modification, we proceed as in I by making a partial wave analysis to obtain precisely I(23) except that the integral I_A is now replaced by

$$I_A' = I_A + \tfrac{2}{3}I_F \tag{7}$$

with

$$I_F = \int_0^\infty u_l^{\pm}(k_1,r)H_l(k_f,r)k_{1s,ns}(r)\,r\,dr \tag{8}$$

and

$$k_{1s.ns}(r) = -\frac{1}{r^4}\int_0^r t^2 R_{ns}(t)U_{1s\to p}(t)dt. \tag{9}$$

We have applied this modification of I to the 1s $\to$ 2s transitions in H and He^+. For this case

$$k_{2s}(x) = \frac{5{\cdot}214549}{x^4}\left[1-\left(1+\frac{3}{2}x+\frac{9}{8}x^2+\frac{9}{16}x^3+\frac{27}{128}x^4 + \frac{3^4}{2^4\times 56}x^5+\frac{3^4}{2^6\times 56}x^6\right)e^{-3x/2}\right] \tag{10}$$

$$\underset{x\to 0}{=} \frac{1}{2\sqrt{2}}\left(-\frac{2}{5}x+\frac{1}{2}x^2-\frac{1}{4}x^3+\frac{3}{64}x^4+\frac{1}{64}x^5+\ldots\right). \tag{10'}$$

The results are tabulated below, and compared with the unorthogonalized results of I. The coupling effect studied here is unimportant for energies greater than 100 eV in e–H collisions and at corresponding energies in e–He^+ collisions as regards total cross sections.

The results for hydrogen in the near threshold region are, as is shown in figure 1, in close agreement with those of Geltman and Burke (1970) and of a recent application of the algebraic variational method by Callaway and Wooten (1974). They remain consistent with the experimental results, discussed in I, when these are renormalized.

In this case the effect of coupling has been to increase the cross section, especially the $l = 0$ partial cross section, I_F being the same sign as I_A for $l = 0$.

The effect in He^+ is quite different. Our previous results are reduced by 18% at threshold (though they are still within 50% of the experimental values of Peart and Dolder (1972)), I_F now being of opposite sign to I_A for $l = 0$. The cancellation between I_A and I_F for small l is somewhat compensated for by the comparatively long range nature of $k_{ns}(r)$ compared with the exponential decrease of $h_{1s,ns}(r)$, so that the higher partial cross sections are now more important. The present results for He^+ (1s $\to$ 2s) disagree by almost a factor of three (at threshold) with the close coupling calculations of Burke and Taylor (1969), which however lies a factor of two above experiment. This is surprising in view of the agreement obtained for atomic hydrogen. Further work on the 1s $\to$ np (n = 2,3) transitions is in progress, and may clarify the situation.

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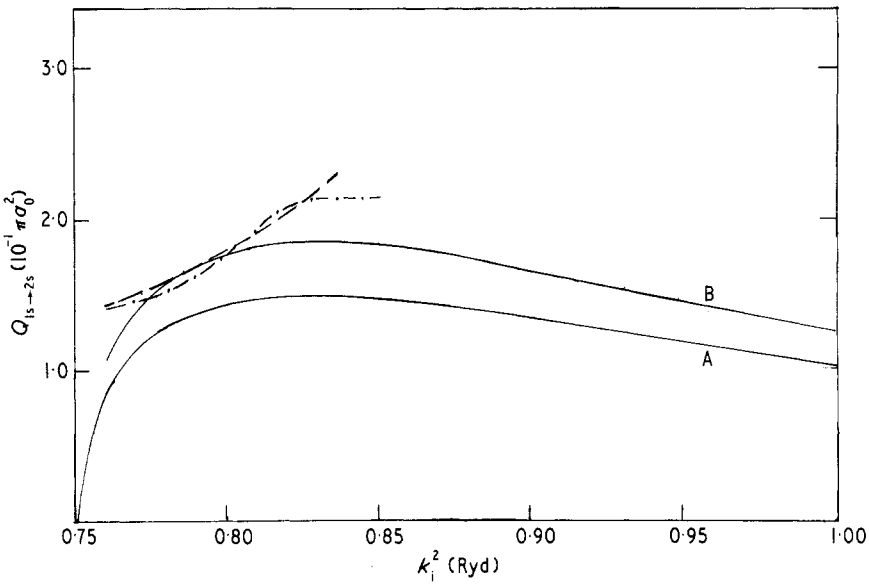

Figure 1. Electron impact excitation cross sections for H(1s → 2s). Curve A unorthogonalized results of (I); curve B this paper including coupling. Dashed curve (BG) close-coupling (Geltman and Burke 1970). Dash-dot curve: algebraic variational method (Callaway and Wooten 1974).

Table 1. (*a*) hydrogen: Q_u, unorthogonalized results of I; Q, this paper in units of $10^{-2}\pi a_0^2$.

k_i^2(Ryd)	0·76	0·77	0·78	0·80	0·81	0·83	0·85	0·90	0·95	1·0
Q_u	8·53	11·2	12·8	14·3	14·7	14·9	14·7	13·4	12·1	10·9
Q	10·6	14·0	15·9	17·8	18·2	18·4	18·1	16·4	14·4	12·7
k_i^2(Ryd)	1·1	1·2	1·5	2·0	3·0	4·0	7·35			
Q_u	9·41	8·33	9·17	9·99	9·17	7·82	5·01			
Q	10·3	9·02	8·29	8·79	8·33	7·32	4·96			

(*b*) He^+, as above but cross sections in units of $10^{-3}\pi a_0^2$.

k_i^2(Ryd)	3·005	3·01	3·04	3·60	3·2	3·3	3·4	3·5
Q_u	8·16	8·19	8·35	8·45	9·13	9·55	—	10·26
Q	6·68	6·70	6·84	6·93	7·50	7·89	8·23	8·54
k_i^2(Ryd)	3·6	4·0	5·0	6·0	8·0	10·0		
Q_u	10·6	11·35	—	11·2	9·70	8·08		
Q	8·81	9·62	10·22	9·94	8·78	7·68		

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