A NEW SOLVER FOR THE TIME-DEPENDENT SCHRÖDINGER EQUATION ON UNBOUNDED DOMAINS

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ABSTRACT

I will introduce a new numerical method for the solution of the time-dependent Schrödinger equation in free space. Using a pseudospectral-type method with the real Fourier axis deformed to a properly chosen complex contour, I will show that traditional artificial boundary conditions can be avoided, in a controlled manner, as long as the usual assumption of a compactly-supported potential holds. I will obtain a numerical method which is high-order accurate in space and time, has quasi-optimal computational complexity, operates on Cartesian grids in any dimension, naturally permits time-dependent potentials and spatially-uniform applied fields, and can allow solutions to leave the computational domain and return later. I will present results from simulations of absorption and photoemission spectroscopy using time-dependent density functional theory which suggest the method enables the use of significantly smaller computational domain sizes than the complex absorbing potentials presently in common use.

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