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LETTER TO THE EDITOR

Neutralization of protons in energetic collisions with hydrogen-like beryllium ions

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Abstract. A theoretical study of hydrogen production in collisions between protons and hydrogen-like beryllium ions Be^{3+} is reported, for a proton impact energy range between 100 keV and 3 MeV. Cross sections are obtained in close-coupled atomic-orbital calculations within the semiclassical impact parameter method. The presented results are relevant to design and interpretation of current experiments at JET where a substantial flux of neutral hydrogen is observed to be generated at the centre of the tokamak plasma.

Neutralization of protons in collisions with hydrogen-like ions $A^{(Z-1)+}$ of atomic impurities A plays an important role in the interpretation of current experiments that study energy distribution of energetic protons in tokamak plasmas (Korotkov and Gondhalekar 1994a, b). The use of the neutral hydrogen flux generated in the plasma for diagnostics requires the knowledge of accurate cross sections for hydrogen production in a wide range of energies. At present, the accurate theoretical neutralization cross sections are available only in a narrow range of the scaled impact energy $E_p = E/Z^2$, $E_p \leqslant 1$, where E is the proton energy measured in the laboratory system. These cross sections were obtained in close-coupled (CC) calculations of Winter (1982, 1987) for $Z = 2$–6, and, in a wider range of E_p, in the CC calculations of Ermolaev and McDowell (1987) for $Z = 3$. For hydrogen-like ions of beryllium (the main impurity in tokamak plasmas), the range treated by Winter is between 0.125 and 1.00 ($50 \leqslant E \leqslant 400$ keV) whereas the range important for applications starts at energies corresponding to the cross section maximum (≈ 200 keV for Be^{3+}) and extends up to 3 MeV. Though for E above the maximum the cross sections can be estimated from the distorted-wave (DW) approach (Mukherjee and Sil 1980, Grozdanov and Kristic 1988) its accuracy and validity range has not been yet established by any independent calculation. Therefore it was important to extend the CC calculations of neutralization beyond the energy range considered by Winter (1987).

In this communication are reported CC calculations of the main neutralization process

$$p + Be^{3+}(1s) \rightarrow H(n\ell) + Be^{4+} \qquad n = 1, 2 \tag{1}$$

where the beryllium ion is initially in the ground state.

Calculations have been carried out using a modified version of an earlier developed close-coupling semiclassical impact parameter code (Ermolaev 1984, 1990) for one- and pseudo-one-electron systems that uses a two-centre atomic orbital (AO) expansion, in terms of Slater type orbitals (STO). A basis of 35 AO states (five on the projectile and 30 on the target ion) was used in the calculations and the corresponding eigenenergies are listed in

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Table 1. Scaled eigenenergies E_i/Z^2 of the 35-state AO basis (in au).

H centre, $Z = 1$			
1s	-0.5		
2s	-0.125		
ϵ_1s	0.155 58		
2p	-0.125		
Be^{3+} centre, $Z = 4$			
1s	-0.5	2p	-0.125
2s	-0.125	3p	$-0.055\,56$
3s	$-0.055\,56$	4p	$-0.031\,25$
4s	$-0.031\,25$	5p	$-0.018\,95$
5s	$-0.019\,56$	ϵ_1p	0.007 84
$\tilde{6}$s	$-0.004\,21$	ϵ_2p	0.178 75
ϵ_1s	0.043 02	3d	$-0.055\,56$
ϵ_2s	0.227 79	4d	$-0.031\,25$
ϵ_3s	1.594 5	$\tilde{5}$d	$-0.009\,39$

table 1. This basis is somewhat smaller than the largest Sturmian basis of 45 states employed by Winter (1987) for the beryllium calculations. However, it was expected that the present choice of 1s, 2s, $2p_0$ and $2p_1$ bound states as well as one positive-energy s state centred on the projectile would be adequate for assessing the rate of convergence of the CC calculations and for producing good estimates of the main capture cross sections, particularly for high energies towards the asymptotic region where the $1/n^3$ rule ultimately holds for capture into H(n). *In view of a significant coupling between the dominant excitation and ionization* channels and a relatively weak charge transfer to the impinging proton, target-centred bound states with $n \leqslant 5$ and a number of positive-energy s and p pseudostates were included in the basis.

The neutralization cross sections have been computed in the range $100 \leqslant E \leqslant 3000$ keV. Neutralization cross sections for capture into the ground state of hydrogen, $\sigma(1s)$, are presented in figure 1 where they are compared with the Sturmian CC results of Winter (1987) and the DW calculations. In the region of the cross section maximum (150 and 200 keV), the present calculations give capture that differs by 5–10% from Winter's 45-state calculation. For energies below the maximum (100 keV) and above it (400 keV), the cross sections differ by some 20%. It can be seen, at the same time, that the CDW result of Mukherjee and Sil (1980) and the boundary corrected first Born approximation (B1B) of Grozdanov and Kristic (1988) are both surprisingly close to Winter's calculation for 400 keV. For $E > 400$ there are no independent CC data that would allow the accuracy of the computed $1s \to 1s$ neutralization to be tested but comparison with the DW data can be carried out. Both sets of the cross sections come close together at 700 keV. For higher energies, the CC and B1B cross sections are in accord with each other to within some 10% but the CDW gradually diverges from the CC and B1B results. The disagreement increases with energy and reaches 100% for 2 MeV. For comparison, the OBK cross sections (Omidvar 1967) are also shown in figure 1. It can be seen that even at the highest energy of 3 MeV considered here the asymptotic relation ${}^{\mathrm{B1B}}\sigma = 0.661\,{}^{\mathrm{OBK}}\sigma$ (see e.g. Bransden and McDowell 1992) does not hold yet so that the use of the CC theory is justified in the full energy range (or the use of the B1B for $E > 1$ MeV as the present calculations may suggest).

The total CC neutralization cross sections σ_t are displayed in table 2 together with the partial cross sections $\sigma(1s)$ and $\sigma(n \geqslant 2)$, where they are compared with those obtained by Winter (1987). We note that the basis of Winter contains 20 projectile-centred and 25 target-centred states constructed from selected sets of Sturmian functions with n up to 8

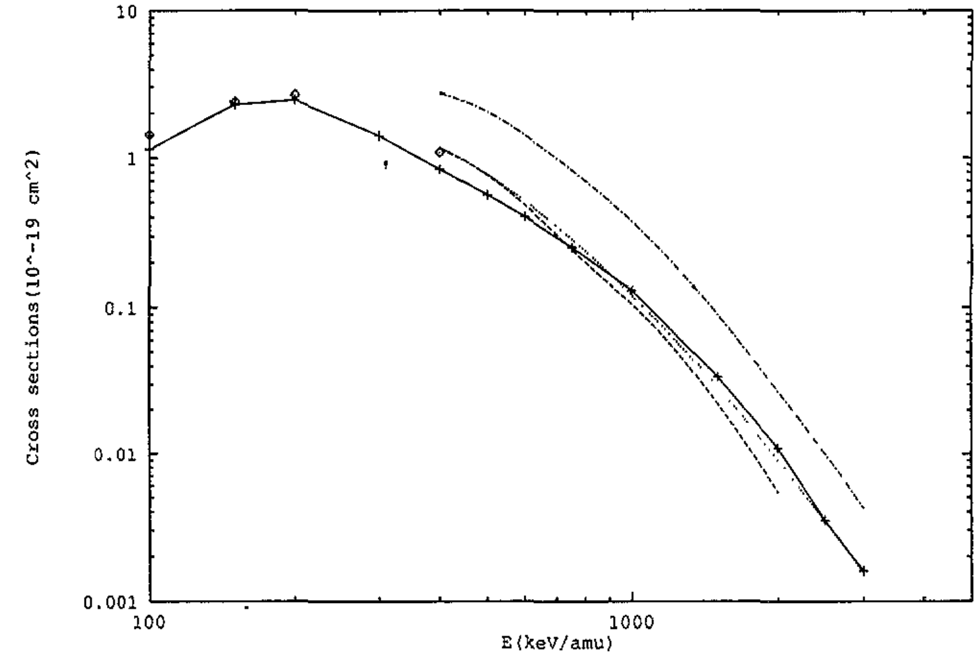

Figure 1. p + Be^{3+}(1s) collisions. Capture into H(1s). —— + ——, 35-state AO expansion, present; ◇, 45-state Sturmian expansion, Winter (1987); - - - -, BIB, Grozdanov and Kristic (1988); – – –, CDW, Mukherjee and Sil (1980). — · —, OBK, Omidvar (1967).

Table 2. Neutralization in p + Be^{3+} collisions. Close-coupled cross sections for production of H(n) (in 10^{-19} cm^2.

	1s		$n \geqslant 2$		Total	
E (keV)	a	b	a	b	a	b
100	1.14	1.43	0.28	0.50	1.42	1.93
150	2.28	2.39	0.46	0.47	2.74	2.85
200	2.45	2.64	0.39	0.35	2.84	2.99
400	0.83	1.08	0.26	0.24	1.09	1.32

[a] Present 35-state AO basis.
[b] Winter (1987), 45-state Sturmian basis.

and ℓ up to 2. It is difficult to judge, by comparison with the present 35 AO basis, which specific Sturmian states mainly contribute to the convergence of σ_t at 100 and 400 keV. For E = 100 keV, as table 2 shows, the difference between the present σ_t and those of Winter comes from both σ(1s) and $\sigma(n \geqslant 2)$. However, for E above 100 keV, the present $\sigma(n = 2)$ are remarkably close to Winter's $\sigma(n \geqslant 2)$. It appears that the two sets of σ_t are at variance with each other entirely due to the difference between the AO and Sturmian values of σ(1s) .

The present calculations show that $\sigma(n \geqslant 2)$ constitute some 15–20% of σ(1s), depending on E. This is somewhat higher but not very different from the prediction of the $1/n^3$ scaling rule. It is also found that capture into the $n = 2$ excited states of neutral hydrogen predominantly occurs into H(2s). Charge transfer into H(2p) constitutes only 20% of the partial $\sigma(n = 2)$ cross section at 200 keV. Its contribution rapidly decreases for

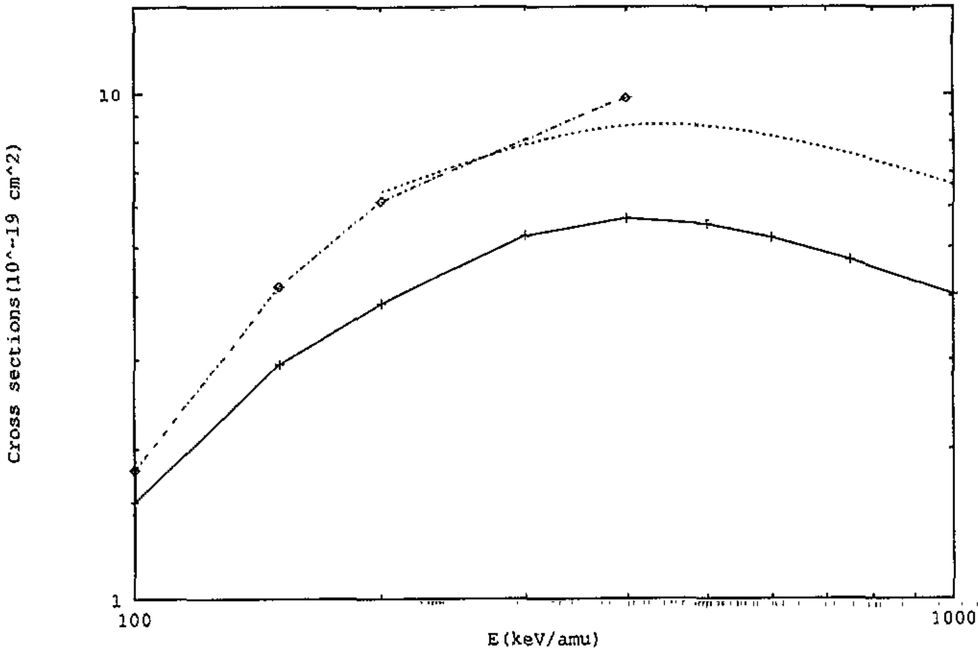

Figure 2. Ionization of $Be^{3+}(1s)$ in collisions with p. ——+——, 35-state AO expansion, present; — · —◇— · —, 45-state Sturmian expansion, Winter (1987); - - - -, Born, Bates and Griffing (1953).

higher energies becoming less than 5% at 1 MeV.

The solution of the rearrangement problem (1) with the expansion basis of table 1 also allows us to obtain, in the course of the calculations, direct excitation and ionization cross sections. As usual, ionization is computed using the projection method. Table 1 shows that the target bound states are well separated from the continuum, with the exception of the $\tilde{6}s$ and $\tilde{5}d$ states which had to be first projected onto the full spectrum of the target bound states in order to extract from them the contribution from the continuum. A small correction for capture into the projectile continuum estimated from the positive-energy target s state, was added to direct ionization to obtain the total ionization. The result is shown in figure 2 together with the ionization cross sections of the 45 Sturmian state calculation of Winter (1987) and the Born ionization (Bates and Griffing 1953). The Born cross sections lie *below* Winter's cross sections in the region of the *ionization maximum*, for $E > 200$ keV. This may suggest that his calculations overestimate ionization, at least at 400 keV, though the possible source of such an effect remains unclear. The present results, obtained with a limited number of positive energy pseudostates, probably underestimate the ionization cross sections.

In conclusion, a 35-state AO basis has been employed within the close-coupled semiclassical impact parameter method, to obtain cross sections for production of hydrogen in energetic $p+Be^{3+}$ collisions. In the intermediate energy range, coupling between charge-transfer and ionization channels has been taken into account by including some positive-energy pseudostates in the basis. It appears that there are two separate energy regions, one below and another one above the neutralization maximum, where the theoretical data for capture into the ground state of atomic hydrogen definitely show a scatter larger than 10%, the accuracy required in the current JET experiments. Further studies of the problem, with the aim of establishing the convergence of the computed cross sections, are in progress.

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