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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,

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

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

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

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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.

Up to our knowledge, compact finite difference method has not yet been applied to SPS. In this paper, we first present Crank-Nicolson compact finite difference scheme (**CNCFD**) which preserves the conservation laws of energy and mass on the discrete level. However, when applying CNCFD to SPS, we have to solve a nonlinear equation each step which is quite expensive in the view of computation time. Therefore, we propose a semi-implicit compact finite difference scheme (**SICFD**) and also establish optimal error estimates for both schemes.

The paper is organized as follows. In Section 2, we present two compact finite difference schemes and their corresponding error estimates in Theorem 2.1 and Theorem 2.2. In Section 3, optimal error estimate of CNCFD method is presented by energy method and a *priori* bound in l^∞ norm is obtained by inverse inequality. The optimal error estimate of SICFD method is established by energy method and mathematical induction in Section 4. Extensive numerical results are reported to support our error estimates in the Section 5. Finally, some conclusions are made in the last section. Through out the paper, we adopt the standard Sobolev spaces and their corresponding norms and the commonly used constant C does not depend on mesh size h or time step τ if not stated otherwise.

2 Numerical methods and main results

In this section, we introduce CNCFD and SICFD in 1-d for the sake of simplicity. Extensions of CNCFD and SICFD to higher dimensions are possible and similar.

For the wave function ψ decays exponentially fast and constant shif of self-consistent Poisson potential does not affect the physical observation $\rho=|\psi|^2$, therefore in computational practice we could always truncate the whole space to bounded domain. The 1-d truncated SPS on bounded domain $[a,b]$ reads as

$$\begin{aligned}
&i\partial_t\psi(x,t)=\left[-\frac{1}{2}\partial_x^2+V(x)+\beta\Phi(x,t)\right]\psi(x,t), && x\in(a,b), && (2.1)\\
&-\partial_x^2\Phi(x,t)=|\psi(x,t)|^2, && x\in(a,b), && (2.2)\\
&\psi(x,0)=\psi_0(x), && x\in[a,b], && (2.3)
\end{aligned}$$

subject to Dirichlet boundary condition

$$\psi(a,t)=\psi(b,t)=0, \qquad \Phi(a,t)=\Phi(b,t)=0. \tag{2.4}$$

The 1-d computational domain $\Omega=[a,b]$ is discretized as $x_j=a+jh, j=0,1,\cdots,M-1,M$ with $h=\frac{b-a}{M}$ and M being a positive integer. Define the function space

$$X_M=\{u=(u_j)_{j\in\mathcal{T}_M^0}\,|\,u_0=u_M=0\}\subset\mathbb{C}^{M+1},$$

where $\mathcal{T}_M^0=\{j\,|\,j=0,1,\cdots,M-1,M\}$. Choose time step $\tau:=\Delta t$ and denote the time $t_n=n\tau, n=0,1,\cdots$. Let ψ_j^n be the numerical approximation of $\psi(x_j,t_n)$ and $\psi^n\in X_M$ be the numerical solution at time t_n. The standard finite difference operators are listed as follows:

$$\delta_x^+ u_j^n = \frac{u_{j+1}^n - u_j^n}{h}, \quad \delta_x^- u_j^n = \frac{u_j^n - u_{j-1}^n}{h}, \quad \delta_x u_j^n = \frac{u_{j+1}^n - u_{j-1}^n}{2h},$$
$$\delta_t^+ u_j^n = \frac{u_j^{n+1} - u_j^n}{\tau}, \quad \delta_t^- u_j^n = \frac{u_j^n - u_j^{n-1}}{\tau}, \quad \delta_t u_j^n = \frac{u_j^{n+1} - u_j^{n-1}}{2\tau},$$
$$\mu_t u_j^n = \frac{u_j^n + u_j^{n+1}}{2}, \quad \delta_x^2 u_j^n = \frac{u_{j+1}^n - 2u_j^n + u_{j-1}^n}{h^2}.$$

2.1 Compact finite difference method

Before presenting the compact finite difference scheme for SPS, we would first make a brief introduction of compact finite difference approximation to the Poisson equation.

For Poisson equation with homogeneous Dirichlet boundary condition

$$\partial_x^2 \phi(x) = f(x), \quad x \in (a,b) \qquad \text{with} \qquad \phi(a) = \phi(b) = 0. \tag{2.5}$$

By Taylor expansion,

$$\delta_x^2 \phi(x_j) = \frac{\phi(x_j+h) - 2\phi(x_j) + \phi(x_j-h)}{h^2}$$

approximates $\partial_x^2 \phi(x)$ as

$$\begin{aligned} \delta_x^2 \phi(x_j) &= (\partial_x^2 \phi)(x_j) + \frac{h^2}{12}(\partial_x^4 \phi)(x_j) + \mathcal{O}(h^4) \\ &= f(x_j) + \frac{h^2}{12}(\partial_x^2(\partial_x^2 \phi))(x_j) + \mathcal{O}(h^4) \\ &= f(x_j) + \frac{h^2}{12}(\partial_x^2 f)(x_j) + \mathcal{O}(h^4) \\ &= f(x_j) + \frac{h^2}{12}(\delta_x^2 f)(x_j) + \mathcal{O}(h^4). \end{aligned} \tag{2.6}$$

Then the Poisson equation could be approximated by $\delta_x^2 \phi_j = (1 + \frac{h^2}{12}\delta_x^2) f_j$ with fourth order accuracy. Let $\phi_h, f_h \in X_M$ and denote $A_h = (a_{ij})_{(M-1)\times(M-1)}$, $\Delta_h = B_h^{-1} A_h$ as the standard central finite difference and fourth order approximation of ∂_x^2 respectively, where $B_h = \mathbb{I} + \frac{h^2}{12} A_h$ and A_h is a tri-diagonal matrix with $a_{ii} = -\frac{2}{h^2}, a_{i,i+1} = a_{i,i-1} = \frac{1}{h^2}$. Let $I_h : \mathbb{C}^{M+1} \to \mathbb{C}^{M-1}$ be the standard identity projection operator, i.e.,

$$(I_h u) = (u_1, \cdots, u_{M-1})^T \in \mathbb{C}^{M-1}, \quad \forall\, u = (u_0, \cdots, u_M)^T \in \mathbb{C}^{M+1}.$$

Thus the numerical Poisson potential ϕ_h and the second order derivative $f_h = (\partial_x^2 \phi)_h$ are approximated as

$$I_h f_h = \Delta_h (I_h \phi_h), \qquad I_h \phi_h = \Delta_h^{-1}(I_h f_h). \tag{2.7}$$

2.2 Numerical methods

Based on the fourth order compact finite difference discretization, the conservative Crank-Nicolson compact finite difference scheme (**CNCFD**) for SPS reads as follows:

$$i\delta_t^+\psi_j^n = -\frac{1}{2}\Big(\Delta_h I_h \mu_t \psi^n\Big)_j + V_j \mu_t \psi_j^n + \beta \mu_t \Phi_j^n \mu_t \psi_j^n, \qquad j\in\mathcal{T}_M, \quad n\geq 0, \tag{2.8}$$

where

$$-\Delta_h I_h \Phi^n = I_h(|\psi^n|^2), \qquad -\Delta_h I_h \Phi^{n+1} = I_h(|\psi^{n+1}|^2), \tag{2.9}$$

and the index set $\mathcal{T}_M$ is defined as $\mathcal{T}_M=\{j\mid j=1,2,\cdots,M-1\}$.

The boundary condition (2.4) is discretized as

$$\psi_0^n=\psi_M^n=0, \qquad \Phi_0^n=\Phi_M^n=0, \qquad n=0,1,\cdots, \tag{2.10}$$

and the initial value is discretized as

$$\psi_j^0=\psi_0(x_j), \qquad j\in\mathcal{T}_M^0. \tag{2.11}$$

We apply iteration method to solve the nonlinear equation. Given $\psi^n\in X_M$, to solve ψ^{n+1} in (2.8), one could solve its linearized equation, i.e.,

$$i\frac{\psi_j^{*,s+1}-\psi_j^n}{\tau} = -\frac{1}{4}\Big[\Delta_h I_h(\psi^{*,s+1}+\psi^n)\Big]_j + \left[V_j+\beta\frac{\Phi_j^{*,s}+\Phi_j^n}{2}\right]\frac{\psi_j^{*,s+1}+\psi_j^n}{2}, \tag{2.12}$$

until the $\psi^{*,s}$ converges up to given accuracy that is sufficiently small so as to preserve the conservation of mass and energy on discrete level.

As to be stated in Section 3, the above CNCFD scheme conserves the mass and energy. However, due to the nonlinearity of Poisson potential, one has to solve a nonlinear equation which is quite expensive in the view of computation time. Therefore we come up with a semi-implicit compact finite difference method (**SICFD**).

The semi-implicit compact finite difference method, a three-level scheme, reads as follows:

$$i\delta_t\psi_j^n = -\frac{1}{2}\left[\Delta_h I_h\Big(\frac{\psi^{n+1}+\psi^{n-1}}{2}\Big)\right]_j + V_j\frac{\psi_j^{n+1}+\psi_j^{n-1}}{2} + \beta\Phi_j^n\psi_j^n, \quad n\geq 1, \tag{2.13}$$

and the Poisson potential, boundary condition and the initial value are determined the same way as in CNCFD. The first step value ψ_j^1 could be computed by an at least second order accuracy scheme in time, for example, a second order modified Euler method, i,e.,

$$\psi_j^1=\psi_j^0-i\tau\left[-\frac{1}{2}\Big(\Delta_h I_h\psi^{(1)}\Big)_j+V_j\psi_j^{(1)}+\beta\Phi_j^{(1)}\psi_j^{(1)}\right], \quad j\in\mathcal{T}_M, \tag{2.14}$$

$$\psi_j^{(1)}=\psi_j^0-i\frac{\tau}{2}\left[-\frac{1}{2}\Big(\Delta_h I_h\psi^0\Big)_j+V_j\psi_j^0+\beta\Phi_j^0\psi_j^0\right], \qquad j\in\mathcal{T}_M, \tag{2.15}$$

where Poisson potential $\Phi^{(1)}$ and Φ^0 are evaluated by scheme (2.9).

Thanks to the equally spaced stencils, Eqs. (2.13) and (2.13) can be accelerated by discrete sine transform (DST) that would help reduce the computational cost from $\mathcal{O}(M^3)$ (direct linear system solver) to $\mathcal{O}(M\log(M))$ and we refer to [21] for more details on DST. Extensions of DST acceleration method to higher dimensions are similar and straightforward.

2.3 Main error estimate results

Before presenting the main error estimates, we would like first to introduce some notations and definitions. For any $u,\ v\in X_M$, $w\in\mathbb{C}^{M-1}$, we define inner product and norms as

$$\begin{aligned}
&\|u\|_{l^2}^2=h\sum_{k=1}^{M-1}|u_k|^2,\qquad \|\delta_x^+u\|_{l^2}^2=h\sum_{k=0}^{M-1}|\delta_x^+u_k|^2,\qquad \|u\|_{l^\infty}=\max_{j\in\mathcal{T}_M^0}|u_j|,\\
&(\delta_x^+u,\delta_x^+v)=h\sum_{k=0}^{M-1}(\delta_x^+u_k)(\delta_x^+\overline{v_k}),\qquad \langle u,w\rangle=\overline{\langle w,u\rangle}=h\sum_{k=1}^{M-1}u_k\overline{w_k},\\
&E_h(u)=\frac{1}{2}\langle-\Delta_hI_hu,u\rangle+\frac{\beta}{2}\langle\Delta_h^{-1}I_h|u|^2,|u|^2\rangle+\langle Vu,u\rangle,\\
&\mathcal{E}(u)=\frac{1}{2}\langle-\Delta_hI_hu,u\rangle+\langle Vu,u\rangle,
\end{aligned}$$

where $\overline{u_k}$ denotes the conjugate of u_k.

We make the following assumptions:

$$\begin{aligned}
(A):\quad &\psi\in C^0([0,T];W^{7,\infty}(\Omega)\cap H_0^2(\Omega))\cap C^1([0,T];W^{4,\infty}(\Omega))\\
&\quad\cap C^2([0,T];W^{3,\infty}(\Omega))\cap C^4([0,T];L^\infty(\Omega)),
\end{aligned}$$

where $0\le T\le T_{\max}$ with $T_{\max}$ being the maximal existing time [23,24].

(B): The external potential V(x) is smooth.

Denote $M_1=\max_{0\le t\le T}\|\psi\|_{L^\infty}$ and define the error function $e^n\in X_M$ as

$$e_j^n=\psi(x_j,t_n)-\psi_j^n,\qquad j\in\mathcal{T}_M^0,\quad n=0,1,\cdots.$$

Theorem 2.1. *For the CNCFD method, under assumptions (A) and (B), there exists h_0 and τ_0 such that for any $0<h<h_0$ and $0<\tau<\tau_0$, the error function satisfies that*

$$\|e^n\|_{l^2}+\|\delta_x^+e^n\|_{l^2}\le C(h^4+\tau^2),\qquad 0\le n\le\frac{T}{\tau},\tag{2.16}$$

where the constant C depends on Ω but not on h or τ.

Theorem 2.2. *For the SICFD method, under assumptions (A) and (B), there exists h_0 and τ_0 such that for any $0<h<h_0, 0<\tau<\tau_0$ and $\tau\le h$, the error function satisfies that*

$$\|e^n\|_{l^2}+\|\delta_x^+e^n\|_{l^2}\le C(h^4+\tau^2),\qquad 0\le n\le\frac{T}{\tau},\tag{2.17}$$

where the constant C depends on Ω but not on h or τ.

Remark 2.1. In higher dimensions, if the wave function ψ and Poisson potential φ are both specified with homogeneous Dirichlet boundary condition on bounded computation domain, higher order compact finite difference discretizations of $\Delta\psi$ and φ are still applicable and we refer the reader to [7,19,29] for more details, thus the numerical methods proposed here can be generalized to higher dimensions.

Remark 2.2. Error analysis in higher dimensions are possible in the framework of our proof. All the key inequalities involved could be adapted therein. The inverse inequality used to obtain a *priori* bound in the l^∞ norm in Section 3 can be extended to higher dimensions. The maximum principle theorem still holds and we refer to [14] for details. We remark that the work on error analysis in higher dimensions is still on-going.

3 Error estimates for the CNCFD method

In this section, we will give detailed proof of the main results by energy method with inequalities presented in the following lemma.

Let $u,v\in X_M$, then u,v satisfy the following inequalities:

Lemma 3.1.

$$\langle u,\delta_x^2v\rangle=-(\delta_x^+u,\delta_x^+v)=\langle\delta_x^2u,v\rangle,\qquad\langle A_hI_hu,v\rangle=\langle u,\delta_x^2v\rangle,\tag{3.1}$$

$$\|u\|_{l^\infty}\le\sqrt{b-a}\,\|\delta_x^+u\|_{l^2},\qquad\|u^2\|_{l^\infty}\le\sqrt{2}\,\|u\|_{l^2}\,\|\delta_x^+u\|_{l^2},\tag{3.2}$$

$$\langle-\Delta_h^{-1}I_h|u^2|,|u^2|\rangle\le\varepsilon\,\|\delta_x^+u\|_{l^2}^2+C_\varepsilon\,\|u\|_{l^2}^6.\tag{3.3}$$

Proof. The equality (3.1) can be verified using summation by parts as

$$\begin{aligned}\langle u,\delta_x^2v\rangle&=h\sum_{k=1}^{M-1}u_k\,\frac{\overline{v_{k+1}}-2\overline{v_k}+\overline{v_{k-1}}}{h^2}\\&=-h\sum_{k=0}^{M-1}\Big(\frac{u_{k+1}-u_k}{h}\Big)\Big(\frac{\overline{v_{k+1}}-\overline{v_k}}{h}\Big)\\&=-(\delta_x^+u,\delta_x^+v)=\langle\delta_x^2u,v\rangle.\end{aligned}$$

$\langle A_hI_hu,v\rangle=\langle\delta_x^2u,v\rangle$ can be proved by definition.

Proof of (3.2). For any $u\in X_M$,

$$\begin{aligned}|u_j| &= \Big|\sum_{k=1}^{j}(u_k-u_{k-1})\Big| = \Big|\sum_{k=1}^{j}\delta_x^+ u_{k-1}\sqrt{h}\sqrt{h}\Big| \\ &\le \Big(h\sum_{k=1}^{j}|\delta_x^+ u_{k-1}|^2\Big)^{\frac{1}{2}}(hj)^{\frac{1}{2}} \le \sqrt{b-a}\,\|\delta_x^+ u\|_{l^2},\end{aligned}$$

take maximum over index $j\in\mathcal{T}_M^0$, we could get

$$\|u\|_{l^\infty}\le\sqrt{b-a}\,\|\delta_x^+ u\|_{l^2}.$$

Similarly,

$$u_j^2=\sum_{k=1}^{j}u_k^2-u_{k-1}^2=\sum_{k=1}^{j}\Big(\frac{u_k-u_{k-1}}{h}\sqrt{h}\Big)\Big((u_k+u_{k-1})\sqrt{h}\Big),$$

take absolute value on both sides, we have

$$\begin{aligned}|u_j^2| &\le \Big(h\sum_{k=1}^{j}|\delta_x^+ u_{k-1}|^2\Big)^{1/2}\Big(h\sum_{k=1}^{j}|u_k+u_{k-1}|^2\Big)^{1/2} \\ &\le \sqrt{2}\,\|u\|_{l^2}\,\|\delta_x^+ u\|_{l^2}.\end{aligned}$$

Then by taking maximum over $j\in\mathcal{T}_M^0$, we could get

$$\|u^2\|_{l^\infty}\le\sqrt{2}\|u\|_{l^2}\,\|\delta_x^+ u\|_{l^2}.$$

The inequality

$$\langle-\Delta_h^{-1}I_h|u^2|,|u^2|\rangle\le\varepsilon\|\delta_x^+ u\|_{l^2}^2+C_\varepsilon\|u\|_{l^2}^6$$

is useful in estimating the Poisson interaction energy. Herein the Δ_h^{-1} approximates inverse Poisson operator.

$$\begin{aligned}|\langle-\Delta_h^{-1}I_h|u^2|,|u^2|\rangle| &= \left|\sum_{k=1}^{M-1}(-\Delta_h^{-1}I_h|u|^2)_k\,|u_k|^2h\right| \\ &\le \|u\|_{l^2}^2\,\|\Delta_h^{-1}I_h|u|^2\|_{l^\infty}\le C\,\|u\|_{l^2}^2\,\||u|^2\|_{l^\infty} \\ &\le C\,\|u\|_{l^2}^3\,\|\delta_x^+ u\|_{l^2}\le\varepsilon\,\|\delta_x^+ u\|_{l^2}^2+C_\varepsilon\,\|u\|_{l^2}^6,\end{aligned}$$

where we use discrete maximum principle in $\|\Delta_h^{-1}I_h|u|^2\|_{l^\infty}$ estimate and in last equality we apply Young inequality with ε being any positive real number. □

In order to analyze the H^1 error, we need to investigate some related matrix in detail. The following lemma establish some useful properties of approximation matrix $A_h,B_h,\Delta_h\in\mathbb{R}^{M-1\times M-1}$.

Lemma 3.2 (Properties of related approximation matrix). *For any $u,v\in X_M$ and matrix A_h,B_h,Δ_h, we have*

$$\|A_h^{-1}I_hu\|_{l^\infty}\le C\|u\|_{l^\infty},\quad \|A_h^{-1}I_hu\|_{l^2}\le\frac{(b-a)^2}{\pi^2}\|u\|_{l^2},\tag{3.4}$$

$$\|B_hI_hu\|_{l^\infty}\le\|u\|_{l^\infty},\qquad \|B_h^{-1}I_hu\|_{l^\infty}\le\frac{3}{2}\|u\|_{l^\infty},\tag{3.5}$$

$$\|B_hI_hu\|_{l^2}\le\|u\|_{l^2},\qquad \|B_h^{-1}I_hu\|_{l^2}\le\frac{3}{2}\|u\|_{l^2},\tag{3.6}$$

$$\langle -A_hI_hu,u\rangle\le\langle -\Delta_hI_hu,u\rangle\le\frac{3}{2}\langle -A_hI_hu,u\rangle,\tag{3.7}$$

where the constant C depends on Ω but not on h or u.

Proof. By applying discrete maximum principle in [14], one can get $\|A_h^{-1}I_hu\|_{l^\infty}\le C\|u\|_{l^\infty}$ where the constant C depends on Ω but not on h or u. Standard contradiction argument would lead us to $\|B_h^{-1}I_hu\|_{l^\infty}\le\frac{3}{2}\|u\|_{l^\infty}$. If examining entries of B_h carefully, one can get

$$\|B_h\|_{l^\infty}=\max_{1\le i\le M-1}\sum_{j=1}^{M-1}|(B_h)_{ij}|\le 1,$$

thus we finish the proof of $\|B_hI_hu\|_{l^\infty}\le\|u\|_{l^\infty}$.

Note that $-A_h,B_h$ are commutable positive definite matrix, then they have the same eigenvectors. The j-th eigenvalue of $-A_h$ equals to $\lambda_j(-A_h)=\frac{2}{h^2}(1-\cos(\frac{\pi j}{M}))$, $j=1,2,\cdots,M-1$ and the j-th eigenvalue of B_h is $\lambda_j(B_h)=1-\frac{1}{6}(1-\cos(\frac{\pi j}{M}))\in(\frac{2}{3},1)$, then we have

$$\lambda_j(-A_h^{-1})=\frac{h^2}{2}\frac{1}{1-\cos(\frac{\pi j}{M})}$$

which implies that

$$\|A_h^{-1}\|_{l^2}=\max_{1\le j\le M-1}|\lambda_j(-A_h^{-1})|\le\frac{(b-a)^2}{\pi^2}.$$

Thus we obtain

$$\|A_h^{-1}I_hu\|_{l^2}\le\frac{(b-a)^2}{\pi^2}\|u\|_{l^2}.$$

Similarly, we have

$$\|B_h\|_{l^2}=\max_{1\le j\le M-1}|\lambda_j(B_h)|\le 1,\qquad \|B_h^{-1}\|_{l^2}=\max_{1\le j\le M-1}|\lambda_j(B_h^{-1})|\le\frac{3}{2}.$$

Therefore we get $\|B_hI_hu\|_{l^2}\le\|u\|_{l^2}$, $\|B_h^{-1}I_hu\|_{l^2}\le\frac{3}{2}\|u\|_{l^2}$.

The last inequality states the equivalence of two kinetic energies. Notice $\langle -A_h I_h u, u\rangle = \|\sqrt{-A_h} I_h u\|_{l^2}^2$, $\langle -\Delta_h I_h u, u\rangle = \|\sqrt{-\Delta_h} I_h u\|_{l^2}^2$, and denote $S=\sqrt{-A_h}$, $T=\sqrt{B_h}$ with $ST=TS$. Then we have

$$\begin{aligned}
\|\sqrt{-A_h} I_h u\|_{l^2} &= \|S I_h u\|_{l^2} = \|T(T^{-1}S) I_h u\|_{l^2} \\
&\le \|T\|_{l^2} \|(T^{-1}S) I_h u\|_{l^2} \le \|T\|_{l^2} \|\sqrt{-\Delta_h} I_h u\|_{l^2}, \\
\|\sqrt{-\Delta_h} I_h u\|_{l^2} &= \|(T^{-1}S) I_h u\|_{l^2} \le \|T^{-1}\|_{l^2} \|S I_h u\|_{l^2} \le \|T^{-1}\|_{l^2} \|\sqrt{-A_h} I_h u\|_{l^2},
\end{aligned}$$

which implies

$$\begin{aligned}
\langle -A_h I_h u, u\rangle &= \|\sqrt{-A_h} I_h u\|_{l^2}^2 \le \|T\|_{l^2}^2 \langle -\Delta_h I_h u, u\rangle, \\
\langle -\Delta_h I_h u, u\rangle &= \|\sqrt{-\Delta_h} I_h u\|_{l^2}^2 \le \|T^{-1}\|_{l^2}^2 \langle -A_h I_h u, u\rangle.
\end{aligned}$$

For $\|B_h\|_{l^2}$ is bounded, we can conclude that $\|T^{-1}\|_{l^2}^2 = \|B_h^{-1}\|_{l^2} \le \frac{3}{2}$, $\|T\|_{l^2}^2 \le 1$. Thus we prove the equivalence inequality. $\square$

Since the fourth order compact finite difference scheme has been proposed before, the following lemma completes the error analysis.

Lemma 3.3 (Error estimates of compact finite difference scheme)**.** *For Poisson equation* (2.5)*, let* $f_{\rm ext}=(f(x_0),f(x_1),\cdots,f(x_M))^T$, $\phi_{\rm ext}=(\phi(x_0),\phi(x_1),\cdots,\phi(x_M))^T$ *be the exact solution and* $f_h=(f_0,f_1,\cdots,f_M)^T$, $\phi_h=(\phi_0,\phi_1,\cdots,\phi_M)^T$ *be the numerical approximation obtained by the fourth order compact finite difference scheme.*

Assume $\phi(x)\in C^6([a,b])$, $f(x)\in C^4([a,b])$*, if* $f(x)$ *is known, we get*

$$\|\phi_h - \phi_{\rm ext}\|_{l^\infty} = \mathcal{O}(h^4, \partial_x^4 f).$$

Inversely, with $\phi(x)$ *being known,*

$$\|f_h - f_{\rm ext}\|_{l^\infty} = \mathcal{O}(h^4, \partial_x^6 \phi).$$

Proof. The proof is mainly based on Taylor formula with integral remainder and discrete maximum principle of elliptic equation.

Firstly, if $\phi(x)\in C^6([a,b])$, $f(x)\in C^4([a,b])$, by Taylor formula, we have

$$\begin{aligned}
\delta_x^2\phi(x_j) &= (\partial_x^2\phi)(x_j) + \frac{h^2}{12}(\partial_x^4\phi)(x_j) + \mathcal{R}_j^{\rm I} \\
&= f(x_j) + \frac{h^2}{12}(\partial_x^2 f)(x_j) + \mathcal{R}_j^{\rm I} \\
&= f(x_j) + \frac{h^2}{12}\delta_x^2 f(x_j) + \mathcal{R}_j^{\rm I} + \mathcal{R}_j^{\rm II},
\end{aligned}$$

where

$$\mathcal{R}_j^{\mathrm{I}}=\frac{1}{5!h^2}\int_0^h (h-s)^5\left[\phi^{(6)}(x_j+s)+\phi^{(6)}(x_j-s)\right]\mathrm{d}s,$$
$$\mathcal{R}_j^{\mathrm{II}}=-\frac{1}{72}\int_0^h (h-s)^3\left[f^{(4)}(x_j+s)+f^{(4)}(x_j-s)\right]\mathrm{d}s.$$

To solve the Poisson equation in (2.5), we apply the compact finite difference method as $-\Delta_h I_h\phi_h=I_h f_{\mathrm{ext}}$. Then $A_h I_h(\phi_{\mathrm{ext}}-\phi_h)=\mathcal{R}^{\mathrm{I}}+\mathcal{R}^{\mathrm{II}}$, by discrete maximum principle, it can be concluded that

$$\|\phi_h-\phi_{\mathrm{ext}}\|_{l^\infty}\le C\|\mathcal{R}^{\mathrm{I}}+\mathcal{R}^{\mathrm{II}}\|_{l^\infty}\le Ch^4\|\partial_x^4 f\|_{L^\infty},$$

where $\mathcal{R}^{\mathrm{I}},\mathcal{R}^{\mathrm{II}}\in\mathbb{C}^{M-1}$ and the constant C depends on Ω but not on $f(x)$ or h.

Reversely, the second derivative of $\phi(x)$ was approximated by $I_h f_h=\Delta_h I_h\phi_{\mathrm{ext}}$ and the equation $B_h I_h(f_h-f_{\mathrm{ext}})=(\mathcal{R}^{\mathrm{I}}+\mathcal{R}^{\mathrm{II}})$ holds. Then we have

$$\|f_h-f_{\mathrm{ext}}\|_{l^\infty}\le\frac{3}{2}\|\mathcal{R}^{\mathrm{I}}+\mathcal{R}^{\mathrm{II}}\|_{l^\infty}\le Ch^4\|\partial_x^6\phi\|_{L^\infty}.$$

The proof is complete. □

Remark 3.1. One must have noticed that the approximation errors in f_{ext}, ϕ_{ext} are globally dependent on $\phi(x)$ and $f(x)$ respectively, and this is quite different from the cubic nonlinear or other local nonlinear Schrödinger equations.

Lemma 3.4 (Conservation of mass and energy)**.** *For the CNCFD scheme* (2.8) *with* (2.10) *and* (2.11)*, for any time step $\tau>0$ and mesh size $h>0$ and initial data ψ_0. It conserves the mass and energy in the discretized level, i.e.,*

$$\|\psi^n\|_{l^2}=\|\psi^0\|_{l^2},\qquad E_h(\psi^n)=E_h(\psi^0). \tag{3.8}$$

Proof. One can apply a similar process as in [5], so we omit it for brevity. □

Lemma 3.5 (Solvability of the difference equation)**.** *For any given ψ^n, under assumptions (A) and (B), there exists a solution $\psi^{n+1}\in X_M$ satisfies* (2.8)*. There exists $\tau_0>0$ such that the solution is unique for $0<\tau<\tau_0$.*

Proof. Proof for existence and uniqueness of CNCFD are similar to those in [1]. Rewrite (2.8) as

$$\psi^{n+1/2}=\psi^n+i\frac{\tau}{2}F^n(\psi^{n+1/2}),\qquad n=0,1,\cdots,$$

where $F^n: X_M\to X_M$ is defined as

$$(F^n(u))_j=-\frac{1}{2}(A_h I_h u)_j+V_j u_j+\beta\left[-A_h^{-1}I_h\left(\frac{|\psi^n|^2+|2u-\psi^n|^2}{2}\right)\right]_j u_j.$$

Define the map $G^n: X_M \to X_M$ as

$$G^n(u) = u - \psi^n - i\frac{\tau}{2}F^n(u), \qquad u \in X_M,$$

and it is continuous. Moreover,

$$\mathrm{Re}\langle G^n(u),u\rangle = \|u\|_{l^2}^2 - \mathrm{Re}\langle \psi^n,u\rangle \geq \|u\|_{l^2}(\|u\|_{l^2} - \|\psi^n\|_{l^2}), \qquad u \in X_M,$$

which implies

$$\lim_{\|u\|_{l^2}\to\infty} \frac{|\langle G^n(u),u\rangle|}{\|u\|_{l^2}} = \infty.$$

Thus G^n is surjective according to theorem in [13], that is to say, there exists a solution $u_0 \in X_M$ satisfying $G^n(u_0) = 0$.

We can use standard energy argument to prove uniqueness of (2.8). Assume $u,v \in X_M$ satisfies Eq. (2.8) for given ψ^n. Denote $w = u - v \in X_M$, we have

$$i\frac{w_j}{\tau} = -\frac{1}{2}\frac{(\Delta_h I_h w)_j}{2} + \frac{V_j w_j}{2} + \beta\chi_j, \qquad j \in \mathcal{T}_M,$$

where

$$\chi_j := \frac{1}{4}\left[-\Delta_h^{-1} I_h(|u|^2 + |\psi^n|^2)\right]_j (u_j + \psi_j^n) - \frac{1}{4}\left[-\Delta_h^{-1} I_h(|v|^2 + |\psi^n|^2)\right]_j (v_j + \psi_j^n).$$

Multiply both sides (3.9) by $\overline{w_j}h$ and then take imaginary part of the summation over $j \in \mathcal{T}_M$, we can get

$$\begin{aligned}
\frac{\|w\|_{l^2}^2}{\tau} &= \left|\frac{\beta}{4}h\sum_{j=1}^{M-1}\Big(\Delta_h^{-1} I_h(|u|^2 + |\psi^n|^2)\Big)_j |w_j|^2 + \Big(\Delta_h^{-1} I_h(|u|^2 - |v|^2)\Big)_j (v_j + \psi_j^n)\overline{w_j}\right| \\
&\leq C\|w\|_{l^2}^2(\|u\|_{l^\infty}^2 + \|\psi^n\|_{l^\infty}^2) + C(\|v\|_{l^\infty} + \|\psi^n\|_{l^\infty})\|w\|_{l^2}\|\Delta_h^{-1} I_h(|u|^2 - |v|^2)\|_{l^2} \\
&\leq C(\|u\|_{l^\infty}^2 + \|v\|_{l^\infty}^2 + \|\psi^n\|_{l^\infty}^2)(\|w\|_{l^2}^2 + \||u|^2 - |v|^2\|_{l^2}^2).
\end{aligned}$$

As stated before, the CNCFD scheme preserves the mass and energy in the discretized level, by applying inequalities in (3.2)-(3.3), we have

$$\begin{aligned}
E_h(u) &= \langle -\Delta_h I_h u, u\rangle + \frac{\beta}{2}\langle \Delta_h^{-1} I_h |u|^2, |u|^2\rangle + h\sum_{k=1}^{M-1} V_k u_k \overline{u_k} \\
&\geq \|\delta_x^+ u\|_{l^2}^2 - |\beta|\varepsilon\|\delta_x^+ u\|_{l^2}^2 - C_\varepsilon\|u\|_{l^2}^6 - C\|u\|_{l^2}^2,
\end{aligned}$$

where the last inequality holds due to Assumption (B) that V is bounded on finite interval, thus we have

$$\|\delta_x^+ u\|_{l^2}^2 \leq E_h(\psi^0) + C_\varepsilon\|\psi^0\|_{l^2}^6 + C\,\|\psi^0\|_{l^2}^2. \tag{3.9}$$

By simple calculations, we have

$$\||u|^2-|v|^2\|_{l^2}^2=h\sum_{j=1}^{M-1}\left[u_j(\overline{u_j}-\overline{v_j})+(u_j-v_j)\overline{v_j}\right]^2\le C\left(\|u\|_{l^\infty}^2+\|v\|_{l^\infty}^2\right)\|w\|_{l^2}^2.$$

Put together all the inequalities listed above, we have

$$\begin{aligned}\|w\|_{l^2}^2&\le C\tau\|w\|_{l^2}^2\left(\|u\|_{l^\infty}^2+\|v\|_{l^\infty}^2+\|\psi^n\|_{l^\infty}^2+1\right)^2\\&\le C\tau\|w\|_{l^2}^2\left(\|\delta_x^+u\|_{l^2}^2+\|\delta_x^+v\|_{l^2}^2+\|\delta_x^+\psi^n\|_{l^2}^2+C_0\right)^2\\&\le C\tau\|w\|_{l^2}^2\left(E_h(\psi^0)+C_\varepsilon\|\psi^0\|_{l^2}^6+C_0\right)^2,\end{aligned}$$

where C_0 is a constant that does not depend on h or ψ. There exists τ_0 such that $|C\tau(E_h(\psi^0)+C_\varepsilon\|\psi^0\|_{l^2}^6+C_0)^2|\le\frac{1}{2}$ for any $0\le\tau\le\tau_0$, which implies that

$$\|w\|_{l^2}^2=\|u-v\|_{l^2}^2=0\quad\Longrightarrow\quad u=v,$$

thus we finish the proof of uniqueness. □

Denote the local truncation error of CNCFD scheme by η^n, which is defined as

$$\begin{aligned}\eta_j^n:=&\,i\delta_t^+\psi(x_j,t_n)+\frac{1}{2}\left[\Delta_hI_h\mu_t\psi(\cdot,t_n)\right]_j-V(x_j)\mu_t\psi(x_j,t_n)\\&-\beta\left[-\Delta_h^{-1}I_h\mu_t|\psi(\cdot,t_n)|^2\right]_j\mu_t\psi(x_j,t_n),\qquad j\in\mathcal{T}_M,\quad n\ge0,\end{aligned}$$

where $\psi(\cdot,t_n)=(\psi(x_0,t_n),\psi(x_1,t_n),\cdots,\psi(x_M,t_n))^T\in X_M$.

Lemma 3.6 (Local truncation error)**.** *Under assumptions (A) and (B), the local truncation error for CNCFD satisfies*

$$\begin{aligned}&\|\eta^n\|_{l^\infty}=\mathcal{O}(h^4+\tau^2),&&\|\eta^n\|_{l^2}=\mathcal{O}(h^4+\tau^2),&&0\le n\le\frac{T}{\tau},\\&\|\delta_x^+\eta^n\|_{l^2}=\mathcal{O}(h^4+\tau^2),&&\|\delta_x^+\eta^n\|_{l^\infty}=\mathcal{O}(h^4+\tau^2),&&0\le n\le\frac{T}{\tau}.\end{aligned}$$

Proof. Firstly, by Taylor formula with integral remainder, we have

$$\begin{aligned}&\delta_t^+\psi(x_j,t_n)=(\partial_t\psi)(x_j,t_{n+\frac{1}{2}})+\mathcal{Q}_j^{n+\frac{1}{2}}(\psi),\\&V(x_j)\mu_t\psi(x_j,t_n)=V(x_j)\psi(x_j,t_{n+\frac{1}{2}})+V(x_j)\mathcal{P}_j^{n+\frac{1}{2}}(\psi),\\&\Delta_hI_h\mu_t\psi(x_j,t_n)=(\partial_x^2\psi)(x_j,t_{n+\frac{1}{2}})+\mathcal{P}_j^{n+\frac{1}{2}}(\partial_x^2\psi)+\left[B_h^{-1}\mu_t\mathcal{R}^n(\psi)\right]_j,\end{aligned}$$

where $\mathcal{Q}_j^{n+\frac{1}{2}},\mathcal{P}_j^{n+\frac{1}{2}},\mathcal{R}_j^n$ are defined as

$$\begin{aligned}
\mathcal{Q}_j^{n+\frac{1}{2}}(f(x,t)) &= \frac{1}{4\tau}\int_0^\tau (\tau-s)^2\left[\partial_t^3 f(x_j,t_{n+\frac{1}{2}}+s)+\partial_t^3 f(x_j,t_{n+\frac{1}{2}}-s)\right]\mathrm{d}s,\\
\mathcal{P}_j^{n+\frac{1}{2}}(f(x,t)) &= \int_0^\tau (\tau-s)\left[\partial_t^2 f(x_j,t_{n+\frac{1}{2}}+s)+\partial_t^2 f(x_j,t_{n+\frac{1}{2}}-s)\right]\mathrm{d}s,\\
\mathcal{R}_j^n(f(x,t)) &= \frac{1}{5!\,h^2}\int_0^h (h-s)^5\left[f^{(6)}(x_j+s,t_n)+f^{(6)}(x_j-s,t_n)\right]\mathrm{d}s\\
&\quad -\frac{1}{72}\int_0^h (h-s)^3\left[f^{(6)}(x_j+s,t_n)+f^{(6)}(x_j-s,t_n)\right]\mathrm{d}s.
\end{aligned}$$

Let $\Phi(\cdot,t_n)=(\Phi(x_0,t_n),\Phi(x_1,t_n),\cdots,\Phi(x_M,t_n))^T\in X_M$, then

$$\left[-\Delta_h^{-1}I_h\mu_t|\psi(\cdot,t_n)|^2\right]_j=\Phi(x_j,t_{n+\frac{1}{2}})+\mathcal{P}_j^{n+\frac{1}{2}}(\Phi)-\left[A_h^{-1}\mu_t\mathcal{R}^n(\Phi)\right]_j,$$

thus

$$\begin{aligned}
&\left[-\Delta_h^{-1}I_h\mu_t|\psi(\cdot,t_n)|^2\right]_j\mu_t\psi(x_j,t_n)\\
=&\left[\Phi(x_j,t_{n+\frac{1}{2}})+\mathcal{P}_j^{n+\frac{1}{2}}(\Phi)-\left(A_h^{-1}\mu_t\mathcal{R}^n(\Phi)\right)_j\right]\left[\psi(x_j,t_{n+\frac{1}{2}})+\mathcal{P}_j^{n+\frac{1}{2}}(\psi)\right].
\end{aligned}$$

By discrete maximum principle of elliptic equation, we have

$$\|\Phi\|_{L^\infty}\le C\||\psi|^2\|_{L^\infty},\qquad \|\partial_t^2\Phi\|_{L^\infty}\le C\|\partial_t^2|\psi|^2\|_{L^\infty},$$

therefore,

$$\begin{aligned}
&\left|\left[-\Delta_h^{-1}I_h\mu_t|\psi(\cdot,t_n)|^2\right]_j\mu_t\psi(x_j,t_n)-(\Phi\psi)(x_j,t_{n+\frac{1}{2}})\right|\\
=&\left|\Phi(x_j,t_{n+\frac{1}{2}})\mathcal{P}_j^{n+\frac{1}{2}}(\psi)+\left[\psi(x_j,t_{n+\frac{1}{2}})+\mathcal{P}_j^{n+\frac{1}{2}}(\psi)\right]\left[\mathcal{P}_j^{n+\frac{1}{2}}(\Phi)-\left(A_h^{-1}\mu_t\mathcal{R}^n(\Phi)\right)_j\right]\right|\\
\le& h^4(\|\partial_x^6\Phi\|_{L^\infty}\|\psi\|_{L^\infty})+\tau^2(\|\psi\|_{L^\infty}^2\|\partial_t^2\psi\|_{L^\infty}+\|\psi\|_{L^\infty}\|\partial_t^2\Phi\|_{L^\infty})+\mathcal{O}(h^4\tau^2+\tau^4)\\
\le& h^4(\|\partial_x^4|\psi|^2\|_{L^\infty}\|\psi\|_{L^\infty})+\tau^2(\|\psi\|_{L^\infty}^2\|\partial_t^2\psi\|_{L^\infty}+\|\psi\|_{L^\infty}\|\partial_t^2|\psi|^2\|_{L^\infty})+\mathcal{O}(h^4\tau^2+\tau^4).
\end{aligned}$$

Finally, local truncation error η_j^n can be written in integral form as

$$\begin{aligned}
\eta_j^n=&i\mathcal{Q}_j^{n+\frac{1}{2}}(\psi)+\frac{1}{2}\mathcal{P}_j^{n+\frac{1}{2}}(\partial_x^2\psi)+\frac{1}{2}\left[B_h^{-1}\mu_t\mathcal{R}^n(\psi)\right]_j-\left[V(x_j)+\beta\Phi(x_j,t_{n+\frac{1}{2}})\right]\mathcal{P}_j^{n+\frac{1}{2}}(\psi)\\
&-\beta\left[\psi(x_j,t_{n+\frac{1}{2}})+\mathcal{P}_j^{n+\frac{1}{2}}(\psi)\right]\left[\mathcal{P}_j^{n+\frac{1}{2}}(\Phi)-\left(A_h^{-1}\mu_t\mathcal{R}^n(\Phi)\right)_j\right].
\end{aligned}$$

Thus we can get

$$\left|\eta_j^n\right| \le C\tau^2\left(\|\partial_t^2\psi\|_{L^\infty}+\|\partial_t^3\psi\|_{L^\infty}+\|\partial_t^2\partial_x^2\psi\|_{L^\infty}+\|\psi\|_{L^\infty}^2\|\partial_t^2\psi\|_{L^\infty}+\|\psi\|_{L^\infty}\|\partial_t^2|\psi|^2\|_{L^\infty}\right)$$
$$+Ch^4(\|\partial_x^6\psi\|_{L^\infty}+\|\partial_x^4|\psi|^2\|_{L^\infty}\|\psi\|_{L^\infty})+\mathcal{O}(h^4\tau^2+\tau^4),$$

and this would lead us to $\|\eta^n\|_{l^\infty}=\mathcal{O}(h^4+\tau^2)$ and $\|\eta^n\|_{l^2}=\mathcal{O}(h^4+\tau^2)$.

To evaluate $\delta_x^+\eta_j^n$, we just need to estimate the nonlocal term error, i.e., $\left(B_h^{-1}\mu_t\mathcal{R}^n(\psi)\right)_j$ and $\left(A_h^{-1}\mu_t\mathcal{R}^n(\Phi)\right)_j$, because the local term could be dealt with by standard technique [1]. We just take $\delta_x^+\left(B_h^{-1}\mu_t\mathcal{R}^n(\psi)\right)_j$ as an example and the other term is estimated the same way.

Notice $B_h^{-1}\mu_t\mathcal{R}^n(\psi)\in X_M$ and denote

$$\mathcal{R}^n(\psi)=(\mathcal{R}_1^n(\psi),\cdots,\mathcal{R}_{M-1}^n(\psi))^T,\quad \mathcal{R}_x^n(\psi)=(\delta_x^+\mathcal{R}_1^n(\psi),\cdots,\delta_x^+\mathcal{R}_{M-2}^n(\psi))^T,$$
$$g_j=\left[B_h^{-1}\mu_t\mathcal{R}^n(\psi)\right]_j,\quad \mathcal{G}=(g_1,\cdots,g_{M-1})^T,\quad \mathcal{G}_x=(\delta_x^+g_1,\cdots,\delta_x^+g_{M-2})^T.$$

Reformulate the equation, we get

$$\mathcal{G}_x=B_h^{-1}\mu_t\mathcal{R}_x^n+B_h^{-1}\mathbf{b},\tag{3.10}$$

with $\mathbf{b}=\frac{1}{12}(\delta_x^+g_0,0,\cdots,0,\delta_x^+g_{M-1})_{M-2}^T$.

Then by taking l^2 norm on both sides, we have

$$\sum_{j=1}^{M-2}|\delta_x^+g_j|^2h\le C\sum_{j=1}^{M-2}(|\delta_x^+\mathcal{R}_j^n|^2+|\delta_x^+\mathcal{R}_j^{n+1}|^2)h+(|\delta_x^+g_0|^2+|\delta_x^+g_{M-1}|^2)h$$

and $\delta_x^+g_0$ can be estimated as

$$|\delta_x^+g_0|=\left|\frac{g_1-g_0}{h}\right|=\left|\frac{g_1}{h}\right|=\left|\frac{[B_h^{-1}\mu_t\mathcal{R}^n(\psi)]_1}{h}\right|=\left|\frac{\sum_{j=1}^{M-1}(B_h^{-1})_{1,j}\mu_t\mathcal{R}_j^n(\psi)}{h}\right|$$
$$\le C\sum_{j=1}^{M-1}d_j\,\frac{\mu_t\mathcal{R}_j^n(\psi)}{h}\le C\sum_{j=1}^{M-1}\frac{12}{(4+2\sqrt{6})^j}\,\frac{\mu_t\mathcal{R}_j^n(\psi)}{h}\le Ch^4\|\partial_x^7\psi\|_{L^\infty},$$

where $d_j\triangleq[B_h^{-1}]_{1,j}$ satisfies $|d_j|\le\frac{12}{(4+2\sqrt{6})^j}$, $j=1,2,\cdots,M-1$ and the last inequality holds because $\partial_x^6\psi(a)=\partial_x^6\psi(b)=0$ under regularity assumptions (A) and (B).

Similarly, $|\delta_x^+g_{M-1}|\le Ch^4\|\partial_x^7\psi\|_{L^\infty}$. Therefore $\|\delta_x^+g\|_{l^2}\le C\,h^4\|\partial_x^7\psi\|_{L^\infty}$. Taking maximum norm of (3.10) on both sides and using inequality (3.5), we can have $\|\delta_x^+g\|_{l^\infty}\le Ch^4\|\partial_x^7\psi\|_{L^\infty}$. Thus, we obtain

$$\|\delta_x^+\eta^n\|_{l^2}=\mathcal{O}(h^4+\tau^2),\quad \|\delta_x^+\eta^n\|_{l^\infty}=\mathcal{O}(h^4+\tau^2),\quad 0\le n\le\frac{T}{\tau}.$$

The proof is complete. ∎

Theorem 3.1 (l^2 norm estimate)**.** *Under assumptions (A) and (B), there exist h_0 and τ_0 such that for any $0<h<h_0$, $0<\tau<\tau_0$ and $\tau\le h$, the error function satisfies that*

$$\|e^n\|_{l^2}\le C(\tau^2+h^4),\qquad 0\le n\le\frac{T}{\tau},\tag{3.11}$$

where the constant C does not depend on h or τ.

Proof. Choose a smooth function $\alpha\in C^\infty([0,\infty))$, which is defined as

$$\alpha(\rho)=\begin{cases}1, & 0\le\rho\le 1,\\ \in[0,1], & 1<\rho<2,\\ 0, & \rho\ge 2.\end{cases}$$

Define truncating function $F_{M_0}(\rho)$ as

$$F_{M_0}(\rho)=\alpha(\frac{\rho}{M_0})\rho,\qquad 0\le\rho\le\infty,\qquad M_0=2(1+M_1^2)\ge 0,$$

so that $F_{M_0}(\rho)$ satisfies the following Lipschitz condition, that is,

$$|F_{M_0}(\rho_1)-F_{M_0}(\rho_2)|\le C|\sqrt{\rho_1}-\sqrt{\rho_2}|,\qquad 0\le\rho_1,\rho_2\le\infty.$$

Introduce an auxiliary scheme of $\phi\in X_M$, taking $\phi^0=\psi^0$ as the initial value, which is given by

$$i\delta_t^+\phi_j^n=-\frac{1}{2}[\Delta_h I_h\mu_t\phi^n]_j+V_j\mu_t\phi_j^n+\beta\mu_t\left[-\Delta_h^{-1}I_hF_{M_0}\left(|\phi^n|^2\right)\right]_j\mu_t\phi_j^n.\tag{3.12}$$

Herein, ϕ_j^n can be viewed as another approximation of $\psi(x_j,t_n)$. Define the 'auxiliary error' function $\widetilde{e^n}\in X_M$

$$\widetilde{e_j^n}=\psi(x_j,t_n)-\phi_j^n,\qquad j\in\mathcal{T}_M^0,\quad n\ge 0.$$

The corresponding local truncation error $\widetilde{\eta^n}$ is defined as

$$\begin{aligned}\widetilde{\eta_j^n}=&\,i\delta_t^+\psi(x_j,t_n)+\frac{1}{2}[\Delta_h I_h\mu_t\psi(\cdot,t_n)]_j-V(x_j)\mu_t\psi(x_j,t_n)\\&-\beta\mu_t\left[-\Delta_h^{-1}I_hF_{M_0}(|\psi(\cdot,t_n)|^2)\right]_j\mu_t\psi(x_j,t_n).\end{aligned}\tag{3.13}$$

Similarly, the local truncation error $\|\widetilde{\eta^n}\|_{l^\infty}=\mathcal{O}(h^4+\tau^2)$, $0\le n<\frac{T}{\tau}$. Subtracting (3.13) form (3.12), we have

$$i\delta_t^+\widetilde{e_j^n}=-\frac{1}{2}\left[\Delta_h I_h\mu_t\widetilde{e^n}\right]_j+V_j\mu_t\widetilde{e_j^n}+\widetilde{\xi_j^n}+\widetilde{\eta_j^n},\tag{3.14}$$

with

$$\widetilde{\xi_j^n}=\beta\mu_t\left[-\Delta_h^{-1}I_hF_{M_0}(|\psi(\cdot,t_n)|^2)\right]_j\mu_t\psi(x_j,t_n)-\beta\mu_t\left[-\Delta_h^{-1}I_hF_{M_0}(|\phi^n|^2)\right]_j\mu_t\phi_j^n.$$

Let

$$\Phi_j^n=\left[-\Delta_h^{-1}I_hF_{M_0}(|\phi^n|^2)\right]_j,\qquad \widetilde{\Phi_j^n}=\left[-\Delta_h^{-1}I_hF_{M_0}(|\psi(\cdot,t_n)|^2)\right]_j,$$

we have

$$\begin{aligned}\left|\mathrm{Im}\langle\widetilde{\xi_j^n},\widetilde{e_j^n}+\widetilde{e_j^{n+1}}\rangle\right|&=|\beta|\left|\mathrm{Im}\langle\mu_t(\widetilde{\Phi_j^n}-\Phi_j^n)\mu_t\psi(x_j,t_n)-\mu_t\Phi_j^n\mu_t\widetilde{e_j^n},2\mu_t\widetilde{e_j^n}\rangle\right|\\&=|\beta|\left|\mathrm{Im}\langle\mu_t(\widetilde{\Phi_j^n}-\Phi_j^n)\mu_t\psi(x_j,t_n),2\mu_t\widetilde{e_j^n}\rangle\right|.\end{aligned}$$

Denote $v,w\in\mathbb{C}^{M-1}$ as

$$v_j=F_{M_0}(|\psi(x_j,t_n)|^2)-F_{M_0}(|\phi_j^n|^2),\qquad w_j=\widetilde{e_j^n}+\widetilde{e_j^{n+1}},\qquad j=1,2,\cdots,M-1.$$

Then by the Lipschitz condition of F_{M_0}, we have

$$|v_j|\le C\big|\,|\psi(x_j,t_n)|-|\phi_j^n|\,\big|\le C|\psi(x_j,t_n)-\phi_j^n|=C|\widetilde{e_j^n}|,\qquad j=1,2,\cdots,M-1.$$

Therefore, by Cauchy-Schwartz inequality, we obtain

$$\begin{aligned}\left|\mathrm{Im}\langle\mu_t(\widetilde{\Phi_j^n}-\Phi_j^n)\mu_t\psi(x_j,t_n),2\mu_t\widetilde{e_j^n}\rangle\right|&\le C\rho(A_h^{-1})\sum_{j=1}^{M-1}(|v_j|^2+|w_j|^2)h\\&\le C(\|\widetilde{e^n}\|_{l^2}^2+\|\widetilde{e^{n+1}}\|_{l^2}^2),\end{aligned}$$

and

$$\begin{aligned}|\langle\widetilde{\eta_j^n},\mu_t\widetilde{e_j^n}\rangle|&\le C\|\widetilde{\eta^n}\|_{l^2}\|\mu_t\widetilde{e^n}\|_{l^2}\le C(\|\widetilde{\eta^n}\|_{l^2}^2+\|\mu_t\widetilde{e^n}\|_{l^2}^2)\\&\le C(\|\widetilde{\eta}^n\|_{l^\infty}^2+\|\widetilde{e^n}\|_{l^2}^2+\|\widetilde{e^{n+1}}\|_{l^2}^2).\end{aligned}$$

Multiply both sides of Eq. (3.14) by $2h\mu_t\overline{\widetilde{e_j^n}}$ and sum up over index $j\in\mathcal{T}_M$, after taking imaginary parts, we have

$$\|\widetilde{e^{n+1}}\|_{l^2}^2-\|\widetilde{e^n}\|_{l^2}^2\le C\tau(\|\widetilde{\eta^n}\|_{l^\infty}^2+\|\widetilde{e^{n+1}}\|_{l^2}^2+\|\widetilde{e^n}\|_{l^2}^2),\qquad 0\le n<\frac{T}{\tau}.$$

Applying discrete Gronwall inequality [28], we have

$$\|\widetilde{e^n}\|_{l^2}\le C(h^4+\tau^2),\qquad 0\le n\le\frac{T}{\tau},$$

and

$$\|\widetilde{e^n}\|_{l^\infty}\le\|\widetilde{e^n}\|_{l^2}h^{-1/2}\le C\left(h^{\frac{7}{2}}+\frac{\tau^2}{\sqrt{h}}\right)\le Ch,\quad \tau\le h,$$

thus

$$|\phi_j^n| \le |\psi(x_j,t_n)| + |\widetilde{e_j^n}| \le \frac{\sqrt{M_0}}{2} + Ch \le \sqrt{M_0},$$

which infers $F_{M_0}(|\phi_j^n|^2) = |\phi_j^n|^2$ and

$$\phi_j^n = \psi_j^n, \quad e_j^n = \widetilde{e_j^n}, \quad j = 1,2,\cdots,M-1, \quad 0 \le n \le \frac{T}{\tau}.$$

The proof is complete. □

Remark 3.2. In fact, the restriction on the grid ratio, i.e. $\tau \le h$, could be removed. By using inequality (3.9) and the 1D Sobolev inequality (3.2), we could obtain a *priori* uniform bound in l^∞ norm as $\|\psi^n\|_{l^\infty} \le C(E_h(\psi^0) + \|\psi^0\|_{l^2})$. Then by standard energy method, we could obtain the l^2 and H^1 error analysis. Please refer to [27] for details.

Remark 3.3. However, the argument above relies heavily on discrete Sobolev inequality and in higher dimensions we could get such a *priori* estimate. While the above proof, which is borrowed from [1], overcomes this problem by introducing an auxiliary function and using an inverse inequality and it could be extended to higher dimensions.

Next, we continue to prove Theorem 2.1.

Proof. The local truncation equation (3.14) is reduced as

$$i\delta_t^+ e_j^n = -\frac{1}{2}[\Delta_h I_h \mu_t e^n]_j + V_j \mu_t e_j^n + \xi_j^n + \eta_j^n, \tag{3.15}$$

where

$$\xi_j^n = \beta\left[-\Delta_h^{-1} I_h \mu_t |\psi(\cdot,t_n)|^2\right]_j \mu_t \psi(x_j,t_n) - \beta\left[-\Delta_h^{-1} I_h \mu_t |\psi^n|^2\right]_j \mu_t \phi_j^n \tag{3.16}$$

satisfies

$$\|\delta_x^+ \xi^n\|_{l^2} \le C\left((h^4+\tau^2)^2 + \|e^n\|_{l^2} + \|e^{n+1}\|_{l^2} + \|\delta_x^+ e^n\|_{l^2} + \|\delta_x^+ e^{n+1}\|_{l^2}\right). \tag{3.17}$$

Rewrite (3.15) as

$$e_j^{n+1} - e_j^n = -i\tau(\mathcal{L}_j^n + \xi_j^n + \eta_j^n),$$

where $\mathcal{L}_j^n$ is defined as

$$\mathcal{L}_j^n = -\frac{1}{2}[\Delta_h I_h \mu_t e^n]_j + V_j \mu_t e_j^n, \qquad j = 1,2,\cdots,M-1, \quad n \ge 0.$$

Multiply both sides of Eq. (3.15) by $2h\,\overline{e_j^{n+1}-e_j^n}$ and sum up over index $j\in\mathcal{T}_M$, after taking real parts, we have

$$\begin{aligned}\mathcal{E}(e^{n+1})-\mathcal{E}(e^n)&=-2\,\mathrm{Re}\langle\xi^n+\eta^n,e^{n+1}-e^n\rangle\\&=-2\,\mathrm{Re}\langle\xi^n+\eta^n,-i\tau(\mathcal{L}^n+\xi^n+\eta^n)\rangle\\&=2\tau\,\mathrm{Im}\langle\xi^n+\eta^n,\mathcal{L}^n\rangle.\end{aligned}$$

By Cauchy-Schwartz inequality and equivalent energies inequality, we have

$$\begin{aligned}\left|\langle\eta^n,\mathcal{L}^n\rangle\right|&\le\left|\langle\eta^n,-\frac{1}{2}\Delta_h I_h\mu_t e^n\rangle\right|+\left|\langle\eta^n,V\mu_t e^n\rangle\right|\\&\le C\left(\left|\langle(-\Delta_h)^{\frac{1}{2}}I_h\eta^n,(-\Delta_h)^{\frac{1}{2}}I_h\mu_t e^n\rangle\right|+\|e^n\|_{l^2}^2+\|e^{n+1}\|_{l^2}^2+(h^4+\tau^2)^2\right)\\&\le C\left(\|(-A_h)^{\frac{1}{2}}I_h\eta^n\|_{l^2}^2+\|(-A_h)^{\frac{1}{2}}I_h\mu_t e^n\|_{l^2}^2+(h^4+\tau^2)^2\right)\\&\le C\left(\|\delta_x^+\eta^n\|_{l^2}^2+\|\delta_x^+e^n\|_{l^2}^2+\|e^{n+1}\|_{l^2}^2+(h^4+\tau^2)^2\right)\\&\le C\left((h^4+\tau^2)^2+\|\delta_x^+e^n\|_{l^2}^2+\|\delta_x^+e^{n+1}\|_{l^2}^2\right).\end{aligned}$$

Similarly, we have

$$\begin{aligned}\left|\langle\xi^n,\mathcal{L}^n\rangle\right|&\le\left|\langle\xi^n,-\frac{1}{2}\Delta_h I_h\mu_t e^n\rangle\right|+\left|\langle\xi^n,V\mu_t e^n\rangle\right|\\&\le C\left(\|\delta_x^+\xi^n\|_{l^2}^2+\|\delta_x^+e^n\|_{l^2}^2+\|\delta_x^+e^{n+1}\|_{l^2}^2+\|e^n\|_{l^2}^2+\|e^{n+1}\|_{l^2}^2\right)\\&\le C\left((h^4+\tau^2)^2+\|\delta_x^+e^n\|_{l^2}^2+\|\delta_x^+e^{n+1}\|_{l^2}^2+\|e^n\|_{l^2}^2+\|e^{n+1}\|_{l^2}^2\right),\end{aligned}$$

where the last inequality holds because of (3.17).

Thus, we have

$$|\mathrm{Im}\langle\xi^n+\eta^n,\mathcal{L}^n\rangle|\le C(h^4+\tau^2)^2+\mathcal{E}(e^{n+1})+\mathcal{E}(e^n).$$

Combing the above inequalities, we get

$$\mathcal{E}(e^{n+1})-\mathcal{E}(e^n)\le C\tau\left[(h^4+\tau^2)^2+\mathcal{E}(e^{n+1})+\mathcal{E}(e^n)\right].$$

Then there exists $\tau_0>0$, when $0<\tau\le\tau_0$, by Gronwall inequality,

$$\mathcal{E}(e^n)\le C(h^4+\tau^2)^2,\qquad 0\le n\le\frac{T}{\tau},$$

which, together with Theorem 3.1, finishes the proof of Theorem 2.1. $\square$

Remark 3.4. If we consider the general SPS with local term $|\psi|^{\frac{2}{d}}$, Theorem 2.1 still holds true. We refer to [1] on how to deal with the local term.

4 Error estimates for the SICFD method

In this section, we present optimal error estimate for the SICFD method (2.13)-(2.15) with initial value (2.11) and Dirichlet boundary condition (2.10) in discrete l^2 and H^1 norm.

First, we prove the solvability and uniqueness of the SICFD method solution.

Lemma 4.1 (Solvability and uniqueness of the SICFD method)**.** *Under assumptions (A) and (B), for any initial value $\psi^0\in X_M$, there exists a unique solution $\psi^n\in X_M$ of* (2.14)-(2.15) *for $n=1$ and* (2.13) *for $n>1$.*

Proof. The lemma holds true for $n=1$. First, we prove the uniqueness of (2.13). Given $\psi^n,\psi^{n-1}\in X_M$, suppose there exist two solutions $u,v\in X_M$, i.e.,

$$i\frac{u_j-\psi_j^{n-1}}{2\tau}=-\frac{1}{2}\left[\Delta_h I_h\left(\frac{u+\psi^{n-1}}{2}\right)\right]_j+V_j\frac{u_j+\psi_j^{n-1}}{2}+\beta\Phi_j^n\psi_j^n, \tag{4.1}$$

$$i\frac{v_j-\psi_j^{n-1}}{2\tau}=-\frac{1}{2}\left[\Delta_h I_h\left(\frac{v+\psi^{n-1}}{2}\right)\right]_j+V_j\frac{v_j+\psi_j^{n-1}}{2}+\beta\Phi_j^n\psi_j^n. \tag{4.2}$$

Set $w=u-v$ and subtract (4.2) from (4.1), we have

$$i\frac{w_j}{\tau}=-\frac{1}{2}[\Delta_h I_h w]_j+V_j w_j. \tag{4.3}$$

Multiply both sides of (4.3) by $\overline{w_j}h$ and take imaginary parts of summation over $j\in\mathcal{T}_M$, we get $\|w\|_{l^2}=0$ which implies $u=v$, thus the uniqueness of the solution is proved.

For the solvability, we follow similar process as CNCFD method. Eq. (2.13) can be rewritten as

$$i\psi_j^{n+1}+\frac{\tau}{2}\left[\Delta_h I_h\psi^{n+1}\right]_j-\tau V_j\psi_j^{n+1}+\chi_j=0,$$

where

$$\chi_j=-i\psi_j^{n-1}+\frac{\tau}{2}\left[\Delta_h I_h\psi^{n-1}\right]_j-\tau V_j\psi_j^{n-1}-2\beta\tau\,\Phi_j^n\psi_j^n.$$

Define map $G\colon u\in X_M\rightarrow G(u)\in X_M$ as

$$G(u)=iu_j+\frac{\tau}{2}[\Delta_h I_h u]_j-\tau V_j u_j+\chi_j.$$

The map G is continuous from X_M to X_M and satisfies

$$|\mathrm{Im}\langle G(u),u\rangle|=\big|\|u\|_{l^2}^2+\mathrm{Im}\langle\chi,u\rangle\big|\geq\|u\|_{l^2}^2-\|\chi\|_{l^2}\|u\|_{l^2},$$

which implies

$$\lim_{\|u\|_{l^2}\to\infty}\frac{|\langle G^n(u),u\rangle|}{\|u\|_{l^2}}=\infty.$$

Thus G^n is surjective according to theorem in [13], that is to say, there exists a solution $u_0\in X_M$ satisfying $G^n(u_0)=0$. $\square$

Define local truncation error function η^n for SICFD method as

$$\eta_j^n = i\delta_t\psi(x_j,t_n) + \frac{1}{2}\left[\Delta_h I_h\Big(\frac{\psi(\cdot,t_{n+1})+\psi(\cdot,t_{n-1})}{2}\Big)\right]_j$$
$$-V(x_j)\frac{\psi(x_j,t_{n+1})+\psi(x_j,t_{n-1})}{2} - \beta\left[-\Delta_h^{-1}I_h|\psi(\cdot,t_n)|^2\right]_j\psi(x_j,t_n), \quad n>1, \tag{4.4}$$

and

$$\eta_j^0 = i\delta_t^+\psi(x_j,0) - \left[-\frac{1}{2}\Big(\Delta_h I_h\psi^{(1)}\Big)_j + V(x_j)\psi_j^{(1)} + \beta\Phi_j^{(1)}\psi_j^{(1)}\right], \quad j\in\mathcal{T}_M, \tag{4.5}$$

with

$$\psi_j^{(1)} = \psi_0(x_j) - i\frac{\tau}{2}\left[-\frac{1}{2}\Big(\Delta_h I_h\psi(\cdot,0)\Big)_j + V(x_j)\psi_0(x_j) + \beta\Phi_j^0\psi_0(x_j)\right], \quad j\in\mathcal{T}_M.$$

Then we have

Lemma 4.2 (Local truncation error)**.** *Under assumptions (A) and (B), the local truncation error η^n satisfies*

$$\|\eta^n\|_{l^\infty} \le C(h^4+\tau^2), \quad 0\le n\le\frac{T}{\tau}-1, \qquad \|\delta_x^+\eta^0\|_{l^\infty}\le C(h^3+\tau), \quad \textit{for } \tau\le Ch, \tag{4.6}$$
$$\|\delta_x^+\eta^n\|_{l^\infty} \le C(h^4+\tau^2), \quad 1\le n\le\frac{T}{\tau}-1. \tag{4.7}$$

Proof. When $n=0$, we have

$$\psi_j^{(1)} = \psi(x_j,\tau/2) + i\frac{\tau}{2}\eta_j^{(1)}, \quad j\in\mathcal{T}_M,$$

where truncation error $\eta_j^{(1)}, j\in\mathcal{T}_M$ satisfies

$$\eta_j^{(1)} = i\frac{\psi(x_j,\tau/2)-\psi_0(x_j)}{\tau/2} + \frac{1}{2}[\Delta_h\psi_0]_j - V_j\psi_0(x_j) - \beta\Phi_j^0\psi_0(x_j)$$
$$= \frac{i}{\tau/2}\int_0^\tau(\tau-s)\partial_t^2\psi(x_j,s)\,\mathrm{d}s + \left[B_h^{-1}I_h\mathcal{R}^0(\psi)\right]_j - \beta\left[A_h^{-1}I_h\mathcal{R}^0(\Phi)\right]_j\psi_0(x_j).$$

We can conclude that $\|\eta^{(1)}\|_{l^\infty} = \mathcal{O}(h^4+\tau)$. Then

$$\eta_j^0 = i\frac{\psi(x_j,\tau)-\psi_0(x_j)}{\tau} + \frac{1}{2}\left[\Delta_h I_h\psi^{(1)}\right]_j - V(x_j)\psi_j^{(1)} - \beta\Phi_j^{(1)}\psi_j^{(1)}$$
$$= \mathcal{Q}_j^{\frac{1}{2}}(\psi) + \frac{i\tau}{4}\left[\Delta_h I_h\eta^{(1)}\right]_j + \frac{1}{2}\left[B_h^{-1}I_h\mathcal{R}^{\frac{1}{2}}(\psi)\right]_j - \frac{i\tau}{2}V(x_j)\eta_j^{(1)}$$
$$-\frac{i\tau}{2}\beta\Phi_j^{(1)}\eta_j^{(1)} + \beta\psi(x_j,\tau/2)\big(\Phi(x_j,\tau/2)-\Phi_j^{(1)}\big).$$

By a similar argument, we can obtain $\|\eta^0\|_{l^\infty} \le C(h^4+\tau^2)$ and

$$|\delta_x^+\eta_j^0| \le C\frac{\|\eta_j^0\|_{l^\infty}}{h} \le C(h^3+\tau), \qquad j=0,1,\cdots,M-1$$

for $\tau \le Ch$. Thus, we prove local truncation error for $n=0$. While for $n>1$, by Taylor formula with integral remainder, we get

$$\eta_j^n = \mathcal{Q}_j^{n+\frac{1}{2}}(\psi) + \frac{1}{2}\left[B_h^{-1}I_h\frac{\mathcal{R}^{n+1}(\psi)+\mathcal{R}^{n-1}(\psi)}{2}\right]_j + \frac{1}{2}\mathcal{P}_j^{n+\frac{1}{2}}(\partial_x^2\psi)$$
$$-V(x_j)\mathcal{P}_j^{n+\frac{1}{2}}(\psi) - \beta\left[A_h^{-1}I_h\mathcal{R}^n(\Phi)\right]_j\psi(x_j,t_n).$$

Thus

$$|\eta_j^n| \le Ch^4(\|\partial_x^6\psi\|_{L^\infty} + \|\partial_x^4\psi\|_{L^\infty}\|\psi\|_{L^\infty}) + C\tau^2(\|\partial_t^2\psi\|_{L^\infty} + \|\partial_t^3\psi\|_{L^\infty} + \|\partial_t^2\partial_x^2\psi\|_{L^\infty}),$$

which implies $\|\eta^n\|_{l^\infty} \le C(h^4+\tau^2)$, $1 \le n \le \frac{T}{\tau}-1$. Similarly, we get

$$\delta_x^+\eta_j^n = \delta_x^+\mathcal{Q}_j^{n+\frac{1}{2}}(\psi) + \frac{1}{2}\delta_x^+\left[B_h^{-1}I_h\frac{\mathcal{R}^{n+1}(\psi)+\mathcal{R}^{n-1}(\psi)}{2}\right]_j + \frac{1}{2}\delta_x^+\mathcal{P}_j^{n+\frac{1}{2}}(\partial_x^2\psi)$$
$$+\delta_x^+(V(x_j)\mathcal{P}_j^{n+\frac{1}{2}}(\psi)) - \beta\delta_x^+\left(\left[A_h^{-1}I_h\mathcal{R}^n(\Phi)\right]_j\psi(x_j,t_n)\right),$$

from which we obtain

$$|\delta_x^+\eta_j^n| \le Ch^4(\|\partial_x^7\psi\|_{L^\infty} + \|\partial_x^5\psi\|_{L^\infty}\|\psi\|_{L^\infty} + \|\partial_x^4\psi\|_{L^\infty}\|\partial_x\psi\|_{L^\infty} + \|\partial_x^3\psi\|_{L^\infty}\|\partial_x^2\psi\|_{L^\infty})$$
$$+C\tau^2(\|\partial_x\partial_t^2\psi\|_{L^\infty} + \|\partial_x\partial_t^3\psi\|_{L^\infty} + \|\partial_t^2\partial_x^3\psi\|_{L^\infty}), \qquad 1 \le n \le \frac{T}{\tau}-1,$$

where the nonlocal term $A_h^{-1}I_h\mathcal{R}^n(\Phi)$ and $B_h^{-1}I_h(\mathcal{R}^{n+1}(\psi)+\mathcal{R}^{n-1}(\psi))$ are dealt with similarly. Therefore, we prove the local error estimate. □

Theorem 4.1 (l^2 norm estimate)**.** *Under assumptions (A) and (B), there exist $h_0>0$ and $\tau_0>0$, such that for any $0<h<h_0$, $0<\tau<\tau_0$ and $\tau \le h$, we have*

$$\|e^n\|_{l^2} \le C(h^4+\tau^2), \qquad \|\psi^n\|_{l^\infty} \le 1+M_1, \qquad 1 \le n \le \frac{T}{\tau}. \tag{4.8}$$

Proof. If $\|e^n\|_{l^2} \le C(h^4+\tau^2)$ is known, from $e_j^n = \psi(x_j,t_n)-\psi_j^n$, we can get

$$\|\psi^n\|_{l^\infty} \le \|\psi(\cdot,t_n)\|_{L^\infty} + \|e^n\|_{l^\infty} \le M_1 + h^{-\frac{1}{2}}\|e^n\|_{l^2}$$
$$\le M_1 + C(h^{\frac{7}{2}}+h^{\frac{3}{2}}) \le M_1+1$$

for sufficiently small h and τ. Therefore we only need to verify $\|e^n\|_{l^2}\le C(h^4+\tau^2)$.

We will use mathematical induction to prove the l^2 norm estimate. The initial inequality $\|e^1\|_{l^2}\le C(h^4+\tau^2)$ holds true spontaneously. Now we assume that (4.8) is valid for $0\le n\le m-1\le \frac{T}{\tau}-1$, then we need to confirm that it is still valid when $n=m$. Subtracting (4.4) from (2.13), we have

$$i\delta_t^+ e_j^n=\mathcal{L}_j^n+\xi_j^n+\eta_j^n, \tag{4.9}$$

where

$$\begin{aligned}
&\mathcal{L}_j^n=-\frac{1}{2}\left[\Delta_h I_h\frac{e^{n+1}+e^{n-1}}{2}\right]_j+V_j\frac{e_j^{n+1}+e_j^{n-1}}{2}, && j=1,2,\cdots,M-1,\quad n\ge 0,\\
&\xi_j^n=\beta\left[-\Delta_h^{-1}I_h|\psi(\cdot,t_n)|^2\right]_j\psi(x_j,t_n)-\beta\left[-\Delta_h^{-1}I_h|\psi^n|^2\right]_j\psi_j^n, && j=1,2,\cdots,M-1,\quad n\ge 0.
\end{aligned}$$

Similarly, noticing (3.4) and (3.17), we have

$$\begin{aligned}
&\|\xi^n\|_{l^2}^2\le C\|e^n\|_{l^2}^2, && 1\le n\le m-1,\\
&\|\delta_x^+\xi^n\|_{l^2}^2\le C\left((h^4+\tau^2)^2+\|\delta_x^+e^n\|_{l^2}^2+\|e^n\|_{l^2}^2\right), && 1\le n\le m-1.
\end{aligned}\tag{4.10}$$

Take imaginary parts of the summation on each sides after multiplying (4.9) by $\overline{e_j^{n+1}+e_j^{n-1}}h$, by Cauchy-Schwartz inequality, we have

$$\begin{aligned}
\|e^{n+1}\|_{l^2}^2-\|e^{n-1}\|_{l^2}^2&=2\tau\mathrm{Im}\langle\xi^n+\eta^n,e^{n+1}+e^{n-1}\rangle\\
&\le 2\tau\left[\|e^{n+1}\|_{l^2}^2+\|e^{n-1}\|_{l^2}^2+\|\xi\|_{l^2}^2+\|\eta^n\|_{l^2}^2\right]\\
&\le C\tau(h^4+\tau^2)^2+2\tau(\|e^{n+1}\|_{l^2}^2+\|e^{n-1}\|_{l^2}^2)+C\tau\|e^n\|_{l^2}^2.
\end{aligned}$$

Noticing $e^0=0$ and $\|e^1\|_{l^2}^2\le C(h^4+\tau^2)^2$, when $\tau\le\frac{1}{4}$, sum up the above inequality from $n=1$ to $n=m-1$ and rewrite the inequality, we have

$$\frac{1}{2}(\|e^m\|_{l^2}^2+\|e^{m-1}\|_{l^2}^2)\le C(m-1)\tau(h^4+\tau^2)^2+\|e^1\|_{l^2}^2+(C\tau+4\tau)\sum_{k=1}^{m-1}\|e^k\|_{l^2}^2,$$

which implies

$$\|e^m\|_{l^2}^2\le 2C\Big(T+1\Big)(h^4+\tau^2)^2+2(C\tau+4\tau)\sum_{k=1}^{m-1}\|e^k\|_{l^2}^2. \tag{4.11}$$

Apply Gronwall inequality to (4.11), we get

$$\begin{aligned}
\|e^m\|_{l^2}^2&\le 2C\Big(T+1\Big)(h^4+\tau^2)^2e^{2(C\tau+4\tau)m}\\
&\le 2C\Big(T+1\Big)e^{2(C+4)T}(h^4+\tau^2)^2.
\end{aligned}$$

Hence, the proof is finished. □

Then we continue to prove Theorem 2.2.

Proof. As is stated before, $e^0=0$ and thus Theorem 2.2 holds true.

$$|\delta_x^+ e_j^1|=|\delta_x^+(\psi(x_j,\tau)-\psi_j^1)|=|-i\tau\delta_x^+\eta_j^0|\le C\tau(h^3+\tau)\le C(h^4+\tau^2),$$

which implies Theorem 2.2 is true for $n=1$. Rewrite Eq. (4.9) as

$$e_j^{n+1}-e_j^{n-1}=-2i\tau(\mathcal{L}_j^n+\xi_j^n+\eta_j^n).$$

Multiply both sides of (4.9) by $2h\,\overline{e_j^{n+1}-e_j^{n-1}}$ and sum up both sides over index $j\in\mathcal{T}_M$, after taking real parts, we have

$$\begin{aligned}\mathcal{E}(e^{n+1})-\mathcal{E}(e^{n-1})&=-2\,\mathrm{Re}\langle\xi^n+\eta^n,e^{n+1}-e^{n-1}\rangle\\&=-2\,\mathrm{Re}\langle\xi^n+\eta^n,-2i\tau(\mathcal{L}^n+\xi^n+\eta^n)\rangle\\&=4\tau\,\mathrm{Im}\langle\xi^n+\eta^n,\mathcal{L}^n\rangle.\end{aligned}$$

By Cauchy-Schwartz inequality and equivalent energy inequalities, we have

$$\begin{aligned}|\langle\xi^n,\mathcal{L}^n\rangle|&\le C((h^4+\tau^2)^2+\|\delta_x^+e^{n-1}\|_{l^2}^2+\|\delta_x^+e^n\|_{l^2}^2+\|\delta_x^+e^{n+1}\|_{l^2}^2),\\|\langle\eta^n,\mathcal{L}^n\rangle|&\le C((h^4+\tau^2)^2+\|\delta_x^+e^{n-1}\|_{l^2}^2+\|\delta_x^+e^n\|_{l^2}^2+\|\delta_x^+e^{n+1}\|_{l^2}^2),\end{aligned}$$

for $1\le n\le\frac{T}{\tau}-1$. Thus, we can get

$$\begin{aligned}\mathcal{E}(e^{n+1})-\mathcal{E}(e^{n-1})&\le C\tau(h^4+\tau^2)^2+\tau\left[\|\delta_x^+e^{n-1}\|_{l^2}^2+\|\delta_x^+e^n\|_{l^2}^2+\|\delta_x^+e^{n+1}\|_{l^2}^2\right]\\&\le C\tau(h^4+\tau^2)^2+\tau\left[\mathcal{E}(e^{n-1})+\mathcal{E}(e^n)+\mathcal{E}(e^{n+1})\right].\end{aligned}$$

Then sum up the above inequality from $n=1$ to $n=m-1\le\frac{T}{\tau}-1$, we have, for $\tau\le\frac{1}{4}$ and $\tau\le h$,

$$\frac{1}{2}(\mathcal{E}(e^m)-\mathcal{E}(e^{m-1}))\le C(T+1)(h^4+\tau^2)^2+C\tau\sum_{k=1}^{m-1}\mathcal{E}(e^k),\qquad 1\le m\le\frac{T}{\tau}.$$

Apply discrete Gronwall inequality to the above inequality, we get

$$\frac{1}{2}\|\delta_x^+e^n\|_{l^2}^2\le\mathcal{E}(e^m)\le C(T+1)e^{CT}(h^4+\tau^2)^2.$$

The proof for Theorem 2.2 is complete. □

Lemma 4.3 (l^∞ norm estimate)**.** *For the SICFD method, under assumptions (A) and (B), the l^∞ norm is of order $\mathcal{O}(h^4+\tau^2)$.*

Proof. Since we have obtained $\|\delta_x^+ e^n\|_{l^2} = \mathcal{O}(h^4+\tau^2)$, then the l^∞ norm is valid immediately by inequality (3.2). $\square$

Remark 4.1. If we consider the general SPS with local term $|\psi|^{\frac{2}{d}}$, Theorem 2.2 of the l^2 and H^1 error estimates holds true. We refer to [1] on how to deal with the local term. Compared with (2.8), the SICFD scheme does not require to solve any nonlinear equation, thus it takes up less computational cost and is more appropriate to be extended to higher dimensions.

5 Numerical results

In this section, we present numerical results to verify our error estimates. We choose symmetric computation domain with/without external potential $V(x) = \frac{x^2}{2}$. Let ψ_e be the numerical 'exact' solution obtained with fine mesh h and small time step $\tau = h^2$ at time $T = 0.5$ and $\psi_{h,\tau}$ be the numerical solution with mesh size h and time step τ. Let $e_{h,\tau} = \psi_e - \psi_{h,\tau}$ denote the error function. The initial value is chosen as $\psi_0(x) = e^{-x^2/2}\pi^{-1/4}$. The numerical 'exact' solution is obtained with $h = \frac{1}{256}, \tau = h^2$ on $[-16,16]$.

First, we test the second order temporal accuracy by choosing different time step τ with uniform fine mesh size $h = 1/256$ on interval $[-16,16]$ and the temporal convergence rate is defined as $\log_2(\|e_{h,\tau}\|/\|e_{h,\frac{\tau}{2}}\|)$ with corresponding discrete norm. Table 1, 2, 3 and 4 show errors $\|e\|_{l^2}, \|\delta_x^+ e\|_{l^2}$ and $\|e\|_{l^\infty}$ for CNCFD and SICFD schemes with $\beta = \pm 5$ under external potential $V(x) = 0$ or $V(x) = x^2/2$.

Next, we verify the fourth order spatial accuracy by choosing appropriate mesh size

Table 1: Temporal error analysis of CNCFD at time $T = 0.5$ for different Poisson constant β without external potential, i.e., $V(x) = 0$.

		$\tau=2^{-8}$	$\tau=2^{-9}$	$\tau=2^{-10}$	$\tau=2^{-11}$
$\beta=5$	$\|e\|_{l^2}$	3.720E-03	9.305E-04	2.326E-04	5.811E-05
	Rate	1.999	2.000	2.001	
	$\|\delta_x^+ e\|_{l^2}$	4.752E-03	1.189E-03	2.972E-04	7.426E-05
	Rate	1.999	2.000	2.001	
	$\|e\|_{l^\infty}$	2.447E-03	6.119E-04	1.530E-04	3.821E-05
	Rate	2.000	2.000	2.001	
$\beta=-5$	$\|e\|_{l^2}$	3.633E-03	9.088E-04	2.272E-04	5.676E-05
	Rate	1.999	2.000	2.001	
	$\|\delta_x^+ e\|_{l^2}$	3.131E-03	7.833E-04	1.958E-04	4.892E-05
	Rate	1.999	2.000	2.001	
	$\|e\|_{l^\infty}$	3.024E-03	7.565E-04	1.891E-04	4.724E-05
	Rate	1.999	2.000	2.001	

Table 2: Temporal error analysis of CNCFD at time $T=0.5$ for different Poisson constant β without external potential, i.e., $V(x)=\frac{x^2}{2}$.

		$\tau=2^{-8}$	$\tau=2^{-9}$	$\tau=2^{-10}$	$\tau=2^{-11}$
$\beta=5$	$\|e\|_{l^2}$	3.907E-03	9.774E-04	2.443E-04	6.104E-05
	Rate	1.999	2.000	2.001	
	$\|\delta_x^+ e\|_{l^2}$	3.857E-03	9.650E-04	2.412E-04	6.0268e-05
	Rate	1.999	2.000	2.001	
	$\|e\|_{l^\infty}$	2.650E-03	6.627E-04	1.657E-04	4.138E-05
	Rate	2.000	2.000	2.001	
$\beta=-5$	$\|e\|_{l^2}$	3.564E-03	8.914E-04	2.228E-04	5.567E-05
	Rate	1.999	2.000	2.001	
	$\|\delta_x^+ e\|_{l^2}$	3.618E-03	9.050E-04	2.2623E-04	5.653E-05
	Rate	1.999	2.000	2.001	
	$\|e\|_{l^\infty}$	3.177E-03	7.946E-04	1.987E-04	4.963E-05
	Rate	1.999	2.000	2.001	

Table 3: Temporal error analysis of SICFD at time $T=0.5$ for different Poisson constant β without external potential, i.e., $V(x)=0$.

		$\tau=2^{-8}$	$\tau=2^{-9}$	$\tau=2^{-10}$	$\tau=2^{-11}$
$\beta=5$	$\|e\|_{l^2}$	6.522E-03	1.629E-03	4.069E-04	1.014E-04
	Rate	2.001	2.001	2.004	
	$\|\delta_x^+ e\|_{l^2}$	7.098E-03	1.771E-03	4.423E-04	1.102E-04
	Rate	2.003	2.002	2.005	
	$\|e\|_{l^\infty}$	4.455E-03	1.113E-03	2.780E-04	6.931E-05
	Rate	2.001	2.001	2.004	
$\beta=-5$	$\|e\|_{l^2}$	7.930E-03	1.977E-03	4.935E-04	1.230E-04
	Rate	2.004	2.002	2.005	
	$\|\delta_x^+ e\|_{l^2}$	7.382E-03	1.840E-03	4.593E-04	1.145E-04
	Rate	2.004	2.002	2.005	
	$\|e\|_{l^\infty}$	6.889E-03	1.717E-03	4.287E-04	1.069E-04
	Rate	2.004	2.002	2.005	

h and time step τ and the convergence rate is defined as $\log_2(\|e_{h,\tau}\|/\|e_{\frac{h}{2},\frac{\tau}{4}}\|)$ with corresponding norm. Tables 5 and 6 show errors $\|e\|_{l^2}, \|\delta_x^+ e\|_{l^2}$ and $\|e\|_{l^\infty}$ for the CNCFD method with Poisson coupling constants $\beta=\pm 5$ under external potential $V(x)=0$ or $V(x)=\frac{x^2}{2}$. Tables 7 and 8 show errors $\|e\|_{l^2}, \|\delta_x^+ e\|_{l^2}$ and $\|e\|_{l^\infty}$ for the SICFD method with coupling Poisson constants $\beta=\pm 5$ under external potential $V(x)=0$ or $V(x)=\frac{x^2}{2}$.

Table 9 lists computation time cost by CNCFD and SICFD with different mesh sizes and time step for repulsive SPS ($\beta=5$) at time $T=1.0$ with/without external potential.

Table 4: Temporal error analysis of SICFD at time $T=0.5$ for different Poisson constant β without external potential, i.e., $V(x)=\frac{x^2}{2}$.

		$\tau=2^{-8}$	$\tau=2^{-9}$	$\tau=2^{-10}$	$\tau=2^{-11}$
$\beta=5$	$\|\|e\|\|_{l^2}$	6.780E-03	1.698E-03	4.243E-04	1.060E-04
	Rate	2.002	2.001	2.001	
	$\|\|\delta_x^+ e\|\|_{l^2}$	6.127E-03	1.529E-03	3.820E-04	9.542E-05
	Rate	2.003	2.001	2.001	
	$\|\|e\|\|_{l^\infty}$	4.840E-03	1.209E-03	3.021E-04	7.548E-05
	Rate	2.001	2.000	2.001	
$\beta=-5$	$\|\|e\|\|_{l^2}$	8.206E-03	2.045E-03	5.104E-04	1.272E-04
	Rate	2.005	2.002	2.005	
	$\|\|\delta_x^+ e\|\|_{l^2}$	8.872E-03	2.210E-03	5.517E-04	1.375E-04
	Rate	2.005	2.002	2.005	
	$\|\|e\|\|_{l^\infty}$	7.535E-03	1.878E-03	4.687E-04	1.168E-04
	Rate	2.005	2.002	2.005	

Table 5: Error analysis of CNCFD at time $T=0.5$ for different Poisson constant β without external potential, i.e., $V(x)=0$.

		$h=1/16$ $\tau=2^{-8}$	$h=1/32$ $\tau=2^{-10}$	$h=1/64$ $\tau=2^{-12}$	$h=1/128$ $\tau=2^{-14}$
$\beta=5$	$\|\|e\|\|_{l^2}$	3.465E-02	2.171E-03	1.352E-04	7.964E-06
	Rate	3.996	4.005	4.086	
	$\|\|\delta_x^+ e\|\|_{l^2}$	4.074E-02	2.558E-03	1.593E-04	9.380E-06
	Rate	3.994	4.005	4.086	
	$\|\|e\|\|_{l^\infty}$	2.235E-02	1.399E-03	8.716E-05	5.132E-06
	Rate	3.997	4.005	4.086	
$\beta=-5$	$\|\|e\|\|_{l^2}$	3.444E-02	2.159E-03	1.345E-04	7.919E-06
	Rate	3.996	4.005	4.086	
	$\|\|\delta_x^+ e\|\|_{l^2}$	2.965E-02	1.859E-03	1.158E-04	6.820E-06
	Rate	3.995	4.005	4.086	
	$\|\|e\|\|_{l^\infty}$	2.849E-02	1.786E-03	1.113E-04	6.552E-06
	Rate	3.995	4.005	4.086	

The algorithm was carried out by Linux (version 3.0.0-16) MATLAB (version 7.8.0.347 (R2009a)) on Intel CPU (i3-530). Fig. 1 depicts the long time evolution of the errors of discrete mass and energy for SICFD scheme with mesh size $h=1/16$ when external potential $V(x)=0$ and Poisson constant $\beta=5$.

Based on numerical results shown and not shown here, we can draw the following conclusions: (i) Tables 1-8 confirm the $\mathcal{O}(h^4+\tau^2)$ convergence estimates for the CNCFD and SICFD scheme in l^2, H^1 and l^∞ discrete norms. (ii) The CNCFD scheme conserves

Table 6: Error analysis of CNCFD at time $T=0.5$ for different Poisson constant β with external potential $V(x)=\frac{x^2}{2}$.

		$h=1/16$ $\tau=2^{-8}$	$h=1/32$ $\tau=2^{-10}$	$h=1/64$ $\tau=2^{-12}$	$h=1/128$ $\tau=2^{-14}$
$\beta=5$	$\|\|e\|\|_{l^2}$	3.558E-02	2.230E-03	1.389E-04	8.178E-06
	Rate	3.996	4.005	4.086	
	$\|\|\delta_x^+ e\|\|_{l^2}$	3.234E-02	2.029E-03	1.264E-04	7.440E-06
	Rate	3.995	4.005	4.086	
	$\|\|e\|\|_{l^\infty}$	2.382E-02	1.492E-03	9.292E-05	5.471E-06
	Rate	3.997	4.005	4.086	
$\beta=-5$	$\|\|e\|\|_{l^2}$	3.410E-02	2.138E-03	1.332E-04	7.840E-06
	Rate	3.996	4.005	4.086	
	$\|\|\delta_x^+ e\|\|_{l^2}$	3.547E-02	2.226E-03	1.386E-04	8.163E-06
	Rate	3.995	4.005	4.086	
	$\|\|e\|\|_{l^\infty}$	3.019E-02	1.893E-03	1.179E-04	6.945E-06
	Rate	3.995	4.005	4.086	

Table 7: Error analysis of SICFD at time $T=0.5$ for different Poisson constant β without external potential, i.e., $V(x)=0$.

		$h=1/16$ $\tau=2^{-8}$	$h=1/32$ $\tau=2^{-10}$	$h=1/64$ $\tau=2^{-12}$	$h=1/128$ $\tau=2^{-14}$
$\beta=5$	$\|\|e\|\|_{l^2}$	6.682E-02	4.108E-03	2.551E-04	1.499E-05
	Rate	4.024	4.010	4.089	
	$\|\|\delta_x^+ e\|\|_{l^2}$	7.388E-02	4.532E-03	2.814E-04	1.653E-05
	Rate	4.027	4.010	4.089	
	$\|\|e\|\|_{l^\infty}$	4.371E-02	2.688E-03	1.669E-04	9.806E-06
	Rate	4.023	4.009	4.089	
$\beta=-5$	$\|\|e\|\|_{l^2}$	7.328E-02	4.501E-03	2.796E-04	1.643E-05
	Rate	4.025	4.009	4.089	
	$\|\|\delta_x^+ e\|\|_{l^2}$	1.657E-01	4.023E-03	2.498E-04	1.468e-05
	Rate	4.029	4.009	4.089	
	$\|\|e\|\|_{l^\infty}$	6.209E-02	3.810E-03	2.366E-04	1.391E-05
	Rate	4.027	4.009	4.089	

discrete mass and energy analytically, however, as stated in [1], we have to solve the nonlinear equation accurate enough (up to machine accuracy or nearby) so as to keep the conservation laws numerically. (iii) From Fig. 1, we can observe oscillatory error evolution phenomenon which is similar to that in [1]. (iv) Table 9 shows that the efficiency of SICFD is superior to that of CNCFD with/without external potential. All the linear systems involved in both schemes are accelerated by DST and this make the computation

Table 8: Error analysis of SICFD at time $T=0.5$ for different Poisson constant β without external potential, i.e., $V(x)=\frac{x^2}{2}$.

		$h=1/16$ $\tau=2^{-8}$	$h=1/32$ $\tau=2^{-10}$	$h=1/64$ $\tau=2^{-12}$	$h=1/128$ $\tau=2^{-14}$
$\beta=5$	$\|\|e\|\|_{l^2}$	6.817E-02	4.189E-03	2.601E-04	1.528E-05
	Rate	4.024	4.010	4.089	
	$\|\|\delta_x^+ e\|\|_{l^2}$	5.991E-02	3.674E-03	2.281E-04	1.340E-05
	Rate	4.027	4.010	4.089	
	$\|\|e\|\|_{l^\infty}$	4.663E-02	2.867E-03	1.780E-04	1.046E-05
	Rate	4.024	4.009	4.089	
$\beta=-5$	$\|\|e\|\|_{l^2}$	7.453E-02	4.578E-03	2.843E-04	1.671E-05
	Rate	4.025	4.009	4.089	
	$\|\|\delta_x^+ e\|\|_{l^2}$	8.045E-02	4.930E-03	3.062E-04	1.799E-05
	Rate	4.028	4.010	4.089	
	$\|\|e\|\|_{l^\infty}$	6.706E-02	4.115E-03	2.556E-04	1.502E-05
	Rate	4.027	4.010	4.089	

Table 9: Computation time (in seconds) comparison of CNCFD and SICFD scheme at time $T=1.0$ for Poisson constant $\beta=5$ with/without external potential $V(x)$.

		$h=1/16$ $\tau=2^{-8}$	$h=1/32$ $\tau=2^{-10}$	$h=1/64$ $\tau=2^{-12}$	$h=1/128$ $\tau=2^{-14}$
$V(x)=\frac{x^2}{2}$	CNCFD	3.837	15.039	83.029	577.870
	SICFD	1.289	6.140	37.554	284.854
$V(x)=0$	CNCFD	3.831	15.233	82.103	595.886
	SICFD	0.376	2.228	15.106	110.759

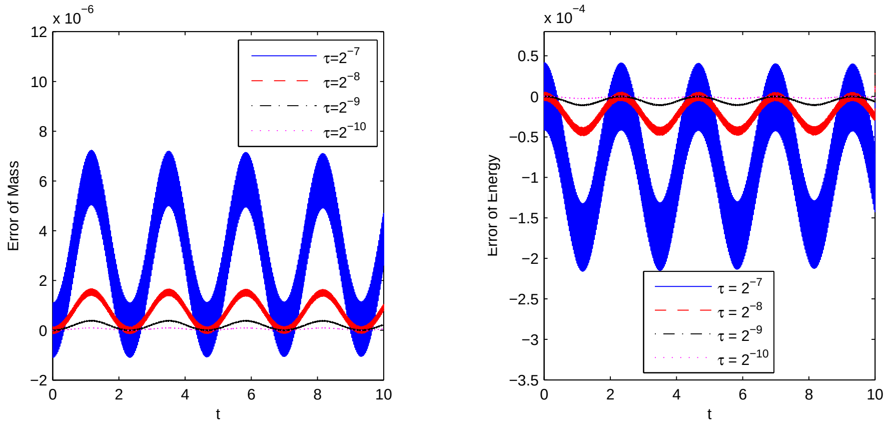

Figure 1: Evolution of the errors of the discrete mass and energy for SICFD scheme with mesh size $h=1/16$ when external potential $V(x)=0$ and Poisson constant $\beta=5$.

time depends almost linearly on mesh size h. The DST accelerated linear system solver can be extended to higher dimensions directly which would still preserve the linear dependency of computation time and mesh size.

6 Conclusions

We presented error analysis of two compact finite difference schemes, i.e., the conservative Crank-Nicolson compact finite difference scheme and the semi-implicit compact finite difference scheme, for the Schrödinger-Poisson system in a bounded domain under proper regularity assumptions on wave function ψ and external potential $V(x)$. Both of the schemes are of order $\mathcal{O}(h^4+\tau^2)$ in discrete l^2, H^1 and l^∞ norms. We analyzed the local truncation error of the compact finite difference for the second derivative and Poisson potential, which is nonlocal, by the discrete maximum principle of the elliptic equation and properties of related approximation matrix. We analyzed the nonlocal approximation term in the local truncation error and global error with Taylor formula with integral remainders. In the proof of CNCFD scheme, we used a Lipschitz function to approximate the nonlinearity so as to obtain l^2 norm estimate and by inverse inequality to get a *priori* bound in l^∞ norm; for SICFD scheme, mathematical induction was used. Extensive numerical results were reported in the last section to confirm our error estimates. In practice, the CNCFD conserves the mass and energy quite well in the discretized level when $\tau=\mathcal{O}(h^2)$ but at each step we have to solve a nonlinear difference equation which could be quite expensive in view of computation time cost, especially in 2-d and 3-d. The SICFD scheme is also unconditional stable and it conserves the mass and energy well and only a linear system is required to be solved each step. In addition, both scheme can be solved within at $\mathcal{O}(M\log(M))$ time/operations with the help of Discrete Sine Transform (DST). The CNCFD and SICFD methods could be extended to Schrödinger-Poisson-Slater system directly.

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