

Variational approach to excitation in $p + \text{Be}^{3+}$ collisions at intermediate and high impact velocities

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Abstract : A variational impact parameter approach, based on the Schwinger principle, is used to study the direct excitation for the single electron $p + \text{Be}^{3+}$ system (the beryllium ion is one of the main impurities in tokamak plasmas). The total cross sections for target excitation are presented in the energy range of 64 KeV to 4 MeV.

1. Variational impact parameter amplitude for direct excitation :

The variational approach reported here uses methods that have been described previously [1, 2] and so will be only briefly recalled.

Let $|\psi^+(z)\rangle$ and $|\psi^-(z)\rangle$ be the scattering wave functions defined, in a collision without rearrangement, by the eikonal Lippmann-Schwinger equations :

$$|\psi_\alpha^+(z)\rangle = |\alpha(z)\rangle + \int_{-\infty}^{+\infty} dz' G_T^+(z-z')V(z')|\psi_\alpha^+(z')\rangle \quad (1a)$$

$$|\psi_\beta^-(z)\rangle = |\beta(z)\rangle + \int_{-\infty}^{+\infty} dz' G_T^-(z-z')V(z')|\psi_\beta^-(z')\rangle \quad (1b)$$

where V is the projectile-target interaction. $|\alpha(z)\rangle$ and $|\beta(z)\rangle$ are the initial and final states of the target, respectively and G_T^\pm the target operator.

The transition amplitude may be written for $\alpha \neq \beta$, as:

$$a_{\beta\alpha}(\vec{\rho}) = \frac{i}{v} \frac{(\beta|V|\psi_\alpha^+)(\psi_\beta^-|V|\alpha)}{(\psi_\beta^-|V-VG_T^+V|\psi_\alpha^+)} \quad (2)$$

where the notation $(\quad|\quad)$ indicates the integration over the electronic coordinates as well as over z only when G_T^+ is does not appear, and over z' when G_T^+ is present.

To the first order in $|\delta\psi_\alpha^+\rangle$ and $|\delta\psi_\beta^-\rangle$, it is easy to show that $\delta a_{\beta\alpha}(\vec{\rho}) = 0$. This means that the expression (2) is stationary for small errors on $|\psi_\alpha^+\rangle$ and on $|\psi_\beta^-\rangle$.

The expression (2) is obviously the eikonal form of the Schwinger principle. By expanding $|\psi_\alpha^+\rangle$ and $|\psi_\beta^-\rangle$ on truncated basis sets $\{|i\rangle\}$ and $\{|j\rangle\}$ respectively (both sets are not necessarily identical but they have the same finite dimension N), one gets a finite set of linear equations for the coefficients by means of the variational condition $\delta a_{\beta\alpha}(\vec{\rho}) = 0$. The insertion of the solutions in eq. (2) leads to :

$$a_{\beta\alpha}(\vec{\rho}) = \left(-\frac{i}{V} \right) \sum_{i=1}^N \sum_{j=1}^N (\beta|V|i)(D^{-1})_{ij} (j|V|\alpha) \quad (3)$$

where $(D^{-1})_{ij}$ is the element (i, j) of the matrix D^{-1} inverse of the matrix D defined by the elements

$$D_{ji} = (j|V - VG_T^+V|i) \quad (4)$$

where $|i\rangle$ and $|j\rangle$ belong to suitable truncated basis sets β_1 and β_2 respectively. V is the target - projectile interaction and G_T^+ the target propagator. G_T^+ has been expanded on the whole discrete spectrum of the target [1]. In the present calculations the contribution of the continuum has been taken into account using an analytical continuation which consists to evaluate the part close to ionisation threshold.

Then, from the expression (4), the born-like term may be written :

$$(j|VG_T^+V|i) = \left(-\frac{i}{V} \right) \sum_{l=0}^{+\infty} \left[\sum_{\nu=l+1}^{+\infty} H_{ji}^{(\nu,l)} + \int_0^{+\infty} dk H_{ji}^{(k,l)} \right] \quad (5)$$

where k is the momentum of a target electron in the continuum.

In (5), the maximum value of ν_0 is evaluated automatically by the code which tests, for each value of ν below the threshold, the ν^{-3} law of matrix elements H_{ji}^ν .

Thus, in the symmetrical situation, the values of k above the threshold, for which the contribution of the continuum becomes negligible, have been found around $k_0 = \frac{2Z_T}{i\nu_0}$.

Then, the sum over the continuous states for a given l is:

$$\int_0^{+\infty} dk H_{ji}^{(k,l)} \approx \int_0^{k_0} dk H_{ji}^{(k,l)} = \frac{k_0}{4} H_{ji}^{(k_0,l)} \quad (6)$$

The evaluation of the contribution of the whole continuum without using an analytical continuation is in progress.

2. Results and discussions :

The figure shows the CC theoretical results from Ermolaev et al [3] for 50 - 300 KeV protons energies using the two - centre AO expansion method with 55 atomic states and pseudostates, along with the present calculations, first Born (B1) and S55 where $\beta_1 = \beta_2 = \{ 1s, 2s, 2p_0, 2p_1, 2p_{-1} \}$.

In the lack of experimental and other theoretical results, and other results of Ermolaev et al for energies above 300 KeV, we note that our results underestimate the cross sections at low energies. On the other hand our B1 and S55 results are close one to the other at energies above the maximum of the excitation cross sections.

At intermediate velocities, the values obtained by the theoretical methods are known to be strongly dependent on the choice of basis set [4].

Starting from view of Slim and Ermolaev [4], our 2s excitation cross sections could be improved as expected, by adding the dominant 1s capture state in the expansion of the scattering wave function $|\psi_{\alpha}^{+}\rangle$ and $|\psi_{\beta}^{-}\rangle$.

These results can allow the deduction of the energy distribution function for the MeV protons in the plasma.

3. References

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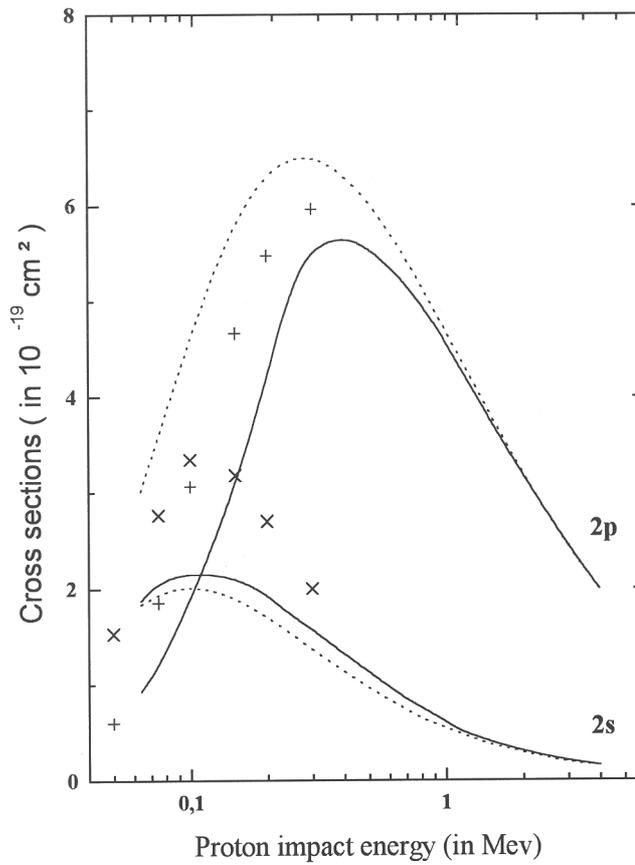


Figure : Total cross section in unit 10^{-19} cm^2 for the $1s \rightarrow 2n$ excitation of Beryllium ion by protons as a function of impact energy in MeV. Present results: — : S55, ---- : B1. Ermolaev et al based on CC calculations [3] : X : 2s, + : 2p.