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LETTER TO THE EDITOR

# On Balmer alpha emission in keV collisions between protons and atomic hydrogen

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**Abstract.** New close-coupled cross sections for direct excitation of H by proton impact and for Balmer alpha emission are reported. Attention is drawn to an apparent disagreement between theoretical and experimental Balmer emission data.

The aim of this letter is to report new theoretical cross sections for direct excitation of atomic hydrogen by proton impact at intermediate energies and to draw attention to an apparent disagreement between the current theoretical and experimental values for cross sections $\sigma_{em}$ for Balmer alpha emission,

$$H^*(n=3) \to H^*(n=2) + h\nu. \tag{1}$$

Collision of protons with atomic hydrogen have been extensively studied experimentally in a wide range of impact velocities. In particular, Park *et al* (1976) measured $n=2$ and $n=3$ excitation cross sections or impact proton energies from 15 to 200 keV lab. Very recently Donnelly *et al* (1991) reported measurements of Balmer alpha emission cross sections due to the primary excitation of atomic hydrogen by proton, $He^+$ and $He^{2+}$ impact in the energy range between 2.5 and 100 keV amu$^{-1}$. Generally, there are two processes populating excited states of H in collisions with p, that is direct excitation

$$p + H(1s) \to p + H^*(nlm) \tag{2}$$

and charge transfer

$$p + H(1s) \to H^*(nlm) + p. \tag{3}$$

Because of its relative simplicity, the p + H system was often used in the past to test various models and approximations in the theory of heavy particle collisions. Consequently, a considerable amount of theoretical data is available for reactions (2) and (3) (Franco and Thomas 1971, Bhadra and Ghosh 1971, Shakeshaft 1978, Bransden *et al* 1979, Reading *et al* 1981, Schoeller *et al* 1986, Ast *et al* 1988, Ermolaev 1988).

The presently reported close-coupled semiclassical impact parameter calculations are an extension of an earlier work of this author (Ermolaev 1984, 1990). As in the earlier work, a rectilinear trajectory was assumed for heavy particles A and B (that is for p and H) and the electronic wavefunction was expanded using a two-centre atomic orbital (TCAO) basis $[u_j^A, u_{j'}^B]$, $j = 1, \ldots, N_A$; $j' = 1, \ldots, N_B$.

In the usual notations, the expansion takes the form

$$\Psi(r, t) = \sum_{j=1}^{N_A} a_j^A(t) u_j^A \eta_j^A + \sum_{j'=1}^{N_B} a_{j'}^B(t) u_{j'}^B \eta_{j'}^B \tag{4}$$

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where $u_j^{A,B}$ and corresponding $\varepsilon_j^{A,B}$ are eigenfunctions and eigenenergies of an electron moving in the central field potentials $V_A$ and $V_B$, respectively, and $\eta_j^{A,B}$ are plane-wave electronic translational factors (PWETF). In the computational scheme adopted, $u_j^{A,B}$ are obtained by diagonalizing Hamiltonians $H_A$ and $H_B$ on linear combinations of the Slater type orbitals (STO). Eigenstates $\varepsilon_j^{A,B}<0$ and $\varepsilon_j^{A,B}>0$ correspond to the discrete spectrum and to the continuum, respectively, associated with A and B.

Following an earlier discussion (Ermolaev 1990), the present calculations employed an asymmetric basis with a single 1s state on projectile A, $N_A=1$, and a large set of $N_B=50$ states with $0\leqslant l\leqslant 3$ centred on target B. Eight s states, sixteen p states, eighteen d states and eight f states were included in the set. In order to test the accuracy of the previous calculations, the number of grid points for interpolating the direct matrix elements was quadrupled and integration of the system of differential equations, for coefficients $a_j^{A,B}$ in equation (4), was carried out in a wider range $\pm 175$ au.

Table 1 presents the $n=3$ direct excitation cross sections $\sigma(3l)$ in the energy range $30\leqslant E\leqslant 200$ keV lab. These cross sections are in agreement with the earlier computed values (Ermolaev 1990) on average within 1-2%.

The Balmer alpha emission cross sections $\sigma_{em}$ were then obtained using the equation

$$\sigma_{em}=\sigma(3s)+0.118\sigma(3p)+\sigma(3d) \tag{5}$$

which shows that the bulk of emission from the 3p level (some 88%) falls on the transition to the ground 1s state. The cross section $\sigma_{em}$ must be corrected for cascades from higher levels of H excited by proton impact. It was pointed out earlier (Williams *et al* 1982) that the cascade correction to the Balmer alpha emission was relatively small. In the present work, only cascades from levels $n=4$, 5 and 6 were considered. Using the transition probabilities (e.g. Bethe and Salpeter 1957) one may obtain cascade contributions to the $n=3$ levels expressed in terms of the direct excitation cross sections for proton impact:

$$\begin{aligned}\sigma_{casc}(3s)=\;&0.0371\sigma(4p)+0.0087\sigma(5s)+0.0381\sigma(5p)+0.0036\sigma(5d)+0.0111\sigma(6s)\\&+0.0396\sigma(6p)+0.0059\sigma(6d)+0.0006\sigma(6f)\end{aligned} \tag{6a}$$

$$\begin{aligned}\sigma_{casc}(3p)=\;&0.4186\sigma(4s)+0.2555\sigma(4d)+0.3069\sigma(5s)+0.0087\sigma(5p)+0.2386\sigma(5d)\\&+0.0936\sigma(5f)+0.2906\sigma(6s)+0.0112\sigma(6p)+0.2345\sigma(6d)\\&+0.1217\sigma(6f)+0.0417\sigma(6g)\end{aligned} \tag{6b}$$

**Table 1.** Direct excitation of hydrogen atom by proton impact. Cross sections for $n=3$ (in $10^{-18}$ cm$^2$).

| $E$ (keV lab) | 3s | 3p | 3d | Total $n=3$ |
|---|---|---|---|---|
| 30.0 | 1.60 | 13.00 | 4.22 | 18.82 |
| 40.0 | 1.94 | 14.70 | 4.45 | 21.09 |
| 50.0 | 2.20 | 15.30 | 4.10 | 21.60 |
| 60.0 | 2.10 | 15.35 | 3.59 | 21.60 |
| 75.0 | 1.84 | 14.81 | 2.85 | 19.50 |
| 85.0 | 1.63 | 14.30 | 2.47 | 18.40 |
| 100.0 | 1.43 | 13.68 | 2.02 | 17.13 |
| 145.0 | 0.97 | 11.92 | 1.28 | 14.17 |
| 200.0 | 0.69 | 10.26 | 0.88 | 11.14 |

$$\sigma_{\mathrm{casc}}(3\mathrm{d}) = 0.0037\sigma(4\mathrm{p}) + \sigma(4\mathrm{f}) + 0.0009\sigma(5\mathrm{s}) + 0.0036\sigma(5\mathrm{p}) + 0.0039\sigma(5\mathrm{d}) + 0.6338\sigma(5\mathrm{f}) + \sigma(5\mathrm{g}) + 0.0014\sigma(6\mathrm{s}) + 0.0029\sigma(6\mathrm{p}) + 0.0063\sigma(6\mathrm{d}) + 0.5127\sigma(6\mathrm{f}) + 0.8369\sigma(6\mathrm{g}) + \sigma(6\mathrm{h}). \quad (6c)$$

The $n = 4$ excitation cross sections of the present work are generally close to the $n^3$ rule estimates. In view of that, the corrected Balmer cross sections were obtained by combining the close-coupled $n = 3$ data with the cascade corrections (6) where the $n^3$ rule estimates of the $n = 4$, 5 and 6 cross sections were used. The summary of these calculations is presented in table 2.

**Table 2.** Balmer alpha emission and cascade corrections. Cross sections in $10^{-18}$ cm$^2$.

| $E$ (keV lab) | $\sigma_{\mathrm{em}}$ ($n = 3$) | $\Delta\sigma_{\mathrm{casc}}$ | $\sigma_{\mathrm{Balmer}}$ |
|---|---|---|---|
| 30.0 | 7.35 | 0.58 | 7.93 |
| 40.0 | 8.12 | 0.66 | 8.78 |
| 50.0 | 8.10 | 0.68 | 8.78 |
| 60.0 | 7.50 | 0.66 | 8.16 |
| 75.0 | 6.44 | 0.61 | 7.05 |
| 85.0 | 5.79 | 0.58 | 6.37 |
| 100.0 | 5.06 | 0.54 | 5.60 |
| 145.0 | 3.66 | 0.44 | 4.10 |
| 200.0 | 2.78 | 0.38 | 3.16 |

A comparison of theoretical results with the recent experimental Balmer cross sections of Donnelly *et al* (1991) is carried out in figure 1. In the same figure, the excitation cross sections of Park *et al* (1976) and the close-coupled results of Shakeshaft (1978), Fritsch and Lin (1983), and Ermolaev (1990) are also shown to illustrate the possible level of agreement between theory and experiment.

It may be useful to give a brief review of the available theoretical results on Balmer alpha emission (see figure 1). At the highest impact energy $E = 225$ keV lab considered, the Born cross sections for Balmer alpha emission are still different from those predicted by close-coupled calculations though the difference is relatively small. The same figure 1 demonstrates that all theoretical models tend to converge to the Born values at certain $E$, beyond the graph. In the intermediate range between 20 and 200 keV lab, say, there is a considerable divergence in the numerical values of the emission cross sections. Coupling between target states is thought to be important and must be taken into account. However, figure 1 shows that the result of this account depends greatly on the choice of the general model. Curve Sc in figure 1 uses the data obtained by Schoeller *et al* (1986) with a set of the $n = 1$, 2 and 3 discrete states on the target, within an approximation where neither ionization nor charge transfer are included explicitly in the model. This overestimates the excitation cross sections as a comparison with the pseudo-state coupled-channel calculations of Bransden *et al* (1979) shows. Hence a similar effect is recorded in the emission cross sections. Below $E = 100$ keV lab, charge transfer becomes a dominant feature of the collision. Its account causes a further decrease of the emission cross sections as, for instance, curves O1 and O2 of the optical potential model (Ast *et al* 1988) may suggest. A very good account of charge transfer is provided at low $E$ by the impact parameter calculations of Shakeshaft (1978). However, the basis used in that work did not take the ionization channel into

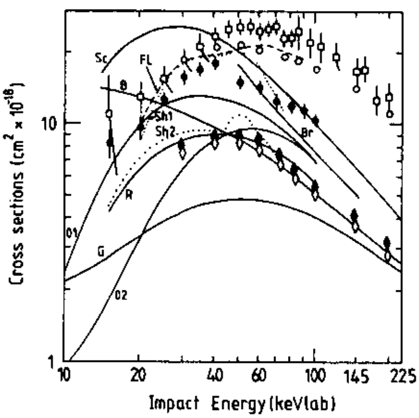


**Figure 1.** Cross sections for Balmer alpha emission from direct target excitation in p+H collisions. (i) $n=3$ excitation. Experiment: ⌽, Park *et al* (1976). Theory (close-coupled, impact parameter, two-centre): Sh1, symmetric AO basis, Shakeshaft (1978); FL, AO$^+$ basis, Fritsch and Lin (1983); ○, asymmetric AO51 basis, Ermolaev (1990) and present calculations. (ii) Balmer alpha emission. Experiment: ⧫, Donnelly *et al* (1991). Theory (without cascade correction): B, Born approximation, Schoeller *et al* (1986); G, Glauber approximation, Franco and Thomas (1971) and Bhadra and Ghosh (1971); Sh2, close-coupled, impact parameter, symmetric two-centre AO basis, Shakeshaft (1978); ◇, close-coupled, impact parameter, asymmetric two-centre AO basis, Ermolaev (1990) and present calculations; O1, one-centre optical, Ast *et al* (1988); O2 two-centre optical, Ast *et al* (1988); Sc, one-centre, without pseudo-states, close-coupling, Schoeller *et al* (1986); R, one-and-a-half centred AO expansion, Reading *et al* (1981); Br, one-centre, impact parameter, with pseudo-states, Bransden *et al* (1979). (iii) Balmer alpha emission (with cascade correction). Theory: ◆, close-coupled, impact parameter, asymmetric two-centre AO basis, present calculations.

consideration. That, in turn, affected to some extent the direct excitation (emission) channel at higher energies $E$. Curve R in figure 1 was obtained with the help of data of Reading *et al* (1981). That work used a basis with a partial account of the charge transfer channel (so-called 'one-and-a-half centre AO expansion') and a good representation of the continuum. In the impact parameter close-coupled model of Ermolaev (1990), a two-centre asymmetric AO51 expansion accounts for all three channels in the course of a single impact-parameter calculation.

A direct comparison with the experimental $n=2$ and $n=3$ excitation cross sections of Park *et al* (1976) normalized in figure 1 to first Born at 200 keV as suggested by Shakeshaft (1976), shows that the asymmetric basis used in the present work may produce very good cross sections for impact energies $E \geqslant 30$ keV lab. However this conclusion appears to be in a conflict with a rather poor agreement between the present theoretical cross sections for Balmer alpha emission and the experimental data of Donnelly *et al* (1991). The theoretical data, as figure 1 demonstrates, may account only for some 50% of the observed emission.

Apparently, no simple explanation of this disagreement can be offered at the moment. Indeed, table 2 and figure 1 show that cascade contributions increase theoretical cross sections by less than 10%. That is not sufficient to account for the difference. Another possible source of the disagreement could be an additional contribution to the emission due to the excited projectile H atoms formed by charge transfer. However, Donnelly *et al* (1991) state that this source has been eliminated. The question of normalization is perhaps less clear since the emission data of Donnelly *et al* (1991) and the excitation data of Park *et al* (1976) were normalized in different ways (Gilbody 1991). On the theoretical side, it has been checked that the overlap between the $n=3$ states and pseudostates of basis (4) is only a few per cent. The author expects the accuracy of the cross sections presented in table 1 to be some 10% or better, within the interval considered. It is possible however that the uncertainty may be higher, perhaps, by a factor of two at the low end of the impact energy interval.

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