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Optimal Error Estimates of Compact Finite Difference Discretizations for the Schrödinger-Poisson System

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Abstract. We study compact finite difference methods for the Schrödinger-Poisson equation in a bounded domain and establish their optimal error estimates under proper regularity assumptions on wave function ψ and external potential $V(x)$. The Crank-Nicolson compact finite difference method and the semi-implicit compact finite difference method are both of order $\mathcal{O}(h^4+\tau^2)$ in discrete l^2,H^1 and l^∞ norms with mesh size h and time step τ. For the errors of compact finite difference approximation to the second derivative and Poisson potential are nonlocal, thus besides the standard energy method and mathematical induction method, the key technique in analysis is to estimate the nonlocal approximation errors in discrete l^∞ and H^1 norm by discrete maximum principle of elliptic equation and properties of some related matrix. Also some useful inequalities are established in this paper. Finally, extensive numerical results are reported to support our error estimates of the numerical methods.

AMS subject classifications: 35Q55, 65M06, 65M12, 65M22, 81-08

Key words: Schrödinger-Poisson system, Crank-Nicolson scheme, semi-implicit scheme, compact finite difference method, Gronwall inequality, the maximum principle.

1 Introduction

The Schrödinger-Poisson system (SPS) is a local single particle approximation of the time-dependent Hartree-Fock system. It reads, in dimensionless form,

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

$$\nabla^2\Phi(\mathbf{x},t)=-|\psi(\mathbf{x},t)|^2,\qquad \mathbf{x}\in\mathbb{R}^d, \tag{1.2}$$

$$\psi(\mathbf{x},t=0)=\psi_0(\mathbf{x}),\qquad \mathbf{x}\in\mathbb{R}^d. \tag{1.3}$$

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The complex-valued function $\psi(\mathbf{x},t)$ stands for the single particle wave function with $\lim_{|\mathbf{x}|\to\infty}|\psi(\mathbf{x},t)|=0$, $V(\mathbf{x})$ is a given external potential, $\Phi(\mathbf{x},t)$ denotes the Poisson potential subject to open boundary condition, and $\beta\in\mathbb{R}$ is the coupling constant. The attractive case ($\beta<0$) is usually called the Schrödinger-Newton (SN) system and it describes the particle moving in its own gravitational potential, while the repulsive case ($\beta>0$) describing electrons travelling in its own Coulomb potential is named as Schrödinger-Poisson (SP) system.

The SPS can be rewritten as nonlinear Schrödinger equation (NLS) as

$$i\partial_t\psi(\mathbf{x},t)=\left[-\frac{1}{2}\Delta+V(\mathbf{x})+\beta\Phi(|\psi|^2,t)\right]\psi(\mathbf{x},t),\quad \mathbf{x}\in\mathbb{R}^d,\quad t>0. \tag{1.4}$$

Here, the Poisson potential is equivalent to $G_d(|\mathbf{x}|)*|\psi|^2$ with $G_d(|\mathbf{x}|)$ representing the Green function of Poisson equation on $\mathbb{R}^d$, which is specified as,

$$G_d(|\mathbf{x}|)=\begin{cases}-\frac{1}{2}|\mathbf{x}|, & d=1,\\ -\frac{1}{2\pi}\ln(|\mathbf{x}|), & d=2,\\ \frac{1}{4\pi}|\mathbf{x}|^{-1}, & d=3.\end{cases} \tag{1.5}$$

There are at least two important invariants of (1.4): the *mass of particles*

$$N(\psi):=\|\psi\|^2=\int_{\mathbb{R}^d}|\psi(\mathbf{x})|^2\,\mathrm{d}\mathbf{x}, \tag{1.6}$$

and the *total energy*

$$E(\psi):=\int_{\mathbb{R}^d}\frac{1}{2}|\nabla\psi|^2+V(\mathbf{x})|\psi|^2+\frac{\beta}{2}\Phi(|\psi|^2)|\psi|^2\,\mathrm{d}\mathbf{x}. \tag{1.7}$$

The NLS has been studied mathematically and numerically extensively. Mathematically, for the well-posedness, smoothing effects and long time behavior of SPS with/without local term (exchange term), we refer to [4, 8, 15, 23, 24] and references therein. Numerically, different efficient and accurate numerical methods had been proposed to solve NLS, such as the time-splitting spectral/pseudospectral method [2, 9], finite difference method [5, 6, 11, 27] and finite element method [18, 22] and so on. Specially, for the Schrödinger-Poisson equation, we refer the reader to [3, 30] for the time splitting pseudospectral method, to [12, 16, 26] for difference method and etc.

Finite difference method is the simplest among them, however, the standard central difference discretization of the Laplacian operator is only of second order accuracy. If combined with the partial differential equation, by carefully designating the finite difference coefficients, one could get higher accuracy with fewer adjacent stencil points, such as the compact finite difference method. For details about compact finite difference method, we refer to [17, 19, 29]. Compact finite difference method was popular and had been applied to different models, such as the cubic nonlinear Schrödinger equation, Helmholtz equation and Navier-Stokes equation [20, 25, 28] and etc.