

B-spline R-matrix with pseudo-states calculations for electron-impact excitation and ionization of beryllium

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Synopsis The B-spline R-matrix-with-pseudostates (BSR) method is employed to treat electron collisions with beryllium atoms. Predictions for elastic scattering, excitation, and ionization are presented for all transitions between the lowest 19 states of beryllium in the energy range from threshold to 150 eV. The sensitivity of the results is checked by comparing data obtained in different approximations with increasing number of pseudo-states.

Beryllium is used as a surface material in the JET project and for the plasma-facing walls in ITER. This calls for accurate electron–beryllium scattering results. Due to the lack of experimental data, researchers in plasma modelling currently have to rely entirely on theoretical predictions. For this reason, it is important to estimate the accuracy of the available theoretical datasets.

Extensive sets of theoretical calculations are indeed available. These data were obtained with advanced methods, such as R-matrix with pseudo-states (RMPS) [1,2], convergent close-coupling (CCC) [3], and time-dependent close-coupling (TDCC) [4]. All these calculations indicate a slow convergence of the close-coupling expansion and large effects from coupling to the target continuum.

In the present work, the B-spline R-matrix method [5] was used to study electron collisions with neutral beryllium over an energy range from threshold to 150 eV. The convergence of the results was checked by comparing data from different models with increasing number of target states, ranging from the distorted-wave approximation to the close-coupling method with 650 continuum pseudo-states. For most excitation cross sections we found very close agreement with the existing results [1-4]. This suggests an accuracy of those datasets within a few percent.

Two new points were revealed in the present calculations. For the first time we obtained converged results for the strong $2s^2 2p$ shape resonance at low energies (see Fig. 1). The position, 0.28 eV, and width, 0.37 eV, of this resonance differ considerably from numerous results obtained with methods based on model potentials [6] or complex rotation [7].

Furthermore, while we obtained close (10%) agreement with RMPS and TDCC ionization cross sections [4] from the ground state, the predictions for ionizing the metastable $(2s2p)^3P$ state differ by a factor of 2 (c.f. Fig. 2). We also found large differences between ionization of the $(2s2p)^3P$ and ^1P states, due to a strong term-dependence of the valence orbitals.

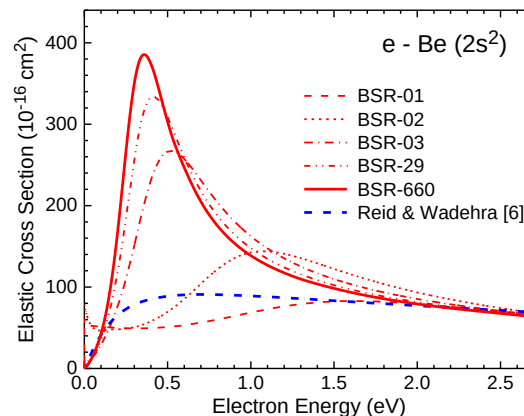


Figure 1. Model dependence of the cross sections obtained for elastic electron scattering from beryllium atoms in their ground state.

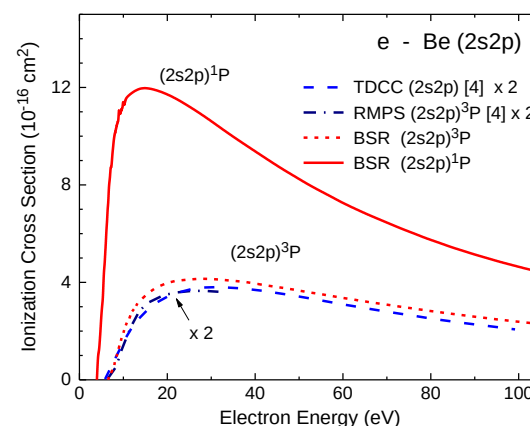


Figure 2. Electron-impact ionization cross sections for neutral Be from the excited $2s2p$ configuration.

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