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Recent advances in numerical solutions of the molecular relativistic time-dependent Dirac equation

Due to recent and prospected technological advances, it is now possible, to consider laser intensities of 10^{23} W/cm² and higher. In this new regime, relativistic and quantum electrodynamics effects start to be important, requiring a theoretical description in terms of the time-dependent Dirac equation. In this presentation, I will present recent advances on the numerical solution of this equation for 3-D axisymmetric geometries using cylindrical coordinates. The numerical method is based on a split-step scheme in coordinate space, which is free from the “fermion doubling” problem and which can be parallelized very efficiently. A new technique to circumvent the coordinate singularity at $r = 0$ using Kirchhoff’s formula will also be described. The numerical method is then utilized to simulate the quantum relativistic dynamics of an electron bound in a diatomic molecule potential and interacting with an ultraintense counterpropagating laser field. These simulations may have applications in quantum imaging for ultraintense laser-matter interaction.