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Comparative Study of Wavelet Basis Set and Finite-Difference Time-Domain Methods for the Time Propagation of Quantum and Classical Systems

EWA NOWARA, IRWIN GOLDBERG, St. Mary’s University (San Antonio, Texas), BRUCE JOHNSON, Rice University, RICHARD LOMBAR-DINI, St. Mary’s University (San Antonio, Texas) — An extensive comparison in error accumulation between a grid point method, in particular finite-difference time-domain (FDTD), and a basis set method using Daubechies wavelets is presented in the modeling of electromagnetic (EM) pulses (classical) in inhomogeneous media and quantum (QM) wavepackets interacting with various potentials. It is demonstrated that the density of wavelet functions needed to attain a certain level of accuracy is far less than needed for grid points (FDTD) translating to savings in computational memory and processing. Since neighboring wavelet basis functions have overlapping support, fictitious wavelet projections created by derivative matching (T.A. Driscoll and B. Fornberg) will be used to handle Dirichlet boundary conditions in both the EM and QM cases in order to prevent rapid error growth.

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