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MODERN METHODS FOR CALCULATIONS OF PHOTOIONIZATION AND ELECTRON IMPACT IONIZATION OF TWO-ELECTRON ATOMS AND MOLECULES

V. V. Serov[a], V. L. Derbov[a], T. A. Sergeeva[a], and S. I. Vinitsky[b]

[a] *Saratov State University, Saratov*
[b] *BLTP, JINR, Dubna*

A review of some recently developed methods of calculating multiple differential cross-sections of photoionization and electron impact ionization of atoms and molecules having two active electrons is presented. The methods imply original approaches to calculating three-particle Coulomb wave functions. The external complex scaling method and the formalism of the Schrödinger equation with a source in the right-hand side are considered. Efficiency of the time-dependent approaches to the scattering problem, such as the paraxial approximation and the method of the expanding coordinate grids, is demonstrated. An original numerical method elaborated by the authors for solving the 6D Schrödinger equation for an atom with two active electrons, based on the Chang-Fano transformation and the discrete variable representation, is formulated. High-efficiency approaches and numerical methods for solving the 6D Schrödinger equation, finally describing the photo- and impact ionization of a two-electron molecule, are presented, including the spheroidal coordinates, the discrete-variable representations, the B-spline expansion, and the finite-element Lobatto quadrature expansion. Basing on numerical simulations, the threshold behavior of angular distributions of two-electron photoionization of the negative hydrogen ion and helium atom, and multiple differential cross-sections of electron impact ionization of hydrogen and nitrogen molecules are analyzed.