Studies on the Electron-Correlation and Relativistic Effects in Target Representation and Low-Energy Collision Calculation

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This work is motivated by a long standing discrepancy between the theoretical models treating the complexity of the resonance structure for low-energy electron scattering. This complexity of the resonance structure for low-energy electron scattering determines the complexity of atomic data calculation. In this respect, current theoretical method and computational tools place more emphasis on the accurate representation of target electron wave functions than the study of other processes. The cross section and rates must be determined at typically tens of thousands of energy values. As the charge number Z on the atomic nucleus increases, relativistic effects become progressively more important in the collision process. In this work we consider how these effects can be accurately represented in low-energy electron collisions with heavy atoms and atomic ions. We have systematically investigated whether the differences in the calculations of atomic data, for the Mg-like S V, S-like Ar III, Li-like Al XI ions and the Fe-peak element Co IV ion, are due to the different treatment of relativistic effects or to the approximation made in solving the resultant scattering equations. We have carried out calculations using several procedures for including electron correlation and relativistic effects, ranging from transforming the non-relativistic K-matrix to solving the Dirac equation in case of the Mg-like S V ion [1,2]. An important question is where can accurate results be obtained using the Breit-Pauli Hamiltonian, and when is it necessary to use the Dirac Hamiltonian. We have addressed this important issue for the S-like Ar III ion [3] and for the Fe-peak element Co IV ion [4, 5].

It has been realized that transitions from autoionizing levels (so-called dielectronic satellites) of highly charged ions provide an outstanding plasma temperature diagnostic. We have performed detailed quantitative description of the level population kinetics responsible for the relatively high line-intensity of the forbidden and intercombination transitions arising from autoionizing states in Li-like Al [6]. Anomalous high intensity X-ray intercombination and two-electron transitions in verifying the conditions stated here have been detected at the nhelix-laser test bed facility at GSI.

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