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A linearized compact finite difference scheme for Schrödinger-Poisson System

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Abstract. In this paper, a novel high accurate and efficient finite difference scheme is proposed for solving the Schrödinger-Poisson System. Applying a local extrapolation technique in time to the nonlinear part makes the proposed scheme linearized in the implementation. In fact, at each time step, only two tri-diagonal linear systems of algebraic equations are solved by using Thomas method. Another feature of the proposed method is the high spatial accuracy on account of adopting the compact finite difference approximation to discrete the system in space. Moreover, the proposed scheme preserves the total mass in discrete sense. Under certain regularity assumptions of the exact solution, the local truncation error of the proposed scheme is analyzed in detail by using Taylor's expansion, and consequently the optimal error estimates of the numerical solutions are established by using the standard energy method and a mathematical induction argument. The convergence order is of O(τ 2 + h4) in the discrete L2-norm and L∞-norm, respectively. Numerical results are reported to measure the theoretical analysis, which shows that the new scheme is accurate and efficient and it preserves well the total mass and energy.

Keywords: Schrödinger-Poisson system, local extrapolation technique, compact finite difference scheme, conservation laws, optimal error estimates.

1. Introduction

The Schrödinger-Poisson system (SPS) appears in nonlinear optics and plasma physics, more often in quantum mechanics and semiconductor theory [1-3]. It is named by Diosi and Penrose who first proposed a model to explain the collapse of quantum wave function. It can also be viewed as a nonlinear correction of the Schrödinger equation with Newtonian gravitational potential. According to the classical model [1], the interaction between a charged particle and electromagnetic field can be described by coupling nonlinear Schrödinger equation and Poisson equation. The dimensionless form of the SPS reads

$$i\partial_t\varphi(\boldsymbol{x},t)=[-\frac{1}{2}\Delta+\mathrm{V}(\boldsymbol{x})+\alpha\Phi(\boldsymbol{x},t)]\varphi(\boldsymbol{x},t),\quad \boldsymbol{x}\in\Omega,\quad t>0, \tag{1.1}$$

$$-\nabla^2\Phi(\boldsymbol{x},t)=|\varphi(\boldsymbol{x},t)|^2,\qquad \boldsymbol{x}\in\Omega, \tag{1.2}$$

$$\varphi(\boldsymbol{x},0)=\varphi_0(\boldsymbol{x}),\qquad \boldsymbol{x}\in\overline{\Omega}. \tag{1.3}$$

Here φ is a complex-valued wave function which represents the single particle wave function with $\lim_{|\boldsymbol{x}|\to\infty}|\varphi(\boldsymbol{x},t)|=0$, $i^2=-1$, V is a given external trapping potential, $\alpha>0$ is the coupling parameter, Φ is the Poisson potential, $\Omega\in R^d$ $(d=1,2,3)$ is a bounded computational domain.

The Schrödinger-Poisson system (SPS) can also be redefined as nonlinear Schrödinger Equation (NLS), i.e,

$$i\partial_t\varphi(\boldsymbol{x},t)=[-\frac{1}{2}\Delta+\mathrm{V}(\boldsymbol{x})+\alpha\,\Phi(|\varphi|^2,t)]\varphi(\boldsymbol{x},t),\quad \boldsymbol{x}\in\Omega,\quad t>0, \tag{1.4}$$

and the Poisson potential $\Phi(x, t)$ is expressed by convolution form

$$\Phi(|\varphi|^2,t)=|\varphi|^2*\mathrm{G}(|x|),$$

where $G(|x|)$ is the Green function of Poisson equation on R^d. Similarly, it easy to see that we have two conserved quantities. The total mass gives in terms of

$$M(t) := \int_{\Omega} |\varphi(\boldsymbol{x},t)|^2 \, d\boldsymbol{x} = \|\varphi(\boldsymbol{x},t)\|^2 \equiv M(0), \quad t \geq 0,$$

and the total energy is

$$E(t) := \int_{\Omega} \left[\frac{1}{2} |\nabla \varphi(\boldsymbol{x},t)|^2 + V(\boldsymbol{x}) |\varphi(\boldsymbol{x},t)|^2 + \frac{\alpha}{2} \Phi\left(|\varphi(\boldsymbol{x},t)|^2 \right) |\varphi(\boldsymbol{x},t)|^2 \right] d\boldsymbol{x} \equiv E(0), \quad t \geq 0.$$

In the past decades, there are extensive researches in basic mathematical analysis carried out for the Schrödinger-Poisson system. Pure theory analysis about the existence of solutions for the SPS can be found in the literature [4-7]. Besides, for the dynamical properties and well-posedness of the SPS, we can read [8-9] and the references therein. In addition to the above basic analyses, numerical analysis is of equal importance. Various accurate and efficient numerical methods have been proposed for the Schrödinger-Poisson system, including the finite element method (FEM) [10-11], finite difference method (FDM) [12-17], and time-splitting or (pseudo-)spectral-type method [8,18-22], such as spectral element method (SEM) [19-20],

spectral Galerkin method [21], splitting Chebyshev collocation method [22].

As far as we know, finite difference method is relatively rare in the numerical analysis of SPS. Ringhofer et al. presented a discrete predictor-corrector SPS preserving energy and mass in [14], where the discretization was based on the Crank-Nicolson scheme. In [14], the theoretical analysis is given, but no numerical experiments are carried out to verify it. Ehrhardt et al. [15] also proposed a Crank- Nicolson-type predictor-corrector scheme with a discrete transparent boundary condition to solve the spherically symmetric SPS, and proved that the scheme satisfies discrete mass and energy conservation exactly by numerical simulation. In [16], Chang et al. constructed a novel two-grid centered difference method for the numerical solutions of the nonlinear Schrödinger-Poisson (SP) eigenvalue problem, they obtained that the convergence rate of eigenvalue computations on the fine grid is O(h3). To enhance the accuracy of convergence, Zhang introduced compact finite difference discretization for SPS in [17]. He confirmed that the Crank-Nicolson compact finite difference (CNCFD) method and the semi- implicit compact finite difference (SICFD) method in their paper are both of order $O(\tau^2 + h^4)$ in the discrete L2-norm, H1-norm and $L\infty$-norm. However, their error estimate results need a weak restriction on the grid ratio in extending their schemes to two or three dimensions.

Compared with the standard difference scheme, the compact scheme can make better use of fewer mesh points to achieve higher precision. Therefore, in view of the basis of [17], we propose a linearized compact finite difference (LCFD) scheme with a local extrapolation technique. This scheme linearizes the nonlinear term which can avoid using iterative method to deal with, and not only spends fewer time in the computation but also improves the better convergence accuracy. Differing from the analysis method used in [17], we establish the optimal error estimates without any restriction on the grid ratios by applying a lifting technique as well as the standard energy method.

The paper has the following basic structure. In Section 2, we give some notations and auxiliary lemmas. A linearized compact finite difference (LCFD) scheme for Schrödinger-Poisson system (SPS) is proposed. In Section 3, we establish the optimal error estimates in the discrete L2-norm and $L\infty$-norm, respectively. In Section 4, numerical experiments are presented to verify our theoretical analysis.

2. Finite difference scheme and auxiliary lemmas

For simplicity, we introduce this numerical method only in one-dimensional cases,extension to two or three dimensions are straightforward. The wave function φ is exponentially decaying,so the problem of one-dimensional Schrödinger-Poisson System will be truncated on bounded domain [a, b] in the calculation. We consider the initial boundary value problem with Dirichlet boundary conditions for SPS (2.1)~(2.4):

$$i\partial_t \varphi = -\frac{1}{2}\partial_{xx}\varphi + V(x)\varphi + \alpha\Phi\varphi, \qquad x \in (a,b), \quad t \in (0,T], \tag{2.1}$$

$$-\partial_{xx}\Phi(x,t) = |\varphi(x,t)|^2, \qquad x \in (a,b), \quad t \in (0,T], \tag{2.2}$$

$$\varphi(x,0) = \varphi_0(x), \qquad x \in [a,b], \tag{2.3}$$

$$\varphi(a,t) = \varphi(b,t) = 0, \quad \Phi(a,t) = \Phi(b,t) = 0, \qquad t \in (0,T]. \tag{2.4}$$