TRANSPARENT BOUNDARY CONDITIONS FOR THE TIME-DEPENDENT SCHRÖDINGER EQUATION WITH A UNIFORM APPLIED FIELD

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Abstract. We consider the problem of constructing transparent boundary conditions for the time-dependent Schrödinger equation (TDSE) with a compactly supported binding potential and a spatially uniform, time-dependent electromagnetic vector potential. Such conditions prevent nonphysical boundary effects from corrupting numerical solutions in a bounded computational domain. We use ideas from potential theory to build an exact transparent condition as a Dirichlet-to-Neumann or Neumann-to-Dirichlet map on an arbitrary domain. The form of the TDSE which we consider supports solutions which may leave a bounded domain and return later. The boundary conditions we derive account for this behavior in a mathematically exact manner. For the one-dimensional case in which the domain is an interval, we propose a simple discretization scheme and a fast algorithm to accelerate the calculation of the boundary condition, which is nonlocal and non-convolutional in time.

Keywords: Time-dependent Schrödinger equation, transparent boundary conditions, laser-molecule interaction

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