

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 $O(\tau^2 + h^4)$ in the discrete L^2 -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

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

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

$$\varphi(\mathbf{x}, 0) = \varphi_0(\mathbf{x}), \quad \mathbf{x} \in \bar{\Omega}. \quad (1.3)$$

Here φ is a complex-valued wave function which represents the single particle wave function with $\lim_{|\mathbf{x}| \rightarrow \infty} |\varphi(\mathbf{x}, t)| = 0$, $i^2 = -1$, 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.,

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

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

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

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

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

and the total energy is

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

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 $O(h^3)$. 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 L_2 -norm, H_1 -norm and L_∞ -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 L_2 -norm and L_∞ -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):

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

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

$$\varphi(x, 0) = \varphi_0(x), \quad x \in [a, b], \quad (2.3)$$

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

Here, Poisson potential Φ and wave function φ satisfy the homogeneous boundary conditions (2.4) respectively.

2.1 Numerical method

We firstly make a uniform mesh division on $[a, b]$. For a positive integer J , choose mesh size $h = \frac{(b-a)}{J}$ and time-step $\tau = \Delta t$. Denote grid points $x_j = a + jh$ ($j = 0, 1, \dots, J$) and time steps $t_n = n\tau$ ($n = 0, 1, 2, \dots$). Define two index sets

$$\Gamma_J^0 := \{j | j = 0, 1, \dots, J-1, J\}, \quad \Gamma_J := \{j | j = 1, 2, \dots, J-2, J-1\},$$

and a space of grid functions

$$X_J := \{w = (w_0, w_1, \dots, w_J) | w_0 = w_J = 0\} \subset C^{J+1}.$$

Let $\varphi^n \in X_J$ be the numerical vector solution at time $t = t_n$, and φ_j^n be the numerical approximation of the exact solution $\varphi(x_j, t_n)$ for $j = 0, 1, 2, \dots, J$ and $n = 0, 1, 2, \dots$. Introduce the following finite difference quotient operators as

$$\begin{aligned} \delta_x^+ w_j^n &= \frac{1}{h}(w_{j+1}^n - w_j^n), & \delta_x^- w_j^n &= \frac{1}{h}(w_j^n - w_{j-1}^n), & \delta_x w_j^n &= \frac{1}{2h}(w_{j+1}^n - w_{j-1}^n), \\ \delta_t^+ w_j^n &= \frac{1}{\tau}(w_j^{n+1} - w_j^n), & \delta_t^- w_j^n &= \frac{1}{\tau}(w_j^n - w_j^{n-1}), & \delta_t w_j^n &= \frac{1}{2\tau}(w_j^{n+1} - w_j^{n-1}), \\ \mu_t w_j^n &= \frac{1}{2}(w_j^{n+1} + w_j^n), & \delta_x^2 w_j^n &= \frac{1}{h^2}(w_{j+1}^n - 2w_j^n + w_{j-1}^n). \end{aligned}$$

Define the matrix operator with order $J-1$ as

$$A_h = \frac{1}{h^2} \begin{pmatrix} -2 & 1 & 0 & \dots & 0 \\ 1 & -2 & 1 & \dots & 0 \\ \vdots & \ddots & \ddots & \ddots & \vdots \\ 0 & \dots & 1 & -2 & 1 \\ 0 & \dots & 0 & 1 & -2 \end{pmatrix}, \quad B_h = I + \frac{h^2}{12} A_h,$$

where A_h is the standard central finite difference, I is an identity matrix and $\Delta_h = B_h^{-1} A_h$ is fourth order approximation of ∂_{xx} . Then we introduce $I_h : C^{J+1} \rightarrow C^{J-1}$ to be the identity projection operator as

$$I_h w = (w_1, w_2, \dots, w_{J-1})^T \in C^{J-1}, \quad \forall w = (w_0, w_1, \dots, w_J)^T \in X_J.$$

Define discrete inner products and norms over X_J as

$$\langle w, v \rangle = h \sum_{j=1}^{J-1} w_j \bar{v}_j = \overline{\langle v, w \rangle}, \quad \langle \delta_x^+ w, \delta_x^+ v \rangle = h \sum_{j=0}^{J-1} (\delta_x^+ w_j) (\delta_x^+ \bar{v}_j),$$

$$\|w\|^2 = h \sum_{j=1}^{J-1} |w_j|^2, \quad \|\delta_x^+ w\|^2 = h \sum_{j=0}^{J-1} |\delta_x^+ w_j|^2, \quad \|w\|_\infty = \max_{j \in \Gamma_J} |w_j|,$$

$$\Psi(w) = \frac{1}{2} \langle -\Delta_h I_h w, w \rangle + \langle V w, w \rangle.$$

Based on the notations above, now we give a linearized compact finite difference (LCFD) schemes for the one-dimensional SPS:

$$i \delta_t^+ \varphi_j^n = -\frac{1}{2} (\Delta_h I_h \mu_t \varphi^n)_j + V_j \mu_t \varphi_j^n + \alpha \left(\frac{3}{2} \Phi_j^n - \frac{1}{2} \Phi_j^{n-1} \right) \mu_t \varphi_j^n, \quad j \in \Gamma_J, n \geq 1, \tag{2.5}$$

$$(-\Delta_h I_h \Phi^n)_j = I_h (|\varphi^n|^2)_j, \quad j \in \Gamma_J, n \geq 1, \tag{2.6}$$

$$\varphi_j^0 = \varphi_0(x_j), \quad j \in I_J^0, \quad (2.7)$$

$$\varphi_0^n = \varphi_J^n = 0, \quad \Phi_0^n = \Phi_J^n = 0, \quad n = 0, 1, \dots \quad (2.8)$$

The proposed scheme applies Crank-Nicolson method to the variables φ_j of SPS equation (2.5) in time direction. Otherwise, by using a local extrapolation technique to discrete the coefficient of the nonlinear term in temporal direction and adopting the centered finite difference method to approximate the other terms, the above scheme is expected to reduce the difficulty in dealing with nonlinear items and the computational cost. Obviously, this three-level scheme can not start by itself, so we use the Taylor's expansion to compute the first step value φ_j^1 :

$$\varphi_j^1 = \varphi_j^0 - i\tau[-\frac{1}{2}\Delta\varphi_0(x_j) + V(x_j)\varphi_0(x_j) + \alpha\Phi_j^0\varphi_0(x_j)], \quad (2.9)$$

where Poisson potential Φ_j^0 can be calculated by scheme (2.6).

2.2 relevant auxiliary lemmas

Lemma 2.1 For any grid functions $u, v \in X_J$, the following expressions hold

$$\begin{aligned} \langle \delta_x w, v \rangle &= -\langle w, \delta_x v \rangle, & \langle \delta_x^2 w, v \rangle &= -\langle \delta_x^+ w, \delta_x^+ v \rangle = \langle w, \delta_x^2 v \rangle, \\ \langle A_h I_h w, v \rangle &= \langle w, \delta_x^2 v \rangle, & \|w\|_\infty &\leq C \|\delta_x^+ w\|. \end{aligned}$$

To estimate the error, we give the following properties for the related approximation matrices A_h, B_h, Δ_h .

Lemma 2.2 [17] For any grid functions $u, v \in X_J$ and approximation matrices A_h, B_h, Δ_h , they hold that

$$\begin{aligned} \|A_h^{-1} I_h w\|_\infty &\leq C \|w\|_\infty, & \|A_h^{-1} I_h w\| &\leq C \|w\|, \\ \|B_h I_h w\|_\infty &\leq \|w\|_\infty, & \|B_h I_h w\| &\leq \|w\|, \\ \|B_h^{-1} I_h w\|_\infty &\leq C \|w\|_\infty, & \|B_h^{-1} I_h w\| &\leq C \|w\|, \\ C_1 \langle -A_h I_h w, w \rangle &\leq \langle -\Delta_h I_h w, w \rangle \leq C_2 \langle -A_h I_h w, w \rangle, \\ C_3 \|A_h I_h w\| &\leq \|\Delta_h I_h w\| \leq C_4 \|A_h I_h w\|, \end{aligned}$$

where C, C_1, C_2, C_3, C_4 are the constants independent of w or h .

3. Error estimates

Before we establish the optimal error estimate, we make two assumptions as follows:

(A) $V(x)$ is the external trapping potential and β is the rotation speed. Assume that there exists a constant $\lambda > 0$ such that

$$V(x) \in C^1(\Omega), \quad V(x) \geq \frac{\lambda^2}{2} x^2, \quad \forall x \in \Omega, \quad |\beta| < \lambda;$$

(B) Assume that the exact solution φ satisfies

$$\varphi \in C^4([0, T]; L^\infty(\Omega)) \cap C^3([0, T]; W^{2,\infty}(\Omega)) \cap C^2([0, T]; W^{3,\infty}(\Omega)) \cap C^1([0, T]; W^{6,\infty}(\Omega)),$$

and $0 < T < T_{\max}$, where T_{\max} is the maximal existing time of the solution [24-25].

According to the proposed scheme (2.5)~(2.9), define the local truncation error function $r^n \in X_J$ as follows:

$$r_j^n = i\delta_t^+ \varphi(x_j, t_n) + \frac{1}{2} \Delta_h I_h \mu_t \varphi(\cdot, t_n) - V_j \mu_t \varphi(x_j, t_n) - \alpha \left[\frac{3}{2} (-\Delta_h)^{-1} I_h |\varphi(\cdot, t_n)|^2 - \frac{1}{2} (-\Delta_h)^{-1} I_h |\varphi(\cdot, t_{n-1})|^2 \right] \mu_t \varphi(x_j, t_n), \quad n \geq 1, \tag{3.1}$$

$$r_j^0 = i\delta_t^+ \varphi_0(x_j) + \frac{1}{2} \Delta_h I_h \varphi(\cdot, 0) - V(x_j) \varphi_0(x_j) - \alpha \Phi(x_j, 0) \varphi_0(x_j), \quad j \in \Gamma_J, \tag{3.2}$$

where $\varphi(\cdot, t_n) = (\varphi(x_0, t_n), \varphi(x_1, t_n), \dots, \varphi(x_J, t_n))^T \in X_J$.

Then by using Taylor's expansion, we can obtain the following estimates of the local truncation error,

Lemma 3.1 (Local truncation error) Under assumptions (A) and (B), the local truncation error $r^n \in X_J$ for the scheme (2.5)~(2.9) satisfies

$$\begin{aligned} \|r^0\|_\infty &\leq C\tau^2, \quad \|\delta_t^+ r^0\|_\infty \leq C\tau^2, \\ \|r^n\|_\infty &\leq C(\tau^2 + h^4), \quad 1 \leq n \leq \frac{T}{\tau} - 1, \\ \|\delta_t^+ r^n\|_\infty &\leq C(\tau^2 + h^4), \quad 1 \leq n \leq \frac{T}{\tau} - 1. \end{aligned}$$

Define the error function $e^n \in X_J$ as

$$e_j^n = \varphi(x_j, t_n) - \varphi_j^n, \quad j \in \Gamma_J^0, \quad n \geq 0.$$

Theorem 3.1 (l^2 -norm estimate) Under assumptions (A) and (B), there exist two constants $\tau_0 > 0$ and $h_0 > 0$ sufficiently small, such that when $0 < \tau \leq \tau_0$ and $0 < h \leq h_0$, we have

$$\|e^n\| \leq C(\tau^2 + h^4), \quad \|\varphi^n\|_\infty \leq 1 + M_1, \quad 1 \leq n \leq \frac{T}{\tau}, \tag{3.3}$$

where $M_1 = \max_{0 \leq t \leq T} \|\varphi\|_{L^\infty}$.

Proof We will prove Theorem 3.1 by mathematical induction. When $n = 1$, it is straightforward to see that

$$|e_j^1| = |\varphi(x_j, t_1) - \varphi_j^1| = |-i\tau_j^0| \leq C(\tau^2 + h^4), \quad j \in \Gamma_J, \tag{3.4}$$

which immediately implies $\|e^1\| \leq C(\tau^2 + h^4)$. Then together with the triangle inequality and the definition of e^n , if τ and h are sufficiently small, we get

$$|\varphi_j^1| \leq |\varphi(x_j, t_1) - e_j^1| + |e_j^1| \leq M_1 + C(\tau^2 + h^4) \leq M_1 + 1, \quad j \in \Gamma_J,$$

so two inequalities above holds true when $n = 1$.

Now we should suppose that (3.3) is valid for all $0 \leq n \leq k-1 \leq \frac{T}{\tau} - 1$, therefore, we have to testify that it is still true when $n = k$. In order to do so, noticing (2.4) and (2.8), subtracting (3.1) from (2.5), we get

$$i\delta_t^+ e_j^n = -\frac{1}{2} (\Delta_h I_h \mu_t e^n)_j + V_j \mu_t e_j^n + R_j^n + r_j^n, \quad j \in \Gamma_J, \quad n \geq 1, \tag{3.5}$$

where R_j^n is defined as

$$\begin{aligned}
 R_j^n &= \alpha \left\{ \frac{3}{2} [(-\Delta_h)^{-1} I_h |\varphi(\cdot, t_n)|^2]_j - \frac{1}{2} [(-\Delta_h)^{-1} I_h |\varphi(\cdot, t_{n-1})|^2]_j \right\} \mu_t \varphi(x_j, t_n) \\
 &\quad - \alpha \left\{ \frac{3}{2} [(-\Delta_h)^{-1} I_h |\varphi^n|^2]_j - \frac{1}{2} [(-\Delta_h)^{-1} I_h |\varphi^{n-1}|^2]_j \right\} \mu_t \varphi_j^n \\
 &= \alpha \left\{ \frac{3}{2} [(-\Delta_h)^{-1} I_h |\varphi(\cdot, t_n)|^2]_j - \frac{1}{2} [(-\Delta_h)^{-1} I_h |\varphi(\cdot, t_{n-1})|^2]_j \right\} \mu_t e_j^n \\
 &\quad + \alpha \left\{ \frac{3}{2} [(-\Delta_h)^{-1} I_h (e^n \bar{\varphi}(\cdot, t_n) + \varphi^n \bar{e}^n)]_j - \frac{1}{2} [(-\Delta_h)^{-1} I_h (e^{n-1} \bar{\varphi}(\cdot, t_{n-1}) + \varphi^{n-1} \bar{e}^{n-1})]_j \right\} \mu_t \varphi_j^n,
 \end{aligned}$$

noticing Lemma 2.2, we have the following estimate

$$\|R^n\|^2 \leq C(\|e^{n+1}\|^2 + \|e^n\|^2 + \|e^{n-1}\|^2).$$

when $1 \leq n \leq k-1$, computing the inner product of (3.5) with $2\mu_t e^n$, and taking imaginary parts, we obtain

$$\begin{aligned}
 \text{Im}\langle i\delta_t^+ e^n, 2\mu_t e^n \rangle &= -\frac{1}{2} \text{Im}\langle \Delta_h I_h \mu_t e^n, 2\mu_t e^n \rangle + \text{Im}\langle V \mu_t e^n, 2\mu_t e^n \rangle \\
 &\quad + \text{Im}\langle R^n, 2\mu_t e^n \rangle + \text{Im}\langle r^n, 2\mu_t e^n \rangle,
 \end{aligned}$$

where

$$\begin{aligned}
 \text{Im}\langle i\delta_t^+ e^n, 2\mu_t e^n \rangle &= \frac{1}{\tau} (\|e^{n+1}\|^2 - \|e^n\|^2), \\
 \text{Im}\langle \Delta_h I_h \mu_t e^n, 2\mu_t e^n \rangle &= \text{Im}\langle V \mu_t e^n, 2\mu_t e^n \rangle = 0, \\
 \text{Im}\langle R^n, 2\mu_t e^n \rangle &\leq C(\|R^n\|^2 + \|e^{n+1}\|^2 + \|e^n\|^2) \\
 &\leq C(\|e^{n+1}\|^2 + \|e^n\|^2 + \|e^{n-1}\|^2), \\
 \text{Im}\langle r^n, 2\mu_t e^n \rangle &\leq C(\|r^n\|^2 + \|e^{n+1}\|^2 + \|e^n\|^2),
 \end{aligned}$$

thus when τ is sufficiently small, we have

$$\|e^{n+1}\|^2 - \|e^n\|^2 \leq C\tau(\|e^{n+1}\|^2 + \|e^n\|^2 + \|e^{n-1}\|^2 + \|r^n\|^2).$$

Summing the above inequality for $1 \leq n \leq k-1$ and applying the discrete Gronwall inequality and Lemma 3.1, besides, noticing $\|e^0\| = 0$ and $\|e^1\| \leq C(\tau^2 + h^4)$, we immediately obtain

$$\begin{aligned}
 \|e^k\|^2 &\leq C\tau \sum_{n=1}^{k-1} \|e^n\|^2 + C(n-1)\tau(\tau^2 + h^4)^2 \\
 &\leq CT(\tau^2 + h^4)^2 e^{CT} \leq C(\tau^2 + h^4)^2,
 \end{aligned}$$

which means that the first inequality in (3.3) holds true when $n = k$. The ‘error’ equation with $n = k-1$ can be rewritten as the following form

$$(\Delta_h I_h \mu_t e^{k-1})_j = -2i\delta_t^+ e_j^{k-1} + 2V_j \mu_t e_j^{k-1} + 2R_j^{k-1} + 2r_j^{k-1}, \quad j \in \Gamma_J. \tag{3.6}$$

Taking the discrete L^2 norm of both sides of the ‘error’ equation (3.6) gives

$$\begin{aligned}
 \|\Delta_h I_h \mu_t e^{k-1}\| &= \|-2i\delta_t^+ e^{k-1} + 2V \mu_t e^{k-1} + 2R^{k-1} + 2r^{k-1}\| \\
 &\leq 2\|\delta_t^+ e^{k-1}\| + 2\|V \mu_t e^{k-1}\| + 2\|R^{k-1}\| + 2\|r^{k-1}\| \\
 &\leq C\tau^{-1}(\tau^2 + h^4) + C(\tau^2 + h^4), \\
 &\leq C\tau^{-1}(\tau^2 + h^4),
 \end{aligned} \tag{3.7}$$

this together with triangle inequality gives

$$\|\Delta_h I_h e^k\| - \|\Delta_h I_h e^{k-1}\| \leq \|\Delta_h I_h e^k + \Delta_h I_h e^{k-1}\| \leq C\tau^{-1}(\tau^2 + h^4). \tag{3.8}$$

Summing (3.8) over k gives

$$\|\Delta_h I_h e^k\| \leq Ck\tau^{-1}(\tau^2 + h^4) \leq C\tau^{-2}(\tau^2 + h^4).$$

Noticing that

$$\begin{aligned} \|e^k\|_\infty &\leq C \|e^k\|^{1/2} (\|\delta_x^+ e^k\| + \|e^k\|)^{1/2} \\ &\leq C \|e^k\|^{1/2} (\|\Delta_h I_h e^k\| + \|e^k\|)^{1/2} \\ &\leq C \tau^{-1} (\tau^2 + h^4) \leq C(\tau + \tau^{-1} h^4). \end{aligned}$$

Hence, for sufficiently small τ and $h \leq \tau$, there is

$$\|e^k\|_\infty \leq 1. \tag{3.9}$$

On the other hand, we have

$$\begin{aligned} \|e^k\|_\infty &\leq C \|e^k\|^{1/2} (\|\delta_x^+ e^k\| + \|e^k\|)^{1/2} \\ &\leq C \|e^k\|^{1/2} (h^{-1} \|e^k\| + \|e^k\|)^{1/2} \\ &\leq Ch^{-1} (\tau^2 + h^4) \leq C(h^{-1} \tau^2 + h^3). \end{aligned}$$

This means that, for sufficiently small h and $\tau \leq h$, there is

$$\|e^k\|_\infty \leq 1. \tag{3.10}$$

Thus, for sufficiently small τ and h , it is always true that

$$\|e^k\|_\infty \leq 1.$$

Then noticing the assumption in Theorem 3.1 and applying the inverse inequality, we can estimate

$$\begin{aligned} |\varphi_j^k| &\leq |e_j^k| + |\varphi(x_j, t_k)| \leq \|e^k\|_\infty + M_1 \\ &\leq \frac{C}{\sqrt{h}} \|e^k\| + M_1 \leq C(h^{-1/2} \tau^2 + h^{3/2}) + M_1 \leq 1 + M_1, \quad j \in \Gamma_j, \end{aligned}$$

when τ and h is sufficiently small, it results to

$$\|\varphi^k\|_\infty \leq 1 + M_1, \quad 1 \leq k \leq \frac{T}{\tau}.$$

Thus, the proof of Theorem 3.1 is finished.

Lemma 3.2 (*l^∞ -norm estimate*) Under the same conditions of Theorem 3.1 with assumptions (A) and (B), we also have

$$\|e^n\|_\infty \leq C(\tau^2 + h^4), \quad 1 \leq n \leq \frac{T}{\tau}.$$

4 Numerical experiments

In this section, numerical experiments are reported to test our theoretical analysis for the linearized compact finite difference scheme (LCFD), which includes the convergence order and the discrete conservation laws. For convenience, we denote

$$E(h, \tau) = \|e^N(h, \tau)\|_\infty, \quad rate_1 = \frac{\ln[E(h_1, \tau)/E(h_2, \tau)]}{\ln(h_1/h_2)}, \quad rate_2 = \frac{\ln[E(h, \tau_1)/E(h, \tau_2)]}{\ln(\tau_1/\tau_2)},$$

where $\|e^N(h, \tau)\|_\infty$ is the maximum norm errors of φ^N at $t_n = n\tau$ with the time-step τ and grid size h .

Example Consider the following initial-boundary value problem

$$\begin{cases} i\partial_t \varphi = -\frac{1}{2} \partial_{xx} \varphi + V \varphi + \alpha \Phi \varphi + g_1(x, t), & x \in (0,1), t \in (0,1], \\ -\partial_{xx} \Phi = |\varphi|^2 + g_2(x, t), & x \in (0,1), t \in (0,1], \end{cases}$$

including

$$\begin{cases} g_1(x, t) = (i - \frac{3}{2} - \frac{x^2}{2} - V)e^{(i+1)t} \sin x \sin \pi x + \pi e^{(i+1)t} \cos x \cos \pi x \\ \quad + \alpha(x-1)e^{(i+2)t+x} \sin^2 x \sin \pi x, \\ g_2(x, t) = 2(\sin x + x \cos x)e^{x+t} - |\sin x \sin \pi x|^2 e^{2t}, \end{cases}$$

then we have the exact solution of this problem

$$\begin{cases} \varphi(x, t) = e^{(i+1)t} \sin x \sin \pi x, \\ \Phi(x, t) = e^{x+t} (1-x) \sin x. \end{cases}$$

To achieve the good stability, we test the accuracy in the spatial and temporal direction separately. Firstly, we take $\alpha = 5$, $V = \frac{x^2}{2}$ and the errors are estimated by using MATLAB software at time $T = 0.5$. In Table 1, the spatial errors computed by the LCFD scheme is listed, which choose a sufficiently small time step $\tau = 0.0001$ for ignoring the temporal errors and different mesh sizes h . In Table 2, the temporal errors of the LCFD scheme are computed with a sufficiently small mesh size $h = 0.0001$ which is also to neglect the spatial errors and different time steps τ . It is obvious to see that the spatial convergence order almost equals 4 in Table 1 and the temporal convergence order almost equals 2 in Table 2, as it supports our theoretical results.

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Table 1. Spatial errors computed by the proposed scheme with $\tau=0.0001$ at $T=0.5$.

h	τ	$E(h, \tau)$	$rate_1$
0.2	0.0001	1.14e-03	—
0.1	0.0001	6.95e-05	4.0359
0.05	0.0001	4.31e-06	4.0113
0.025	0.0001	2.75e-07	3.9702

Table 2. Temporal errors computed by the proposed scheme with $h=0.0001$ at $T=0.5$.

h	τ	$E(h, \tau)$	$rate_2$
0.0001	0.01	5.0171e-05	—
0.0001	0.005	1.2803e-05	1.9704
0.0001	0.0025	3.1981e-06	2.0012
0.0001	0.00125	8.0189e-07	1.9957

In order to show the advantages of the proposed LCFD scheme, we compare it with the Crank Nicolson compact finite difference method (CNCFD) and the semi-implicit compact finite difference method (SICFD) given in [17]. We analyse the error at time $T = 1$ under the maximum norm. For the spatial errors, we choose time step $\tau = 0.0001$ and different h . For the temporal errors, we take mesh size $h = 0.0001$ and different τ . The numerical results are listed in Table 3 and Table 4, which separately present the errors and CPU times of LCFD, CNCFD and SICFD.

From Table 3 and Table 4, the convergence orders of three schemes are of four in the spatial direction and of two in the temporal direction. We can also witness that the proposed LCFD scheme is not only more accurate but also more efficient than CNCFD and SICFD.

Table 3. Spatial errors of the three schemes with $\tau = 0.0001$ and different h at time $T = 1$.

		$h=0.2$	$h=0.1$	$h=0.05$	$h=0.025$
LCFD	$E(h, \tau)$	1.6224e-03	1.0468e-04	6.4671e-06	4.0898e-07
	$rate_1$	—	3.9541	4.0167	3.9830
	CPU time	1.36s	1.44s	1.58s	1.96s
CNCFD	$E(h, \tau)$	1.6221e-03	1.0463e-04	6.4618e-06	4.0545e-07
	$rate_1$	—	3.9545	4.0172	3.9943
	CPU time	3.59s	3.82s	4.42s	5.27s
SICFD	$E(h, \tau)$	1.6221e-03	1.0465e-04	6.4651e-06	4.0653e-07
	$rate_1$	—	3.9542	4.0168	3.9912
	CPU time	1.43s	1.62s	1.76s	2.51s

Table 4. Temporal errors of the three schemes with $h = 0.0001$ and different τ at time $T = 1$.

		$\tau = 0.002$	$\tau = 0.001$	$\tau = 0.0005$	$\tau = 0.00025$
LCFD	$E(h, \tau)$	1.2465e-06	3.1383e-07	7.9113e-08	1.9817e-08
	$rate_2$	—	1.9898	1.9880	1.9972
	CPU time	4.06s	7.97s	15.68s	30.31s
CNCFD	$E(h, \tau)$	1.8577e-06	4.6391e-07	1.1595e-07	2.8975e-08
	$rate_2$	—	2.0016	2.0003	2.0006
	CPU time	10.99s	17.42s	29.17s	63.46s
SICFD	$E(h, \tau)$	4.1135e-06	1.0254e-06	2.5590e-07	6.3939e-08
	$rate_2$	—	2.0042	2.0025	2.0008
	CPU time	4.25s	8.34s	16.24s	31.58s

5 Conclusion

We propose and analyse a new linearized compact finite difference (LCFD) scheme for the Schrödinger-Poisson system in this paper. Different from the Crank-Nicolson compact finite difference (CNCFD) method and the semi-implicit compact finite difference (SICFD) method given in [17], we make the nonlinear part of Schrödinger-Poisson system linearized by using a local extrapolation technique. It only needs to solve two tri-diagonal linear systems of algebraic equations by Thomas method, which computes faster than iteration method in the CNCFD scheme. The proposed method is as high spatial accuracy as the SICFD scheme, on account of applying the compact finite difference approximation to discrete the system in space. In addition, by introducing the standard energy method and a mathematical induction argument, the optimal error estimate converges to $O(\tau^2 + h^4)$ in the discrete L^2 -norm and L^∞ -norm, respectively. Our analysis method for solving the Schrödinger-Poisson system may be a more accurate and efficient choice compared to previous studies.

References

- [1] V. Benci, D. Fortunato, An eigenvalue problem for the Schrödinger-Maxwell equations, *Topol. Methods Nonlinear Anal.*, 11 (1998) 283-293.
- [2] V. Benci, D. Fortunato, Solitary waves of the nonlinear Klein-Gordon equation coupled with Maxwell equations, *Rev. Math. Phys.*, 14 (2002) 409-420.
- [3] G. Vaira, Ground states for Schrödinger-Poisson type systems, *Ric. Mat.*, 60 (2011) 263-297.
- [4] L. Zhao, F. Zhao, On the existence of solutions for the Schrödinger-Poisson equations, *J. Math. Anal. Appl.*, 346 (2008) 155-169.
- [5] J. Wang, L. Tian, J. Xu, F. Zhang, Existence and concentration of positive solutions for semilinear Schrödinger-Poisson systems in R^3 , *Calc. Var.*, 48 (2013) 243-273.
- [6] J. Wang, L. Tian, J. Xu, F. Zhang, Existence of multiple positive solutions for Schrödinger-Poisson systems with critical growth, *Z. Angew. Math. Phys.*, 66 (2015) 2441-2471.
- [7] J. Sun, S. Ma, Ground state solutions for some Schrödinger-Poisson systems with periodic potentials, *J. Differential Equations.*, 260 (2016) 2119-2149.
- [8] Y. Zhang, X. Dong, On the computation of ground state and dynamics of Schrödinger-Poisson-Slater system, *J. Comput. Phys.*, 230 (2011) 2660-2676.
- [9] H. Li, C. Lin, Semiclassical limit and well-posedness of nonlinear Schrödinger-Poisson system, *Electron. J. Differ. Eq.*, 93 (2003) 1-17.
- [10] L. Ram-Mohan, K. Yoo, J. Moussa, The Schrödinger-Poisson self-consistency in layered quantum semiconductor structures, *J. Appl. Phys.*, 95 (2004) 3081-3092.
- [11] C. Chien, B. Jeng, Z. Li, A time-independent approach for computing wave functions of the Schrödinger-Poisson system, *Numer Lin Algebra Appl.*, 15 (2010) 55-82.
- [12] I. Tan, G. Snider, L. Chang, E. Hu, A self-consistent solution of Schrödinger-Poisson equations using a nonuniform mesh, *J. Appl. Phys.*, 68 (1990) 4071-4076.
- [13] A. Trellakis, A. Galick, A. Pacelli, U. Ravaioli, Iteration Scheme for the solution of the two-dimensional Schrödinger Poisson equations in quantum structures, *J. Appl. Phys.*, 81 (1997) 7880-7884.
- [14] C. Ringhofer, J. Soler, Discrete Schrödinger-Poisson Systems Preserving Energy and Mass, *Applied Mathematics Letters.*, 13 (2000) 27-32.
- [15] M. Ehrhardt, A. Zisowsky, Fast calculation of energy and mass preserving solutions of Schrödinger-Poisson systems on unbounded domains, *J. Comput. Appl. Math.*, 187 (2006) 1-28.
- [16] S. Chang, C. Chen, B. Jeng, An efficient algorithm for the Schrödinger-Poisson eigenvalue problem, <https://www.sciencedirect.com/science/journal/03770427J>. *Comput. Appl. Math.*, 205 (2007) 509-532.
- [17] [17] Y. Zhang, Optimal error estimates of compact finite difference discretizations for the Schrödinger-Poisson system. *Commun. Comput. Phys.*, 13 (2013) 1357-1388.
- [18] [18] C. Lubich, On splitting methods for Schrödinger-Poisson and cubic nonlinear Schrödinger equations, *Mathematics of Computation.*, 77 (2008) 2141-2153.
- [19] [19] C. Cheng, Q. Liu, J. Lee, H. Massoud, Spectral Element Method for the Schrödinger-Poisson System, *J. Comput. Electron.*, 3 (2004) 417-421.
- [20] [20] C. Cheng, J. Lee, H. Massoud, Q. Liu, 3-D self-consistent Schrödinger-Poisson solver: the spectral element method, *J. Comput. Electron.*, 7 (2008) 337-341.
- [21] [21] T. Lu, W. Cai, A Fourier spectral-discontinuous Galerkin method for time-dependent 3-D Schrödinger-Poisson equations with discontinuous potentials, *J. Comput. Appl. Math.*, 220 (2008) 588-614.
- [22] H. Wang, Z. Liang, R. Liu, A splitting Chebyshev collocation method for Schrödinger-Poisson system, *Computational & Applied Mathematics.*, 7 (2018) 1-24.
- [23] T. Wang, Maximum norm error bound of a linearized difference scheme for a coupled nonlinear Schrödinger equations, *J. Comput. Appl. Math.*, 235 (2011) 4237-4250.
- [24] H. Steiner, The one-dimensional Wigner-Poisson problem and its relation to the Schrödinger-Poisson problem, *SIAM J. Math. Anal.*, 22 (1991) 957-972.
- [25] H. P. Stimming, The IVP for the Schrödinger-Poisson- X^α equation in one dimension, *Math. Models Methods Appl. Sci.*, 15 (2005) 1169-1180.
- [26] F. E. Browder, Existence and uniqueness theorems for solutions of nonlinear boundary value problems. In: Finn R, ed. *Application of Nonlinear Partial Differential Equations, Proceedings of Symposia in Applied Mathematics.*, 17 (1965) 24-49.
- [27] S. Larsson, V. Thomee, *Partial differential equations with numerical methods*, Springer, 2009.
- [28] W. Bao, Y. Cai, Optimal error estimate of finite difference methods for the Gross-Pitavskii equation with angular momentum rotation, *Math. Comp.*, 82 (2013) 99-128.
- [29] T. Wang, Uniform point-wise error estimates of semi-implicit compact finite difference methods for the nonlinear Schrödinger equation perturbed by wave operator, *J. Math. Anal. Appl.*, 422 (2015) 286-308.