Solving the time-dependent Schroedinger equation with grid-based methods using exterior complex scaling[1] LIANG TAO, LBNL, C. WILLIAM MCCURDY, LBNL and UCDavis, THOMAS N. RESCIGNO, LBNL — We show that exterior complex scaling provides a viable method for suppressing reflections in numerical simulations of the time-dependent Schroedinger equation for strong-field problems, provided the calculations are carried out in the radiation gauge. We show that numerical stability can be achieved without the *ad hoc* use of an untransformed external field and that recently reported instabilities [F. He, C. Ruiz and A. Becker, Phys. Rev. A 75, 053407 (2007)] can be traced to an inappropriate choice of the complex grid. Atomic simulations in 1-,2- or 3-D can be implemented using a discrete variable representation for the radial electron coordinate based on Gauss-Lobatto quadrature and finite-elements (FEM/DVR). For simulations involving diatomic molecules, cylindrical coordinates (ρ, z) can be used, but special care must be taken to avoid slow convergence near $\rho = 0$. We show how a proper FEM/DVR can be constructed in cylindrical coordinates.

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