Photoionization of Cl-like Argon using the Breit-Pauli R-matrix method

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Photoionization of Cl–like Argon using the
Breit–Pauli R–matrix method

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Synopsis Here we present the photoionization cross sections for the ground and metastable states of Cl–like Argon by exploiting the fully relativistic Breit–Pauli R–matrix computer codes to determine these transitions of interest. We compare our work with previous theoretical and experimental results and present a detailed investigation into the model of Ar III, the resonant structure and identification process.

Investigation into the structure of ionic targets is essential for the generation of accurate radiative transitions, of which the bound-free photoionisation (PI) process is to be discussed. Such data is useful in modelling various synthetic spectra through packages such as Cloudy [1]. We focus solely on the PI of Ar II governed by,

\[ \text{hv} + \text{Ar II} \rightarrow \text{Ar III} + e^- \]

in which a direct PI pathway leaves the target Ar III plus the ejected photoelectron, but also indirectly via autoionizing bound states, where the photoelectron is firstly excited into a more energetic state prior to ejection.

Results are obtained through the implementation of large scale Breit–Pauli R–matrix computer codes, to include the one body relativistic operators [2] by availing of the well established R–matrix theory [3]. A delineation of configuration interaction terms are also required to allow for electron correlation effects.

Once an accurate model for Ar III is established, we then compute all PI cross sections in the length gauge defined by,

\[ \sigma = \frac{4\pi^2 a_0^2 \alpha \omega}{3g_i} \sum_{L,lf} |\langle \Psi_f | D| \Psi_i \rangle|^2 \]  

where the wavefunctions of the initial bound state, \( \Psi_i \) and final free state of \( \Psi_f \) are computed over a very fine energy mesh to allow for sharp resolution of the spectra. \( a_0 \equiv \) bohr radius, \( \alpha \equiv \) fine structure constant, \( \omega \equiv \) photon energy and \( g_i \equiv \) statistical weight of initial state.

We compute and present transitions within the intermediate coupling frame for the ground and metastable initial odd states of \( J = 3/2 \) and \( J = 1/2 \) to accessible, dipole allowed final states through Equation (2). A direct comparison with M. Covington et al [6] can be achieved by performing both a 10meV gaussian convolution of the spectra and a weighting comprising of the two initial states. We also conduct a resonance identification procedure using the QB technique [7] which exploits the analytical properties of the R–matrix to identify autoionizing bound states of the indirect path in Equation (1).

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