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Exact Artificial Boundary Condition for the Poisson Equation in the Simulation of the 2D Schrödinger-Poisson System

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Abstract. We study the computation of ground states and time dependent solutions of the Schrödinger-Poisson system (SPS) on a bounded domain in 2D (i.e. in two space dimensions). On a disc-shaped domain, we derive exact artificial boundary conditions for the Poisson potential based on truncated Fourier series expansion in θ, and propose a second order finite difference scheme to solve the r-variable ODEs of the Fourier coefficients. The Poisson potential can be solved within $\mathcal{O}(MN\log N)$ arithmetic operations where M,N are the number of grid points in r-direction and the Fourier bases. Combined with the Poisson solver, a backward Euler and a semi-implicit/leap-frog method are proposed to compute the ground state and dynamics respectively. Numerical results are shown to confirm the accuracy and efficiency. Also we make it clear that backward Euler sine pseudospectral (BESP) method in [33] can not be applied to 2D SPS simulation.

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Key words: 2D Schrödinger-Poisson system, exact artificial boundary condition, backward Euler scheme, semi-implicit/leap-frog scheme, backward Euler sine pseudospectral method.

1 Introduction

The Schrödinger-Poisson system (SPS) is used, e.g., in quantum semiconductor modelling [2, 20]. We shall deal with the 2D (two space dimensions) case [1]. The system

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reads, in rescaled form, as

$$i\partial_t\psi(\mathbf{x},t)=\left(-\frac{1}{2}\Delta+V(\mathbf{x})+\beta\varphi\right)\psi(\mathbf{x},t),\quad \mathbf{x}\in\mathbb{R}^2,\quad t>0, \tag{1.1}$$

$$\psi(\mathbf{x},t=0)=\psi_0(\mathbf{x}),\qquad \mathbf{x}\in\mathbb{R}^2, \tag{1.2}$$

$$-\Delta\varphi(\mathbf{x},t)=|\psi(\mathbf{x},t)|^2,\quad \mathbf{x}\in\mathbb{R}^2,\quad t>0, \tag{1.3}$$

where the complex-valued function $\psi(\mathbf{x},t)$ stands for the wave function and decays to zero at far field, i.e., $\lim_{|\mathbf{x}|\to+\infty}|\psi(\mathbf{x},t)|=0$, $\forall t>0$, ψ_0 is the initial data lying in the energy space $H^1(\mathbb{R}^2)$, $V(\mathbf{x})$ is an external potential and $\beta\in\mathbb{R}$ is a coupling constant that represents the relative strength of the Poisson potential for repulsive case ($\beta>0$) and attractive case ($\beta<0$). Note that the Poisson equation (1.3) can be rewritten as a convolution of the density and the Green's function of Laplace operator as follows

$$\varphi(\mathbf{x},t)=\left(-\frac{1}{2\pi}\ln|\mathbf{x}|\right)*|\psi(\mathbf{x},t)|^2. \tag{1.4}$$

Two important invariants are the mass $M(\psi):=\int_{\mathbb{R}^2}|\psi|^2\mathrm{d}\mathbf{x}$ and the total energy $E(\psi):=\int_{\mathbb{R}^2}\frac{1}{2}|\nabla\psi|^2+V(\mathbf{x})|\psi|^2+\frac{1}{2}\beta\varphi|\psi|^2\mathrm{d}\mathbf{x}$. The ground state ϕ_g is defined as the minimizer of the energy E on the unit sphere $S=\{\phi\,|\,\|\phi\|_{R^2(\mathbb{R}^2)}=1, E(\phi)<\infty\}$, i.e.,

$$\phi_g=\arg\min_{\phi\in S}E(\phi) \tag{1.5}$$

and the ground state energy is denoted as $E^g=E(\phi_g)$.

The SPS is a "weakly" nonlinear Schrödinger equation (NLS) that has been extensively studied analytically and numerically. For a derivation of the Schrödinger-Poisson system from the linear N-body Schrödinger equation with Coulomb interaction, see e.g. [13,14,18]. For a discussion of the dimension reduction from 3D to 2D for the Schrödinger-Poisson system, see e.g. [10,15].

Here we focus on the numerical aspect of reducing the whole space problem to a numerically tractable problem on a bounded domain, with emphasis on the boundary conditions imposed on the Poisson equation.

Several efficient and accurate numerical methods had been proposed to solve SPS, such as the time-splitting spectral/pseudospectral method [11], finite difference method and finite element method [30]. Particularly, for SPS, we refer the reader to [12,17,33] for the time splitting pseudospectral method, to [26,31] for difference method and etc.

For numerical simulations of Schrödinger type equations, the whole space problem is usually truncated on a bounded domain, assuming that the wave function outside the computation domain is negligible. The easiest way is to truncate the wave function on a bounded domain and to use homogeneous Dirichlet boundary conditions (corresponding to reflection due to an infinite potential) or periodic boundary conditions (called "Born-von Karman boundary conditions" in solid state physics) for the wave function and its gradient.