CHRISTOPHE BESSE, Université Lille 1, Cité Scientifique, 59655 Villeneuve d'Ascq Cedex, France
Artifical boundary conditions for the Schrödinger equation with external potential

We are interested in the numerical solving of the Schrödinger equation with variable potential, in one space dimension, on a bounded domain:

$$\begin{cases} i\partial_t u + \partial_x^2 u + V\,u = 0, & (x,t) \in \mathbb{R} \times [0\,;T], \\ u(x,0) = u_0(x), & x \in \mathbb{R}, \end{cases} \tag{1}$$

where u_0 is the initial datum with compact support, T is the final computational time, and $V \in \mathcal{C}^\infty(\mathbb{R} \times \mathbb{R}^+, \mathbb{R})$ is a real potential. In order to numerically solve the equation, we have to compute the solution of the system (eq:Schr-eqn-R) on a bounded space domain. We therefore have to introduce a fictive boundary $\Gamma = \partial\Omega = \{x_l, x_r\}$ to bound the computational domain $\Omega =]x_l, x_r[$. The introduction of this boundary needs the addition of a boundary condition. Ideally, this boundary condition must be transparent with respect to the solution. The solution of the Schrödinger equation on $\Omega \times [0\,;T]$ with the boundary condition must coincide with the restriction on $\Omega \times [0\,;T]$ of the solution of (1) on $\mathbb{R} \times [0\,;T]$.

We will present new results concerning the derivation of an artificial boundary condition when the Schrödinger equation is in presence of a variable potential $V(x,t)$ and its numerical treatment.