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Computational methods in relativistic atomic physics

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Owing to recent advances in accelerator and storage ring techniques, more possibilities arise to study formation of quasi-molecules in slow heavy-ion collisions. Today, these (quasi) molecules are believed to be a versatile tool for investigating a number of fundamental problems in modern physics. In particular, analysis of molecular spectra can provide unique knowledge on the relativistic, many-body and quantum electrodynamics (QED) effects in the non-perturbative domain of high nuclear charges and super strong electromagnetic fields. Moreover, the electron-positron pair production that occurs under such extreme conditions might be utilized to explore the properties and behaviour of physical vacuum and, even, to search for new particles. Theoretical description of super-heavy quasi-molecules is a complicated task which requires solution of the two-center Dirac equation. During the recent years, we have developed several methods for dealing with such a two-center problem. The methods utilize finite basis sets constructed from B-splines and provide an efficient access to a complete (quasi-) molecular spectrum, including not only bound states but also positive- as well as negative-continuum solutions. In my contribution, I will review these novel computational approaches and will show their application for the analysis of the structure and dynamics of quasi-molecules.

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