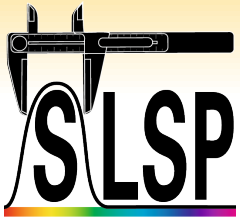

FAC RMatrix for Impact Width and Shift

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Baranger's Formula

The starting point of electron impact width and shift is the Baranger's formula, in the case of FWHM w:

$$w = n_e v \left[\sum_{k \neq i} \sigma_{ik} + \sum_{k \neq f} \sigma_{fk} + \int d\Omega \left| f_i(\Omega) - f_f(\Omega) \right|^2 \right] \qquad (1)$$

Complications from angular momentum coupling treated according to Baranger (1958, PR 112, p856).

Unitarity of the S matrix allows simplications under spherical symmetry (Peach 1996, Atomic, Molecular, Optical Physics Handbook):

$$\begin{aligned} w + i2s &= n_e v \frac{\pi a_0^2}{2E} \Omega(E) \\ \Omega &= \sum_{if} (-1)^{2J_i + 2J_f^T + j + j'} \left(2J_i^T + 1 \right) \times \left(2J_f^T + 1 \right) \\ &\times \begin{Bmatrix} J_f^T & J_i^T & 1 \\ J_i & J_f & j \end{Bmatrix} \begin{Bmatrix} J_f^T & J_i^T & 1 \\ J_i & J_f & j' \end{Bmatrix} \times \left[\delta_{\kappa\kappa'} - S_{ii} S_{ff}^* \right] \end{aligned} \qquad (2)$$

RMatrix Inner Region

We construct a basis set for the $N+1$ electron system using the anti-symmetrized product of target and one electron continuum basis functions with a fixed boundary condition at $r = a$ (Norrington, DARC manual), which diagonalizes the $N+1$ Hamiltonian in the inner region

$$\Psi_k = \sum_{ij} c_{ijk} \mathcal{A} \left[\Phi_i, \phi_{ij} \right]^{J^T \pi} + \sum_m d_{mk} \theta_m (J^T, \pi) \tag{3}$$

Such that Ψ_k is the k-th eigenvector with eigenvalue E_k.

The boundary condition of continuum basis ϕ_{ij} is defined in terms of radial large and small components of the Dirac radial wavefunctions

$$\frac{\mathcal{Q}_{ij}(a)}{\mathcal{P}_{ij}(a)} = \frac{b + \kappa}{2ac} \tag{4}$$

R Matrix at Boundary Surface

The total scatering wavefunction at given energy E is expanded in terms of Ψ_k

$$\Psi(E) = \sum_k A_k(E)\Psi_k \tag{5}$$

Define

$$w_{ik}(r) = \sum_j c_{ijk}\mathcal{P}_{ij}(r) \qquad P_i(r) = \sum_k A_k(E)w_{ik}(r)$$

$$v_{ik}(r) = \sum_j c_{ijk}\mathcal{Q}_{ij}(r) \qquad Q_i(r) = \sum_k A_k(E)v_{ik}(r)$$

and the R matrix

$$R_{ij} = \frac{1}{2a}\sum_k \frac{w_{ik}(a)w_{jk}(a)}{E_k - E} \tag{6}$$

It can be shown

$$P_i(a) = \sum_j R_{ij}\left[2acQ_j(a) - (b+\kappa_j)P_j(a)\right] \tag{7}$$

K Matrix from Boundary Matching

The reactance K matrix is defined through the asymptotic behavior of the continuum wavefunction as $r \to \infty$. For n_o open channels and n_c closed channels, there are $n_o + n_c$ indenpendent solutions in the asymptotic region,

$$P_{ij} \sim \sin\theta_i \delta_{ij} + \cos\theta_i K_{ij} \tag{8}$$

for open channels, and

$$P_{ij} \sim \exp -|k_i| r \tag{9}$$

for closed channels. Solutions with these asymptotic behavior can be integrated inward until the RMatrix boundary at $r = a$, where using the R matrix boundary condition yields a system of linear equations for the reatance matrix K. The S matrix is obtained via

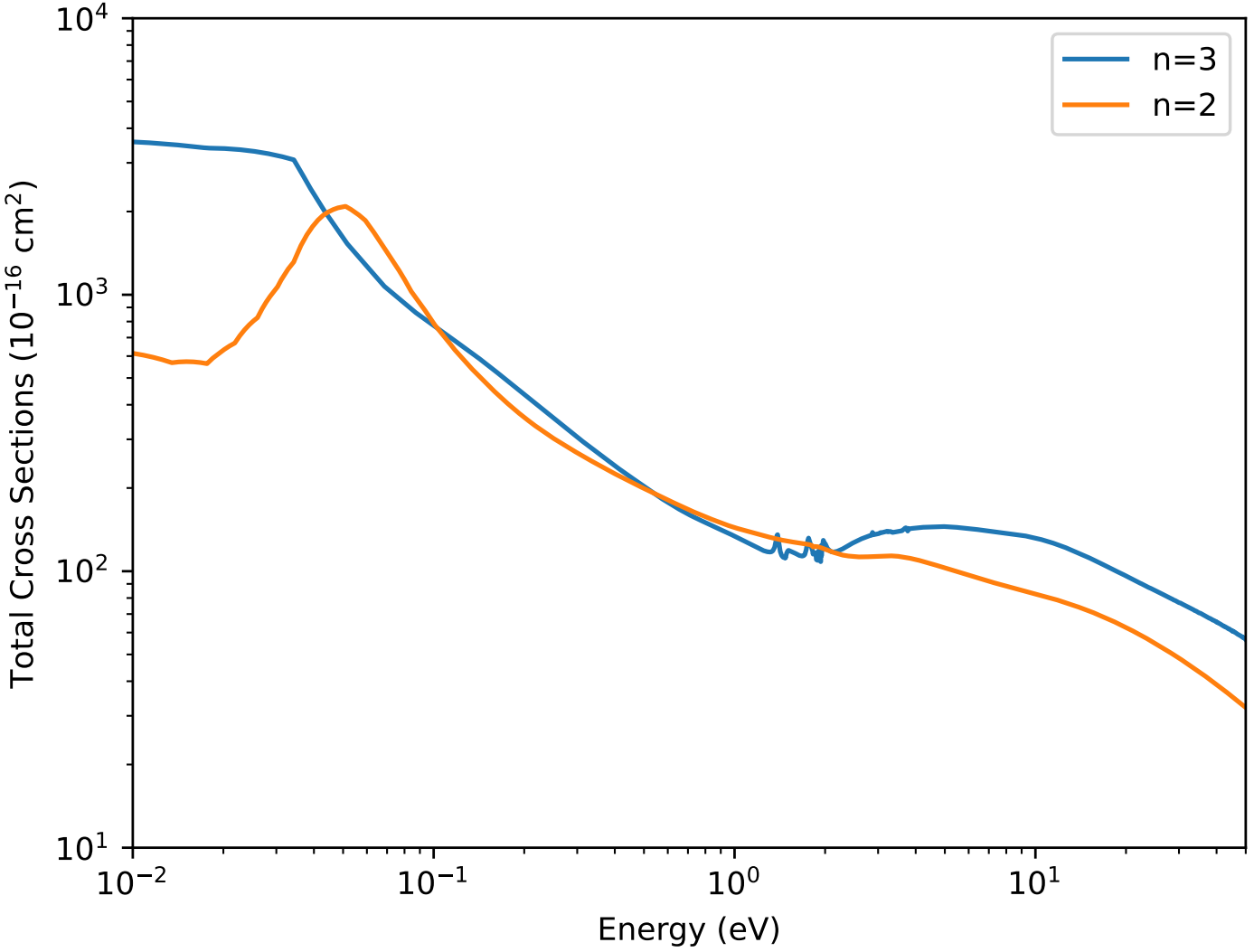
$$S = \frac{1 + iK}{1 - iK} \tag{10}$$

Li I and B III 2s-2p Width and Shift

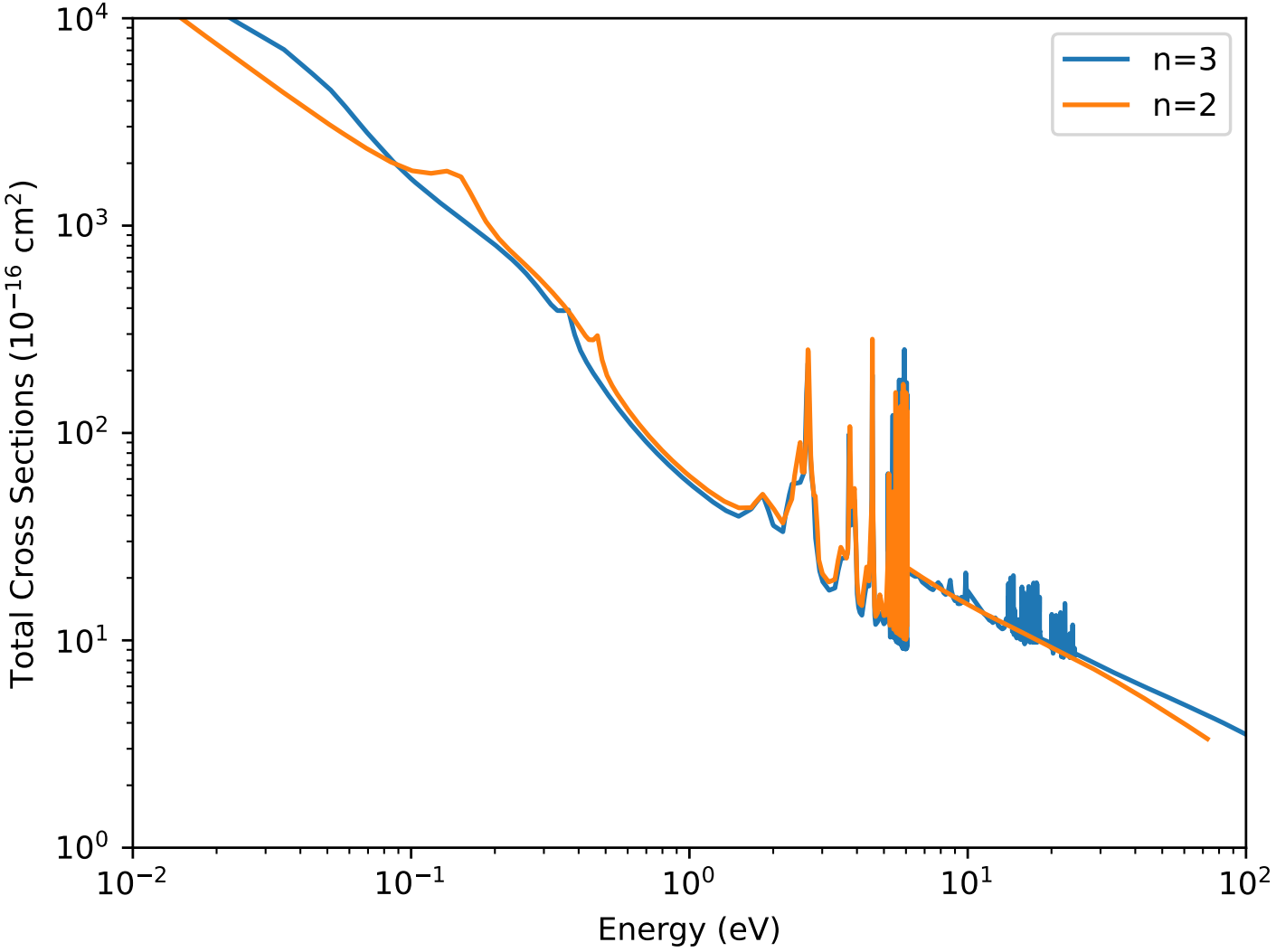
- Default target states, $1s^2 2l$.
- Expanded target states, $1s^2 2l$ and $1s^2 3l$.
- Widths, shifts and partial wave cross sections at requested energy grid for SLSP7.
- Widths and shifts with sufficient energy resolution to resolve electron capture resonances.
- Partial wave expansion up to $l = 100$.

For SLSP7 tabulated results, the default target states are used, and we average over $2p_{1/2}$ and $2p_{3/2}$ fine structure components. The $2p_{1/2} - 2p_{3/2}$ excitation cross sections are also ignored in the submitted results.

Total Cross Section of Li I 2s-2p Width

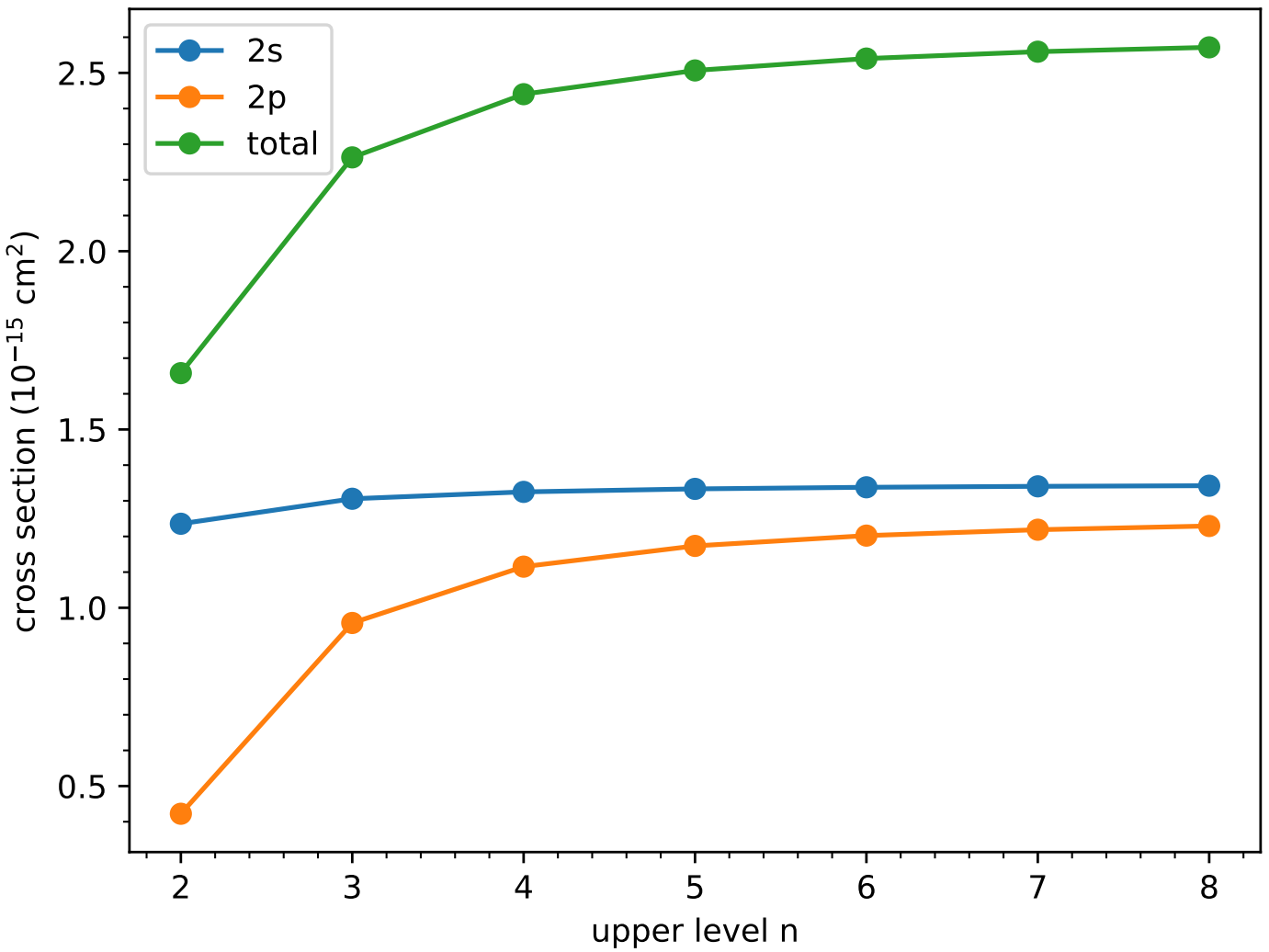


Total Cross Sections of B III 2s-2p Width



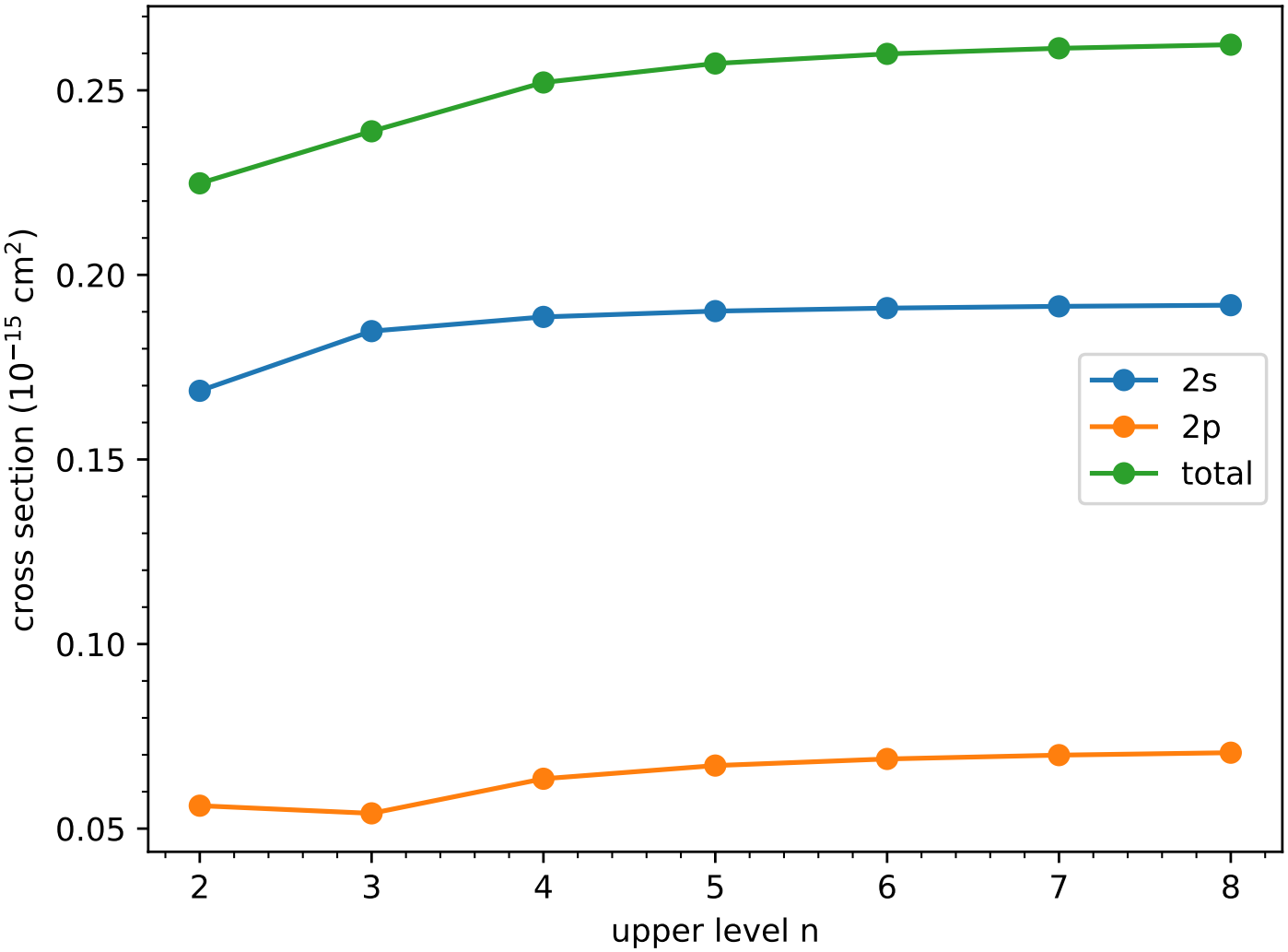
Effects of Excitation to $n > 3$: Li I

Distorted-wave estimation at $E = 100$ eV



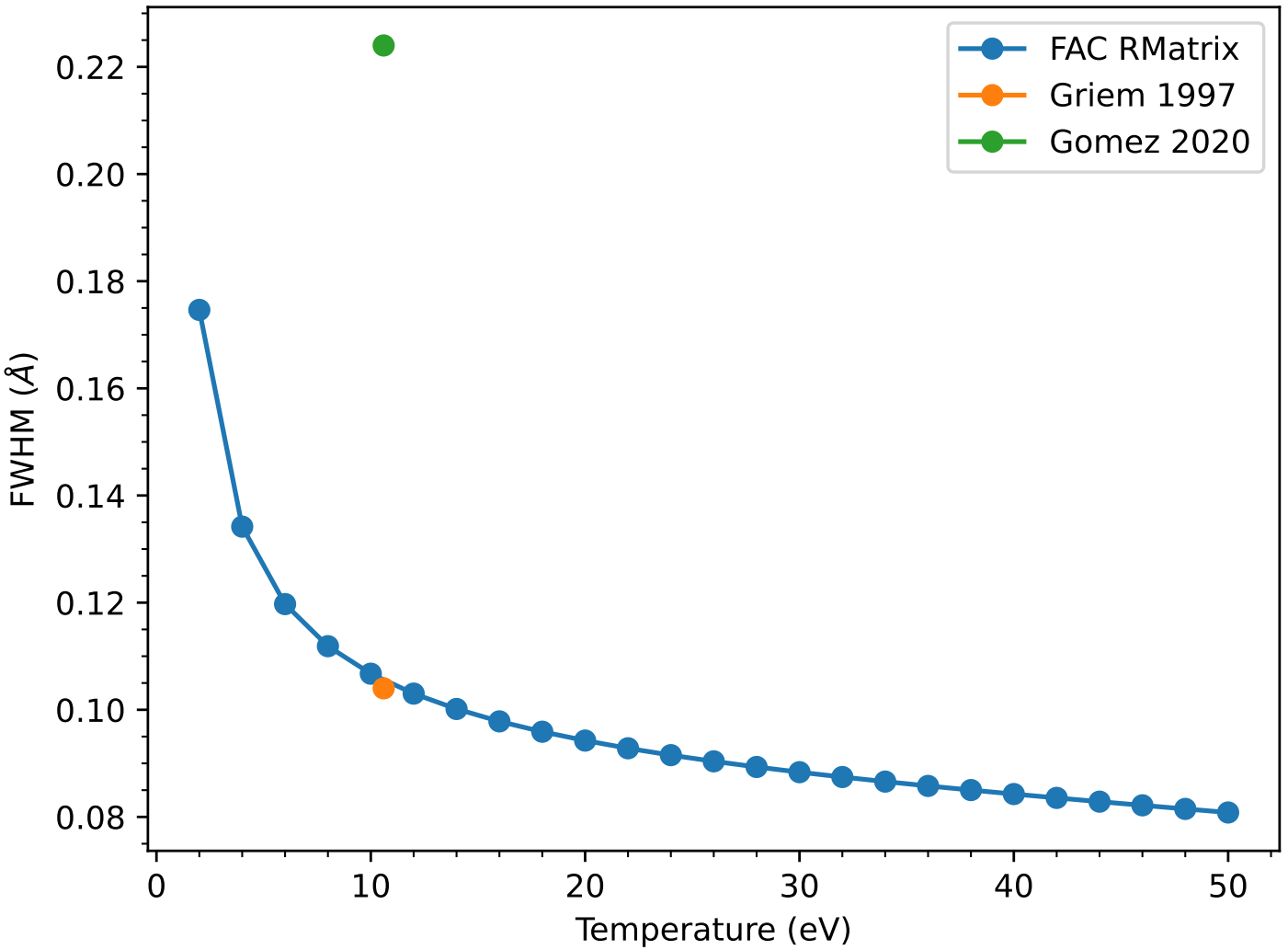
Effects of Excitation to $n > 3$: B III

Distorted-wave estimation at $E = 100$ eV



FWHM of B III 2s-2p in Thermal Plasma

$n_e = 1.8 \times 10^{18} \mathrm{cm}^{-3}$



Comparison of Total Cross sections of B III 2s-2p