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CONSERVATION LAWS AND ERROR ESTIMATES OF SEVERAL CLASSICAL FINITE DIFFERENCE SCHEMES FOR THE NONLINEAR SCHRÖDINGER/GROSS-PITAEVSKII EQUATION*

TINGCHUN WANG†, WEN ZHANG‡, AND CHENYI ZHU§

Abstract. In this paper, several classical implicit finite difference schemes for solving the nonlinear Schrödinger/Gross Pitaevskii (NLS/GP) equation are revisited and analyzed. By introducing a kind of energy functionals, these schemes are proved to preserve the total energy in the discrete sense. Besides the standard energy method, a 'cut-off' technique and a 'lifting' technique are adopted to establish the optimal point-wise error estimates without any restriction on the grid ratios. Numerical results are reported to verify the theoretical analysis.

Key words. NLS/GP equation, finite difference scheme, energy conservation, unconditional convergence, error estimate.

Mathematics Subject Classification. 65M06, 65M12.

1. Introduction.

The nonlinear Schrödinger/Gross-Pitaevskii (NLS/GP) equation is widely used to model the phenomena in many physical fields, such as Quantum physics and nonlinear fibers [2, 3, 16, 23, 30]. A serge of interests have been attracted to numerically study the Cauchy problem or initial-boundary value problem of the NLS/GP equation. Extensive numerical methods including the finite difference method [11, 13, 17, 18, 24, 27, 36, 31, 33, 32, 35], finite element method [19], spectral method [7, 8] and polynomial method [6, 20, 25] have been carried out in literature. For the summary of numerical methods of the NLS/GP equation, we refer to [2, 3]. In this paper, we consider the following one-dimensional NLS/GP equation

$$i\partial_t\psi(x,t) + \alpha\partial_{xx}\psi(x,t) + V(x)\psi(x,t) + f(|\psi(x,t)|^2)\psi(x,t) = 0,$$
$$x \in \Omega, \quad t > 0, \tag{1.1}$$

where α is a nonzero constant, Ω is a bounded computational domain in $\mathbb{R}$, the external potential $V = V(x)$ is a known smooth real-valued function, $\psi = \psi(x,t)$ is the unknown complex-valued wave function, $f = f(s)$ is a known monotone function from $\mathbb{R}^+$ to $\mathbb{R}$, which has different forms in different physical problems [11], such as polynomial function $f(s) = s^\mu (\mu > 0)$, exponential function $f(s) = 1 - e^{-s}$, logarithm function $f(s) = \ln(1+s)$ and rational function $f(s) = -\frac{4s}{(1+s)}$. In the practical computation, ones often take a finite computational domain $\Omega = (a,b)$ with $-a, b \gg 0$. In this paper, we numerically study the NLS/GP equation (1.1) with homogeneous boundary condition

$$\psi(a,t) = \psi(b,t) = 0, \quad t > 0, \tag{1.2}$$

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†School of Mathematics and Statistics, Nanjing University of Information Science and Technology, Nanjing, 210044, China (wangtingchun2010@gmail.com).

‡School of Mathematics and Statistics, Nanjing University of Information Science and Technology, Nanjing, 210044, China (1391070923@qq.com).

§School of Mathematics and Statistics, Nanjing University of Information Science and Technology, Nanjing, 210044, China (445848287@qq.com).

and initial condition

$$\psi(x,0)=\varphi(x), \quad x\in[a,b], \tag{1.3}$$

where $\varphi=\varphi(x)$ is a known smooth complex-valued function. It is easy to verify that the initial-boundary value problem (1.1)-(1.3) preserves the total mass

$$M(t):=\int_a^b|\psi(x,t)|^2dx\equiv M(0):=\int_a^b|\varphi(x)|^2dx, \tag{1.4}$$

and energy

$$\begin{aligned}E(t):=&\int_a^b[-\alpha|\partial_x\psi(x,t)|^2+V(x)|\psi(x,t)|^2]dx+\big(F(|\psi(\cdot,t)|^2),1\big)\\ \equiv E(0):=&\int_a^b[-\alpha|\partial_x\varphi(x)|^2+V(x)|\varphi(x)|^2]dx+\big(F(|\varphi|^2),1\big),\end{aligned} \tag{1.5}$$

where $\big(F(|\psi(\cdot,t)|^2),1\big):=\int_a^b F(|\psi(x,t)|^2)dx$ and $F=F(s)$ is one of primitive functions of $f=f(s)$. In [36], the authors pointed out that the nonconservative schemes may easily show nonlinear blow-up, and they presented a new conservative linear difference scheme for the standard cubic nonlinear Schrödinger equation. In [22], Li and Vu-Quoc also said, "...in some areas, the ability to preserve some invariant properties of the original differential equation is a criterion to judge the success of a numerical simulation." However, there is only one finite difference scheme (see the scheme (2.1) in this paper) which is claimed (see [36]) to preserve the total energy of the NLS/GP equation, and there is no reference to prove that the other classical finite difference schemes of the NLS/GP equation could also preserve the total energy in the discrete sense.

Chang, Jia and Sun proposed and discussed several conservative finite difference schemes of the NLS equation in [11], numerical results show that their schemes preserve the total mass and energy in the discrete sense. In [26, 12], the standard Crank-Nicolson (CN) finite difference scheme was proved to be a symplectic scheme. To the best of our knowledge, there is no reference to claim that the CN scheme could preserve the total energy in the discrete sense, and it is hard to obtain the *a priori* estimate of the numerical solution. Especially, Ge and Marsden pointed out in [15] that the symplectic scheme could not preserve the total energy in the discrete sense for a nonlinear Hamiltonian system. By using a creative and technical induction argument as well as the standard energy method, Guo [17] established the error estimate of the standard CN scheme with a rigorous requirement of the grid ratio. To see more numerical results of the NLS/GP equation, we refer to [2, 3].

In this paper, inspired by the approximation of the energy functionals possessed by the equations studied in [21, 2, 9], we introduce a new type of discrete energy functionals to prove that some other classical finite difference schemes for solving the NLS/GP equation could still preserve the total mass and energy in the discrete sense. Besides, by using the standard energy method and a 'cut-off' technique as well as a 'lifting' technique [34], we establish the optimal point-wise error estimates of the numerical solutions without any restriction on the grid ratios.

The remainder of this paper is organized as follows. In Section 2, we list six classical finite difference schemes for the NLS/GP equation and prove that they preserve the total mass and energy in the discrete sense by introducing a kind of discrete energy functionals. In Section 3, we obtain the *a priori* estimates of the numerical solutions and then establish the optimal point-wise error estimates of these classical schemes without any constrain on the grid ratios. In Section 4, we report some numerical results to test our theoretical analysis. Finally, some concise conclusions are drawn in Section 5.

2. Finite difference schemes and conservation laws. In this section, we revisit several classical finite difference schemes (see [2, 11, 17] and references therein) for solving the problem (1.1)-(1.3) and discuss their conservation laws.

For a positive integer N, choose time-step $\tau = T/N$ and denote time steps $t_n = n\tau,\ n = 0, 1, 2, \cdots, N$, where $0 < T < T_{\max}$ with $T_{\max}$ the maximal existing time of the solution; choose mesh size $h = \frac{b-a}{J}$ with J a positive integer and denote grid points as $x_j = a + jh,\ j = 0, 1, \cdots, J$. Denote ψ_j^n and w_j^n be the numerical approximation, and respectively the exact solution of $\psi(x_j, t_n)$ for $j = 0, 1, 2, \cdots, J$ and $n = 0, 1, 2, \cdots, N$, and denote $\psi^n \in \mathbb{C}^{J+1}$ be the numerical vector solution and respectively $w^n \in \mathbb{C}^{J+1}$ be the exact vector solution at time $t = t_n$. For a grid function $u = \{u_j^n \mid j = 0, 1, 2, \cdots, J;\ n = 0, 1, 2, \cdots, N\}$, we introduce the following finite difference operators:

$$\delta_x^+ u_j^n = \frac{1}{h}\left(u_{j+1}^n - u_j^n\right), \qquad \delta_x^2 u_j^n = \frac{1}{h^2}\left(u_{j-1}^n - 2u_j^n + u_{j+1}^n\right),$$
$$\delta_t^+ u_j^n = \frac{1}{\tau}\left(u_j^{n+1} - u_j^n\right), \qquad \delta_t u_j^n = \frac{1}{2\tau}\left(u_j^{n+1} - u_j^{n-1}\right).$$

We denote the space

$$X_h := \{u = (u_0, u_1, u_2, \cdots, u_J) \mid u_0 = u_J = 0\} \subseteq \mathbb{C}^{J+1},$$

and define discrete inner product and discrete norms over X_h as

$$\langle u, v\rangle := h\sum_{j=1}^{J-1} u_j \overline{v}_j, \quad ||u|| := \langle u, u\rangle^{\frac{1}{2}},$$
$$||u||_\infty := \max_{0\le j\le J} |u_j|, \quad \left|\left|\delta_x^+ u\right|\right| := \left(h\sum_{j=0}^{J-1}\left|\delta_x^+ u_j\right|^2\right)^{\frac{1}{2}},$$

where $\overline{f}$ denotes the conjugate of f. Throughout the paper, we denote C as a generic positive constant which may be dependent on the regularity of the exact solution and the given data but independent of the discrete parameters. A famous energy-preserving finite difference scheme reads (see [2] and references therein)

$$i\delta_t^+\psi_j^n + \alpha\delta_x^2\psi_j^{n+\frac{1}{2}} + V_j\psi_j^{n+\frac{1}{2}} + G(|\psi_j^n|^2, |\psi_j^{n+1}|^2)\psi_j^{n+\frac{1}{2}} = 0,$$
$$j = 1, 2, \cdots, J-1,\ n = 0, 1, 2, \cdots, N-1, \tag{2.1}$$

with boundary condition

$$\psi_0^n = \psi_J^n = 0, \quad n = 1, 2, \cdots, N, \tag{2.2}$$

and initial condition

$$\psi_j^0 = \varphi_j, \quad j = 0, 1, 2, \cdots, J, \tag{2.3}$$

where $\psi_j^{n+\frac{1}{2}} = \frac{1}{2}(\psi_j^n + \psi_j^{n+1})$, $V_j = V(x_j)$, $\varphi_j = \varphi(x_j)$ and

$$G(s_1, s_2) = \int_0^1 f(\theta s_2 + (1-\theta)s_1)d\theta.$$

This scheme preserves the total mass and energy in the discrete sense (see [2] and references therein), i.e.,

$$M^n :=||\psi^n||^2 \equiv M^0, \quad n = 0, 1, 2, \cdots, N, \tag{2.4}$$

$$E^n :=\alpha||\delta_x^+\psi^n||^2 - h\sum_{j=1}^{J-1} V_j|\psi_j^n|^2 - \langle F^n, 1\rangle \equiv E^0, \quad n = 0, 1, 2, \cdots, N, \tag{2.5}$$

where $F^n \in X_h$ with components

$$F_j^n = F(|\psi_j^n|^2). \tag{2.6}$$

Here the discrete functional $\langle F^n, 1\rangle$ can be viewed as the approximation of the functional $(F(\cdot, t_n), 1)$. It is clear that the discrete functional $\langle F^n, 1\rangle$ merely depends on ψ^n. The key nature of the above scheme is the discretization of the nonlinear term, i.e., the definition of $G(s_1, s_2)$. However, there is no other finite difference scheme was claimed in literature to preserve the total energy in the discrete sense. Here, we revisit several classical implicit finite difference schemes and prove that they also preserve the total energy in the discrete sense.

First of all, we consider the following standard Crank-Nicolson finite difference scheme,

$$i\delta_t^+\psi_j^n + \alpha\delta_x^2\psi_j^{n+\frac{1}{2}} + V_j\psi_j^{n+\frac{1}{2}} + f(|\psi_j^{n+\frac{1}{2}}|^2)\psi_j^{n+\frac{1}{2}} = 0,$$
$$j = 1, 2, \cdots, J-1,\ n = 0, 1, 2, \cdots, N-1, \tag{2.7}$$

$$\psi_0^n = \psi_J^n = 0, \quad n = 1, 2, \cdots, N, \tag{2.8}$$

$$\psi_j^0 = \varphi_j, \quad j = 0, 1, 2, \cdots, J. \tag{2.9}$$

It follows from $F(s_2) - F(s_1) = \int_{s_1}^{s_2} f(s)ds$ that

$$\begin{aligned} F(|\psi_j^{n+1}|^2) &= F(|\psi_j^n|^2) + \int_{|\psi_j^n|^2}^{|\psi_j^{n+1}|^2} f(s)ds \\ &= F(|\psi_j^n|^2) + f(|\psi_j^{n+\frac{1}{2}}|^2)(|\psi_j^{n+1}|^2 - |\psi_j^n|^2) + O(\tau^3). \end{aligned} \tag{2.10}$$

This motivates us to introduce a new discrete functional $\langle F^n, 1\rangle$ of grid function $F^n \in X_h$ $(n = 0, 1, \cdots, N)$ which defined by the following recursion formula,

$$F_j^0 = F(|\varphi_j|^2), \quad F_j^{n+1} = F_j^n + f(|\psi_j^{n+\frac{1}{2}}|^2)(|\psi_j^{n+1}|^2 - |\psi_j^n|^2),$$
$$j = 1, 2, \cdots, J-1, \quad n = 0, 1, 2, \cdots, N-1. \tag{2.11}$$

Here, in terms of (2.10) and (2.11), the discrete functional $\langle F^n, 1\rangle$ can be viewed as another approximation of the functional $(F(\cdot, t_n), 1)$.

Corresponding to the conservation laws of the total mass and energy (1.4)-(1.5), the standard Crank-Nicolson scheme (2.7)-(2.9) satisfies the following lemma. i.e., Lemma 2.1. *The standard Crank-Nicolson scheme (2.7)-(2.9) preserves the total mass and energy in the discrete sense, i.e.,*

$$M^n :=||\psi^n||^2 \equiv M^0, \quad n = 0, 1, 2, \cdots, N, \tag{2.12}$$

$$E^n := -\alpha||\delta_x^+\psi^n||^2 + h\sum_{j=1}^{J-1} V_j|\psi_j^n|^2 + \langle F^n, 1\rangle \equiv E^0, \quad n = 0, 1, 2, \cdots, N, \tag{2.13}$$

where F^n is defined in (2.11).

Proof. Computing the inner product of (2.7) with $\psi^{n+1} + \psi^n$, then taking the imaginary part, we obtain

$$\frac{1}{\tau}\left(||\psi^{n+1}||^2 - ||\psi^n||^2\right) = 0, \quad n = 0, 1, 2, \cdots, N-1. \tag{2.14}$$

Let $M^n = ||\psi^n||^2$, then we obtain from (2.14) that

$$M^{n+1} = M^n, \quad n = 0, 1, 2, \cdots, N-1. \tag{2.15}$$

This immediately gives (2.12).

Computing the inner product of (2.7) with $\psi^{n+1} - \psi^n$, then taking the real part, we obtain

$$\begin{aligned} &-\frac{\alpha}{2}\left(||\delta_x^+\psi^{n+1}||^2 - ||\delta_x^+\psi^n||^2\right) + \frac{1}{2}h\sum_{j=1}^{J-1} V_j(|\psi_j^{n+1}|^2 - |\psi_j^n|^2) \\ &+ \frac{1}{2}\left\langle F^{n+1} - F^n, 1\right\rangle = 0, \quad n = 0, 1, 2, \cdots, N-1. \end{aligned} \tag{2.16}$$

This immediately gives (2.13). □

Next, we consider the following linearized Crank-Nicolson scheme:

$$\begin{aligned} &i\delta_t\psi_j^n + \frac{\alpha}{2}\delta_x^2(\psi_j^{n-1} + \psi_j^{n+1}) + \frac{1}{2}V_j(\psi_j^{n-1} + \psi_j^{n+1}) + f(|\psi_j^n|^2)\psi_j^n = 0, \\ &\qquad j = 1, 2, \cdots, J-1,\ n = 1, 2, \cdots, N-1, \end{aligned} \tag{2.17}$$

$$\psi_0^n = \psi_J^n = 0, \quad n = 1, 2, \cdots, N, \tag{2.18}$$

$$\psi_j^0 = \varphi_j, \quad j = 0, 1, 2, \cdots, J. \tag{2.19}$$

Obviously, this is a three-level scheme which could not start by itself, so we need another two-level scheme to compute ψ^1. One method to compute ψ^1 is the Crank-Nicolson scheme (2.7) for $n = 0$. Alternatively, by applying Taylor's expansion to $\psi(x, t_1)$ at the point $(x, 0)$, we obtain

$$\begin{aligned} \psi(x, t_1) &= \psi(x, 0) + \tau\partial_t\psi(x, 0) + \tau^2\int_0^1 \partial_{tt}\psi(x, s\tau)(1-s)ds \\ &= \varphi(x) + \tau\varphi_1(x) + \tau^2\int_0^1 \partial_{tt}\psi(x, s\tau)(1-s)ds, \end{aligned}$$

where $\varphi_1(x) = i[\alpha\partial_{xx}\varphi(x) + V(x)\varphi(x) + f(|\varphi(x)|^2)\varphi(x)]$. This motivates us to design the following two-level scheme to compute ψ^1,

$$\psi_j^1 = \varphi(x_j) + \tau\varphi_1(x_j), \quad j = 1, 2, \cdots, J-1. \tag{2.20}$$

Define a two-component function G from $\mathbb{R}\times\mathbb{R}$ to $\mathbb{R}$ as follows

$$G(r,s)=F(rs), \tag{2.21}$$

where F is a primitive function of f. Let $P_j^k=(\psi_j^k,\overline{\psi_j^k})$ be a point in the plane, then we obtain from Newton-Leibniz formula that

$$\begin{aligned}&\frac{1}{2}\Big(G(\psi_j^{n+1},\overline{\psi_j^{n+1}})+G(\psi_j^n,\overline{\psi_j^n})\Big)-\frac{1}{2}\Big(G(\psi_j^n,\overline{\psi_j^n})+G(\psi_j^{n-1},\overline{\psi_j^{n-1}})\Big)\\&=\frac{1}{2}\int_{P_j^{n-1}}^{P_j^{n+1}}\frac{\partial G}{\partial\vec{l}}dl=\frac{1}{2}\int_{P_j^{n-1}}^{P_j^{n+1}}\nabla G\cdot d\vec{l},\end{aligned} \tag{2.22}$$

where $\vec{l}=(\psi_j^{n+1}-\psi_j^{n-1},\overline{\psi_j^{n+1}-\psi_j^{n-1}})^\top$, $l=|\vec{l}|$, $\nabla G(r,s)=(\partial_rF,\partial_sF)^\top=f(rs)(s,r)^\top$. It is easy to verify that the following numerical approximation with a small remainder of the integral $(\partial_rF,\partial_sF)^\top=f(rs)(s,r)^\top$ holds

$$\begin{aligned}\int_{P_j^{n-1}}^{P_j^{n+1}}\nabla G\cdot d\vec{l}&=\nabla G(P_j^n)\cdot\vec{l}+O(\tau^3)\\&=2f(|\psi_j^n|^2)\mathrm{Re}(\psi_j^n(\overline{\psi_j^{n+1}}-\overline{\psi_j^{n-1}}))+O(\tau^3).\end{aligned} \tag{2.23}$$

Combining (2.22) and (2.23) motivates us to define the discrete functional $\langle G^n+G^{n+1},1\rangle$ of grid function $G^n\in X_h$ defined by G_j^n for $j=0,1,2,\cdots,J,\ n=0,1,2,\cdots,N$ as follows

$$\begin{aligned}&\frac{1}{2}(G_j^n+G_j^{n+1})=\frac{1}{2}(G_j^{n-1}+G_j^n)+f(|\psi_j^n|^2)\mathrm{Re}(\psi_j^n(\overline{\psi_j^{n+1}}-\overline{\psi_j^{n-1}})),\\&\qquad j=0,1,2,\cdots,J,\ n=1,2,\cdots,N-1,\\&G_j^1=F(|\psi_j^1|^2),\quad G_j^0=F(|\psi_j^0|^2),\quad j=0,1,2,\cdots,J.\end{aligned} \tag{2.24}$$

Here the discrete functional $\frac{1}{2}\langle G^n+G^{n+1},1\rangle$ can be viewed as another approximation of the functional $\Big(F(\cdot,t_{n+\frac{1}{2}}),1\Big)$.

Corresponding to the conservation laws of the total mass and energy (1.4)-(1.5), the linearized Crank-Nicolson scheme (2.17)-(2.20) satisfies the following lemma. i.e.,

LEMMA 2.2. *The finite difference scheme (2.17)-(2.20) preserves the total mass and energy in the discrete sense, i.e.,*

$$\begin{aligned}M^n:=&h\sum_{j=1}^{J-1}\mathrm{Re}(\psi_j^{n+1}\overline{\psi_j^n})-\tau\alpha h\sum_{j=1}^{J-1}\mathrm{Im}(\delta_x^+\psi_j^{n+1}\delta_x^+\overline{\psi_j^n})\\&+\tau h\sum_{j=1}^{J-1}V_j\mathrm{Im}(\psi_j^{n+1}\overline{\psi_j^n})\equiv M^0,\quad n=0,1,2,\cdots,N-1,\end{aligned} \tag{2.25}$$

$$\begin{aligned}E^n:=&-\frac{\alpha}{2}(||\delta_x^+\psi^n||^2+||\delta_x^+\psi^{n+1}||^2)+\frac{1}{2}h\sum_{j=1}^{J-1}V_j(|\psi_j^n|^2+|\psi_j^{n+1}|^2)\\&+\frac{1}{2}\langle G^n+G^{n+1},1\rangle\equiv E^0,\quad n=0,1,2,\cdots,N-1,\end{aligned} \tag{2.26}$$

where G^n is defined in (2.24).

Proof. Computing the inner product of (2.17) with ψ^n, then taking the imaginary part, we obtain

$$\frac{1}{2\tau}h\sum_{j=1}^{J-1}\mathrm{Re}(\psi_j^{n+1}\overline{\psi_j^n}-\psi_j^n\overline{\psi_j^{n-1}})-\frac{\alpha}{2}h\sum_{j=1}^{J-1}\mathrm{Im}(\delta_x^+\psi_j^{n+1}\delta_x^+\overline{\psi_j^n}-\delta_x^+\psi_j^n\delta_x^+\overline{\psi_j^{n-1}})$$
$$+\frac{h}{2}\sum_{j=1}^{J-1}V_j\mathrm{Im}(\psi_j^{n+1}\overline{\psi_j^n}-\psi_j^n\overline{\psi_j^{n-1}})=0,\quad n=0,1,2,\cdots,N-1, \tag{2.27}$$

this together with the definition of M^n immediately gives

$$M^n-M^{n-1}=0,\quad n=1,2,\cdots,N-1. \tag{2.28}$$

Then by using successive recursion, we obtain from (2.15) that

$$M^n\equiv M^0,\quad n=0,1,2,\cdots,N-1. \tag{2.29}$$

Computing the inner product of (2.17) with $\psi^{n+1}-\psi^{n-1}$, then taking the real part, we obtain

$$-\frac{\alpha}{2}h\sum_{j=1}^{J-1}(|\delta_x^+\psi_j^{n+1}|^2-|\delta_x^+\psi_j^{n-1}|^2)+\frac{h}{2}\sum_{j=1}^{J-1}V_j(|\psi_j^{n+1}|^2-|\psi_j^{n-1}|^2)$$
$$+h\sum_{j=1}^{J-1}f(|\psi_j^n|^2)\mathrm{Re}(\psi_j^n(\overline{u_j^{n+1}}-\overline{\psi_j^{n-1}}))=0,\quad n=1,2,\cdots,N-1. \tag{2.30}$$

This together with (2.24) gives

$$-\frac{\alpha}{2}(\|\delta_x^+\psi^{n+1}\|^2-\|\delta_x^+\psi^{n-1}\|^2)+\frac{h}{2}\sum_{j=1}^{J-1}V_j(|\psi_j^{n+1}|^2-|\psi_j^{n-1}|^2)$$
$$+\frac{1}{2}\left\langle G^{n+1}-G^{n-1},1\right\rangle=0,\quad n=1,2,\cdots,N-1. \tag{2.31}$$

This immediately gives

$$E^n\equiv E^0,\quad n=1,2,\cdots,N-1. \tag{2.32}$$

This completes the proof of the lemma. □

Except for the above two schemes, many other classical finite difference schemes of the NLS/GP equation preserve the total mass and energy in the discrete sense. Here we consider the following four schemes:

CN-1 scheme

$$i\delta_t^+\psi_j^n+\alpha\delta_x^2\psi_j^{n+\frac{1}{2}}+V_j\psi_j^{n+\frac{1}{2}}+f\left(\frac{1}{2}(|\psi_j^n|^2+|\psi_j^{n+1}|^2)\right)\psi_j^{n+\frac{1}{2}}=0,$$
$$j=1,2,\cdots,J-1,\ n=0,1,2,\cdots,N-1. \tag{2.33}$$

CN-2 scheme

$$i\delta_t^+\psi_j^n + \alpha\delta_x^2\psi_j^{n+\frac{1}{2}} + V_j\psi_j^{n+\frac{1}{2}} + \frac{1}{2}\left[f(|\psi_j^n|^2) + f(|\psi_j^{n+1}|^2)\right]\psi_j^{n+\frac{1}{2}} = 0,$$
$$j = 1, 2, \cdots, J-1,\ n = 0, 1, 2, \cdots, N-1. \tag{2.34}$$

LCN-1 scheme

$$i\delta_t^+\psi_j^n + \alpha\delta_x^2\psi_j^{n+\frac{1}{2}} + V_j\psi_j^{n+\frac{1}{2}} + \frac{1}{2}\left[3f(|\psi_j^n|^2) - f(|\psi_j^{n-1}|^2)\right]\psi_j^{n+\frac{1}{2}} = 0,$$
$$j = 1, 2, \cdots, J-1,\ n = 0, 1, 2, \cdots, N-1. \tag{2.35}$$

LCN-2 scheme

$$i\delta_t\psi_j^n + \frac{\alpha}{2}\delta_x^2(\psi_j^{n-1} + \psi_j^{n+1}) + \frac{1}{2}V_j(\psi_j^{n-1} + \psi_j^{n+1}) + \frac{1}{2}f(|\psi_j^n|^2)(\psi_j^{n-1} + \psi_j^{n+1}) = 0,$$
$$j = 1, 2, \cdots, J-1,\ n = 1, 2, \cdots, N-1. \tag{2.36}$$

By using similar discussion of Lemma 2.1, one can obtain the discrete conservation results of the total mass and energy.

LEMMA 2.3. *The CN-1 scheme possesses the total mass and energy in the discrete sense, i.e.,*

$$M^n := ||\psi^n||^2 \equiv M^0, \quad n = 0, 1, 2, \cdots, N, \tag{2.37}$$
$$E^n := -\alpha||\delta_x^+\psi^n||^2 + h\sum_{j=1}^{J-1} V_j|\psi_j^n|^2 + \langle F^n, 1\rangle \equiv E^0, \quad n = 0, 1, 2, \cdots, N, \tag{2.38}$$

where

$$F_j^0 = F(|\varphi_j|^2), \quad F_j^{n+1} = F_j^n + f\left((|\psi_j^n|^2 + |\psi_j^{n+1}|^2)/2\right)(|\psi_j^{n+1}|^2 - |\psi_j^n|^2),$$
$$j = 0, 1, \cdots, J, \quad n = 0, 1, 2, \cdots, N-1.$$

LEMMA 2.4. *The CN-2 scheme possesses the total mass and energy in the discrete sense, i.e.,*

$$M^n := ||\psi^n||^2 \equiv M^0, \quad n = 0, 1, 2, \cdots, N, \tag{2.39}$$
$$E^n := -\alpha||\delta_x^+\psi^n||^2 + h\sum_{j=1}^{J-1} V_j|\psi_j^n|^2 + \langle F^n, 1\rangle \equiv E^0, \quad n = 0, 1, 2, \cdots, N, \tag{2.40}$$

where

$$F_j^0 = F(|\varphi_j|^2), \quad F_j^{n+1} = F_j^n + \frac{1}{2}\left[f(|\psi_j^n|^2) + f(|\psi_j^{n+1}|^2)\right](|\psi_j^{n+1}|^2 - |\psi_j^n|^2),$$
$$j = 0, 1, \cdots, J, \quad n = 0, 1, 2, \cdots, N-1.$$

LEMMA 2.5. *The LCN-1 scheme possesses the total mass and energy in the discrete sense, i.e.,*

$$M^n :=||\psi^n||^2 \equiv M^1, \quad n = 1, 2, \cdots, N, \tag{2.41}$$

$$E^n := -\alpha||\delta_x^+\psi^n||^2 + h\sum_{j=1}^{J-1} V_j|\psi_j^n|^2 + \langle F^n, 1\rangle \equiv E^1, \quad n = 1, 2, \cdots, N, \tag{2.42}$$

where

$$F_j^1 = F(|\psi_j^1|^2), \quad F_j^{n+1} = F_j^n + \frac{1}{2}\left[3f(|\psi_j^n|^2) - f(|\psi_j^{n-1}|^2)\right](|\psi_j^{n+1}|^2 - |\psi_j^n|^2),$$
$$j = 0, 1, \cdots, J, \quad n = 1, 2, \cdots, N-1.$$

LEMMA 2.6. *The LCN-2 scheme possesses the total mass and energy in the discrete sense, i.e.,*

$$M^n :=\frac{1}{2}(||\psi^n||^2 + ||\psi^{n+1}||^2) \equiv M^0, \quad n = 0, 1, 2, \cdots, N-1, \tag{2.43}$$

$$\begin{aligned} E^n := &-\frac{\alpha}{2}(||\delta_x^+\psi^n||^2 + ||\delta_x^+\psi^{n+1}||^2) + \frac{h}{2}\sum_{j=1}^{J-1} V_j(|\psi_j^n|^2 + |\psi_j^{n+1}|^2) \\ &+ \frac{1}{2}\left\langle G^n + G^{n+1}, 1\right\rangle \equiv E^0, \quad n = 0, 1, 2, \cdots, N-1, \end{aligned} \tag{2.44}$$

where

$$\frac{1}{2}\left(G_j^n + G_j^{n+1}\right) = \frac{1}{2}\left(G_j^{n-1} + G_j^n\right) + \frac{1}{2}f(|\psi_j^n|^2)(|\psi_j^{n+1}|^2 - |\psi_j^{n-1}|^2),$$
$$G_j^0 = F(|\varphi_j|^2), \quad G_j^1 = F(|\psi_j^1|^2), \quad j = 0, 1, \cdots, J, \quad n = 0, 1, 2, \cdots, N-1.$$

REMARK 2.1. Though all the finite difference schemes mentioned in this paper preserve the total mass and energy in the discrete sense, the form of the energy functionals of them are different. The main difference is that the energy functional E^n of the scheme (2.1)-(2.3) merely depends on the numerical solution at the *n-th* level, while the energy functionals of the other six schemes are defined by using a recursive formula.

3. Unconditionally optimal error estimates.

In this section, we firstly establish the *a priori* estimate of the numerical solution of the standard Crank-Nicolson finite difference scheme (2.7)-(2.9), then build the optimal error bound without any constrain on the grid ratios. The numerical analysis can be directly extended to establish the unconditionally optimal point-wise error estimates of other finite difference schemes.

In analyzing the error estimate, we need the the following lemma,

LEMMA 3.1 ([37]). *For any grid function $\mu \in X_h$, there is the inequality*

$$||\mu||_\infty \le C||\mu||^{\frac{1}{2}}(||\delta_x^+\mu|| + ||\mu||)^{\frac{1}{2}}, \quad d = 1, \tag{3.1}$$

$$||\mu||_\infty \le C||\mu||^{1-\frac{d}{4}}(||\Delta_h\mu|| + ||\mu||)^{\frac{d}{4}}, \quad d = 2, 3. \tag{3.2}$$

In the following, for a function $f(x,t)$ over $\Omega \times [0,T]$, we denote

$$||f||_{L^\infty} := \sup_{t\in[0,T]} \sup_{x\in\Omega} |f(x,t)|.$$

Define the local truncation error $\sigma^n \in X_h$ for $n = 0, 1, 2, \cdots, N-1$ as follows

$$\sigma_j^n := i\delta_t^+ w_j^n + \alpha\delta_x^2 w_j^{n+\frac{1}{2}} + V_j w_j^{n+\frac{1}{2}} + f(|w_j^{n+\frac{1}{2}}|^2) w_j^{n+\frac{1}{2}},$$
$$j = 1, 2, \cdots, J-1,\ n = 0, 1, 2, \cdots, N-1, \tag{3.3}$$
$$w_0^n = w_J^n = 0, \quad n = 1, 2, \cdots, N, \tag{3.4}$$
$$w_j^0 = \varphi(x_j), \quad j = 0, 1, 2, \cdots, J. \tag{3.5}$$

By using Taylor's expansion, one can obtain the following lemma:

LEMMA 3.2. *Assuming that* $\psi \in C^4([0,T]; W^{2,\infty}(\Omega)) \cap C^2([0,T]; W^{4,\infty}(\Omega))$, $V \in C(\Omega)$, $f \in C^2([0,\infty))$, *then the local truncation error of the Crank-Nicolson scheme (2.7)-(2.9) satisfies the following estimates,*

$$|\sigma_j^n| \le C(\tau^2 + h^2),\ \ j = 1, 2, \cdots, J-1,\ n = 0, 1, 2, \cdots, N-1,$$
$$|\delta_t^+ \sigma_j^n| \le C(\tau^2 + h^2),\ j = 1, 2, \cdots, J-1,\ n = 0, 1, 2, \cdots, N-2.$$

Define the 'error' function $e^n \in X_h$ for $n = 0, 1, 2, \cdots, N-1$ as

$$e_j^n = w_j^n - \psi_j^n, \tag{3.6}$$

then for the estimate of e^n, there is the following theorem,

THEOREM 3.1. *Under the assumptions in Lemma 3.2, then the numerical solution of the Crank-Nicolson scheme (2.7)-(2.9) converges to the exact solution of the original problem (1.1)-(1.3) in the maximum norm with second order in both spatial and temporal direction, i.e.,*

$$||e^n||_\infty \le C(\tau^2 + h^2), \quad n = 0, 1, 2, \cdots, N-1.$$

Proof. The main difficulty in establishing the error estimate is that the *a priori* estimate of the numerical solution can not be obtained. In [1, 5, 4, 29, 33], this difficulty was overcome by introducing a cut-off function to truncate the coefficient of the nonlinearity to a global Lipschitz function with compact support, which can be achieved if the continuous solution is bounded and the numerical solution is close to the continuous solution. However, the authors only gave the optimal error estimates in the discrete L^2-norm, further more, their results were constrained to the time step. Here, besides the cut-off function technique, we introduce a 'lifting' technique as well as some useful inequalities to establish the optimal error estimates in the discrete H^2-norm (which consequently yields the optimal error estimates in the discrete L^∞-norm) without any constraint on the grid ratios, i.e., (3.1).

Choose a smooth function $\rho(s) \in C^\infty(\mathbb{R})$ such that $\rho(s) = 1$ when $|s| \le 1$, $\rho(s) = 0$ when $|s| \ge 2$, and $0 \le \rho(s) \le 1$ for $s \in \mathbb{R}$. By assumption (B), we can define $M_0 = ||u||_{L^\infty}$, and choose a positive number $B = (M_0 + 1)^2$. For $f(s) \ge 0$ define

$$f_B(s) = f(s)\rho(s/B). \tag{3.7}$$

Then $f_B(s)$ is global Lipschitz and

$$|f_B(s_1) - f_B(s_2)| \le C_B \left|\sqrt{s_1} - \sqrt{s_2}\right|, \quad \forall s_1, s_2 \ge 0. \tag{3.8}$$

Choose $\hat{\psi}^0 = \psi^0$ and define $\hat{\psi}^n \in X_h$ for $n = 0, 1, 2, \cdots, n$ as

$$\begin{aligned} & i\delta_t^+ \hat{\psi}_j^n + \alpha\delta_x^2 \hat{\psi}_j^{n+\frac{1}{2}} + V_j \hat{\psi}_j^{n+\frac{1}{2}} + f_B(|\hat{\psi}_j^{n+\frac{1}{2}}|^2)\hat{\psi}_j^{n+\frac{1}{2}} = 0, \\ & \qquad j = 1, 2, \cdots, J-1, \ n = 0, 1, 2, \cdots, N-1, \end{aligned} \tag{3.9}$$

$$\hat{\psi}_0^n = \hat{\psi}_J^n = 0, \quad n = 1, 2, \cdots, N, \tag{3.10}$$

$$\hat{\psi}_j^0 = \varphi_j, \quad j = 0, 1, 2, \cdots, J. \tag{3.11}$$

In fact, $\hat{\psi}_j^n$ can be viewed as another approximation of $\psi(x_j, t_n)$. Noting that

$$f_B(|\omega_j^{n+\frac{1}{2}}|^2) = f(|\omega_j^{n+\frac{1}{2}}|^2), \quad j = 1, 2, \cdots, J-1, \ \ n = 0, 1, 2, \cdots, N-1,$$

we know that the local truncation error of the scheme (3.9)-(3.11) just is σ^n defined by (3.3)-(3.5). Define the "error" function $\hat{e}^n \in X_h$ for $n = 0, 1, 2, \cdots, N$ as

$$\hat{e}_j^n = w_j^n - \hat{\psi}_j^n. \tag{3.12}$$

Subtracting (3.9)-(3.11) from (3.3)-(3.5) gives the following 'error' equation:

$$\begin{aligned} & i\delta_t^+ \hat{e}_j^n + \alpha\delta_x^2 \hat{e}_j^{n+\frac{1}{2}} + V_j \hat{e}_j^{n+\frac{1}{2}} + \hat{\xi}_j^{n+1} = \sigma_j^n, \\ & j = 1, 2, \cdots, J-1, \ n = 0, 1, 2, \cdots, N-1, \end{aligned} \tag{3.13}$$

where

$$\begin{aligned} \hat{\xi}_j^{n+1} :=& f_B(|w_j^{n+\frac{1}{2}}|^2) w_j^{n+\frac{1}{2}} - f_B(|\hat{\psi}_j^{n+\frac{1}{2}}|^2)\hat{\psi}_j^{n+\frac{1}{2}} \\ =& f_B(|w_j^{n+\frac{1}{2}}|^2)\hat{e}_j^{n+\frac{1}{2}} + \left(f_B(|w_j^{n+\frac{1}{2}}|^2) - f_B(|\psi_j^{n+\frac{1}{2}}|^2)\right)\hat{\psi}_j^{n+\frac{1}{2}}. \end{aligned} \tag{3.14}$$

It follows from (3.7)-(3.8) that

$$||\hat{\xi}^{n+1}|| \le C(||\hat{e}^n|| + ||\hat{e}^{n+1}||). \tag{3.15}$$

Computing the inner product of (3.13) with $\hat{e}^n + \hat{e}^{n+1}$, then taking the imaginary part, we obtain

$$\begin{aligned} & \frac{1}{\tau}(||\hat{e}^{n+1}||^2 - ||\hat{e}^n||^2) \\ =& -\mathrm{Im}(\hat{\xi}^{n+1}, \hat{e}^n + \hat{e}^{n+1}) + \mathrm{Im}(\hat{\sigma}^n, \hat{e}^n + \hat{e}^{n+1}) \\ \le& C\left(||\hat{e}^n||^2 + ||\hat{e}^{n+1}||^2 + ||\sigma^n||^2\right) \\ \le& C\left(||\hat{e}^n||^2 + ||\hat{e}^{n+1}||^2 + (\tau^2 + h^2)^2\right), \quad n = 0, 1, 2, \cdots, N-1, \end{aligned} \tag{3.16}$$

where Lemma 3.2 and (3.15) were used. Then by using Gronwall's inequality and (3.16), we obtain

$$||\hat{e}^n|| \le C(\tau^2 + h^2), \quad n = 1, 2, \cdots, N. \tag{3.17}$$

By using inverse embedding Sobolev inequality, one can obtain

$$||\hat{e}^n||_\infty = h^{-1}||\hat{e}^n|| \le Ch^{-1}(\tau^2+h^2), \quad n=1,2,\cdots,N. \tag{3.18}$$

This means that, if h,τ are small enough and $\tau \le h$, we have

$$||\hat{e}^n||_\infty \le 1, \quad n=1,2,\cdots,N. \tag{3.19}$$

On the other hand, it follows from (3.13) that

$$\begin{aligned}&\delta_x^2(\hat{e}_j^n+\hat{e}_j^{n+1}) = -\frac{2i}{\alpha}\delta_t^+\hat{e}_j^n - \frac{2}{\alpha}V_j\hat{e}_j^{n+\frac{1}{2}} - \frac{2}{\alpha}\hat{\xi}_j^{n+1} + \frac{1}{\alpha}\sigma_j^n,\\ &j=1,2,\cdots,J-1,\ n=0,1,2,\cdots,N-1.\end{aligned} \tag{3.20}$$

Taking the discrete L^2 norm of both sides of (3.20) gives

$$\begin{aligned}&||\delta_x^2\hat{e}^n+\delta_x^2\hat{e}^{n+1}||\\ =&||-\frac{2i}{\alpha}\delta_t^+\hat{e}^n - \frac{1}{\alpha}V_j\hat{e}^{n+\frac{1}{2}} - \frac{1}{\alpha}\hat{\xi}^{n+1} + \frac{1}{\alpha}\sigma^n||\\ \le&C(||\delta_t^+\hat{e}^n||+||\hat{e}^n||+||\hat{e}^{n+1}||+||\hat{\xi}^{n+1}||+||\sigma^n||)\\ \le&C\tau^{-1}(h^2+\tau^2), \quad n=0,1,2,\cdots,N-1.\end{aligned} \tag{3.21}$$

Then, by using Minkovski's inequality, one can obtain from the above inequality that

$$||\delta_x^2\hat{e}^{n+1}||-||\delta_x^2\hat{e}^n|| \le C\tau^{-1}(h^2+\tau^2), \quad n=0,1,2,\cdots,N-1. \tag{3.22}$$

This gives

$$||\delta_x^2\hat{e}^n|| \le C\tau^{-2}(h^2+\tau^2), \quad n=1,2,\cdots,N. \tag{3.23}$$

Then, by using Lemma 3.1, one can obtain from (3.17) and (3.23) that

$$\begin{aligned}||\hat{e}^n||_\infty \le&C||\hat{e}^n||^{\frac{1}{2}}(||\delta_x^+\hat{e}^n||+||\hat{e}^n||)^{\frac{1}{2}}\\ \le&C||\hat{e}^n||^{\frac{1}{2}}(||\delta_x^2\hat{e}^n||+||\hat{e}^n||)^{\frac{1}{2}}\\ \le&C\tau^{-1}(h^2+\tau^2), \quad n=1,2,\cdots,N.\end{aligned} \tag{3.24}$$

This means that, if h,τ are small enough and $\tau \ge h$, we have

$$||\hat{e}^n||_\infty \le 1, \quad n=1,2,\cdots,N. \tag{3.25}$$

Combining (3.19) and (3.25) gives that, for sufficiently small h and τ, we always have

$$||\hat{e}^n||_\infty \le 1, \quad n=1,2,\cdots,N, \tag{3.26}$$

and consequently we obtain

$$||\hat{\psi}^n||_\infty \le ||\psi(\cdot,t_n)||_\infty + ||\hat{e}^n||_\infty \le M_0+1=\sqrt{B}, \quad n=1,2,\cdots,N. \tag{3.27}$$

This implies that

$$f_B(|\hat{\psi}_j^{n+\frac{1}{2}}|^2) = f(|\hat{\psi}_j^{n+\frac{1}{2}}|^2), \quad n=1,2,\cdots,N. \tag{3.28}$$

Hence, the scheme (3.9)-(3.11) just is the standard CN scheme (2.7)-(2.9), and consequently

$$||e^n|| \leq C(\tau^2 + h^2), \quad ||\psi^n||_\infty \leq 1, \quad n = 1, 2, \cdots, N. \tag{3.29}$$

Based on the above *a priori* estimate of the numerical solution, one can use the standard energy method to obtain that

$$||e^n||_\infty \leq C(\tau^2 + h^2), \quad n = 1, 2, \cdots, N. \tag{3.30}$$

Here, we omit the detail proof for brevity.

This completes the proof. □

REMARK 3.1. For brevity, we here just only discuss several finite difference schemes of the NLS/GP equations in one dimension. The conservation laws and the error estimate results can be extended directly to the two- or three-dimensional cases.

4. Numerical results. In order to test our theoretical results, we consider the following initial-boundary value problem of the NLS equaiton,

$$i\partial_t\psi - \partial_{xx}\psi + \frac{x^2}{2}\psi + (|\psi|^2 + |\psi|^4)\psi = 0, \quad x \in (a, b),\ t \in (0, T], \tag{4.1}$$

$$\psi(a, t) = \psi(b, t) = 0, \quad t \in (0, T], \tag{4.2}$$

$$\psi(x, 0) = e^{-\frac{x^2}{2}}, \quad x \in [a, b]. \tag{4.3}$$

Since the exact solution of the problem (4.1)-(4.3) is difficult to be obtained, we here use the numerical solution computed by the standard Crank-Nicolson scheme (2.7) under very fine time step and mesh-size ($\tau = 0.0001$ and $h = 0.0001$) as 'exact' solution. Then we use the numerical solution computed by the six schemes under much bigger h and τ to test our error estimates. For simplicity, we use CN scheme and LCN scheme to denote the Crank-Nicolson scheme (2.7) and the linearized Crank-Nicolson scheme (2.17), respectively.

In the practical computation of the nonlinear schemes, iterations at each time step are unavoidable. Here we adopt the iterative algorithm proposed by Sun in [28] to overcome the difficulty and take the tolerance to be 10^{-8}. For simplicity of notations, we denote

$$\begin{aligned}
&\mathrm{Err}(\tau, h) = \| w^N - \psi^N \|_\infty, \\
&\mathrm{Rate1} = \log\left(\mathrm{Err}(\tau, h_1)/\mathrm{Err}(\tau, h_2)\right) / \log(h_1/h_2), \\
&\mathrm{Rate2} = \log\left(\mathrm{Err}(\tau_1, h)/\mathrm{Err}(\tau_2, h)\right) / \log(\tau_1/\tau_2).
\end{aligned}$$

Due to the good stability, in testing the accuracy in the spatial direction, we list in Table 1 the errors computed by the six schemes under a sufficiently small time-step $\tau = 0.0001$ and different mesh-sizes; in testing the accuracy in the temporal direction, we list in Table 2 the errors computed by the six schemes under a sufficiently small mesh-size $h = 0.0001$ and different time-steps. To test the efficiency of the nonlinear schemes and the linearized schemes, we choose CN-1 scheme and LCN-1 scheme to compute the example by using MATLAB software at time $t = 1$ when $-a = b = 20$ under different h, τ, the results are listed in Table 3. To verify the conservation laws satisfied by the six schemes, we plot in Figures 1-12 the total masses and the total energies computed by the six conservative schemes.

Table 1: Spatial errors of the six schemes under $\tau = 0.0001$ and different h at time $t = 1$.

	$h = 0.4$	$h = 0.2$	$h = 0.1$	$h = 0.08$	$h = 0.04$
CN scheme	2.3754e-002	4.8535e-003	1.1853e-003	7.5667e-004	1.8851e-004
	Rate1	2.29	2.03	2.01	2.00
CN-1 scheme	2.3754e-002	4.8535e-003	1.1853e-003	7.5667e-004	1.8851e-004
	Rate1	2.29	2.03	2.01	2.00
CN-2 scheme	2.3754e-002	4.8535e-003	1.1853e-003	7.5667e-004	1.8851e-004
	Rate1	2.29	2.03	2.01	2.00
LCN scheme	2.3754e-002	4.8536e-003	1.1854e-003	7.5676e-004	1.8860e-004
	Rate1	2.29	2.03	2.01	2.00
LCN-1 scheme	2.3754e-002	4.8535e-003	1.1853e-003	7.5667e-004	1.8851e-004
	Rate1	2.29	2.03	2.01	2.00
LCN-2 scheme	2.3754e-002	4.8536e-003	1.1854e-003	7.5677e-004	1.8861e-004
	Rate1	2.29	2.03	2.01	2.00

Table 2: Temporal errors of the six schemes under $h = 0.0001$ and different τ at time $t = 1$.

	$\tau = 0.1$	$\tau = 0.05$	$\tau = 0.025$	$\tau = 0.02$	$\tau = 0.01$
CN scheme	3.4920e-002	1.0196e-002	2.5955e-003	1.6708e-003	4.2195e-004
	Rate2	1.78	1.97	1.97	1.99
CN-1 scheme	3.4446e-002	1.01758e-002	2.5733e-003	1.6553e-003	4.1675e-004
	Rate2	1.76	1.98	1.99	1.99
CN-2 scheme	3.4451e-002	1.0179e-002	2.5740e-003	1.6557e-003	4.1686e-004
	Rate2	1.76	1.98	1.98	1.99
LCN scheme	7.6361e-002	3.2971e-002	9.9250e-003	6.2162e-003	1.6000e-003
	Rate2	1.21	1.73	2.10	1.96
LCN-1 scheme	3.5413e-002	1.0453e-002	2.4894e-003	1.5902e-003	3.9512e-004
	Rate2	1.76	2.07	2.01	2.01
LCN-2 scheme	8.0535e-002	3.3858e-002	1.0051e-003	6.3367e-003	1.6293e-003
	Rate2	1.25	1.75	2.07	1.96

Table 3: Comparison of errors and CPU times of the CN-1 scheme and LCN-1 scheme at time $t = 1$ when $-a = b = 20$ and under different mesh-size h and time-step τ.

		$h = \tau = 0.001$	$h = \tau = 0.002$	$h = \tau = 0.004$
CN-1 scheme	CPU time	1404s	274s	78s
	Error	4.2254e-006	1.7030e-005	6.8230e-005
LCN-1 scheme	CPU time	118s	29s	8s
	Error	3.9634e-006	1.5998e-005	6.4245e-005

From the results in Tables 1-3, Figures 1-7 and other numerical results not shown here for brevity, we obtain the following observations:

1. The six classical schemes (i.e., the CN, CN-1, CN-2, LCN, LCN-1 and LCN-2 schemes) studied in this paper not only are second-order accurate in both spatial and temporal directions (see Tables 1-3) but also have good stability (see Tables 2-3). These observations are consistent with Theorem 3.1. It is pointed out here that the errors in Table 1 of the six schemes are almost same, the reason is that they have the same discretization in spatial direction.

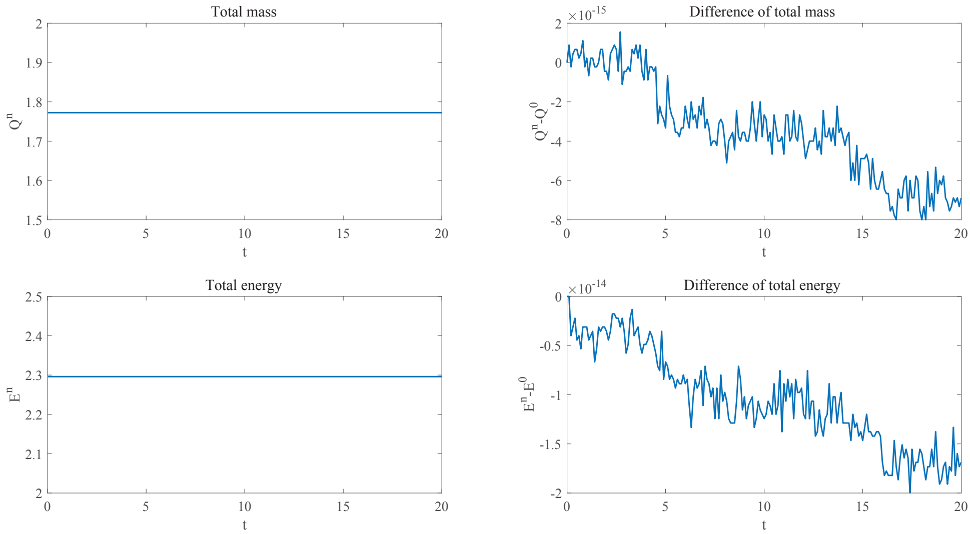

Fig. 1: Total mass (top) and energy (bottom) at different time computed by the CN scheme under $-a = b = 50, T = 20, \tau = h = 0.1$.

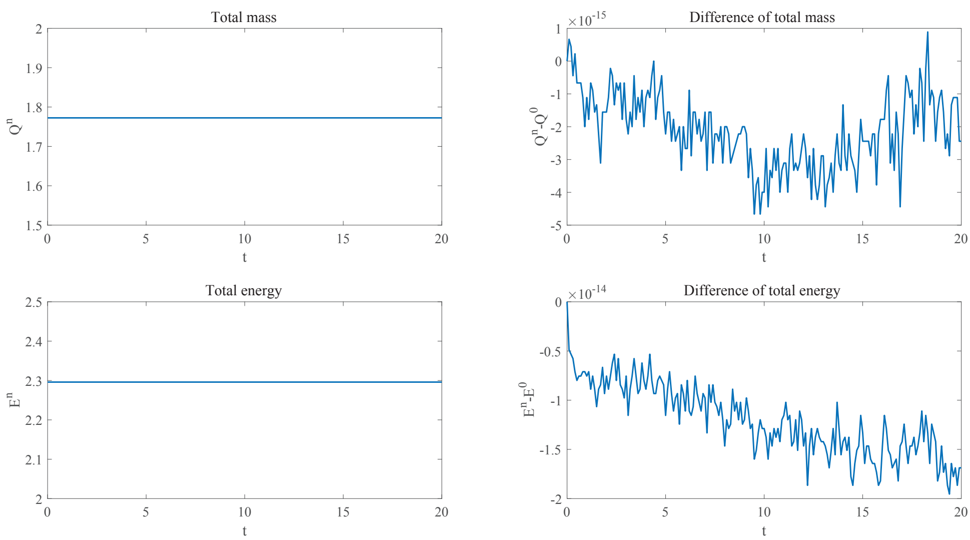

Fig. 2: Total mass (top) and energy (bottom) at different time computed by the CN-1 scheme under $-a = b = 50, T = 20, \tau = h = 0.1$.

2. Just as the energy-preserving scheme (2.1)-(2.3) (see Figure 7), all the other six classical schemes well preserve the total mass and energy in the discrete sense (see Figures 1-6), this verifies Lemmas 2.1-2.6. Furthermore, from Figures 1-7, one can see

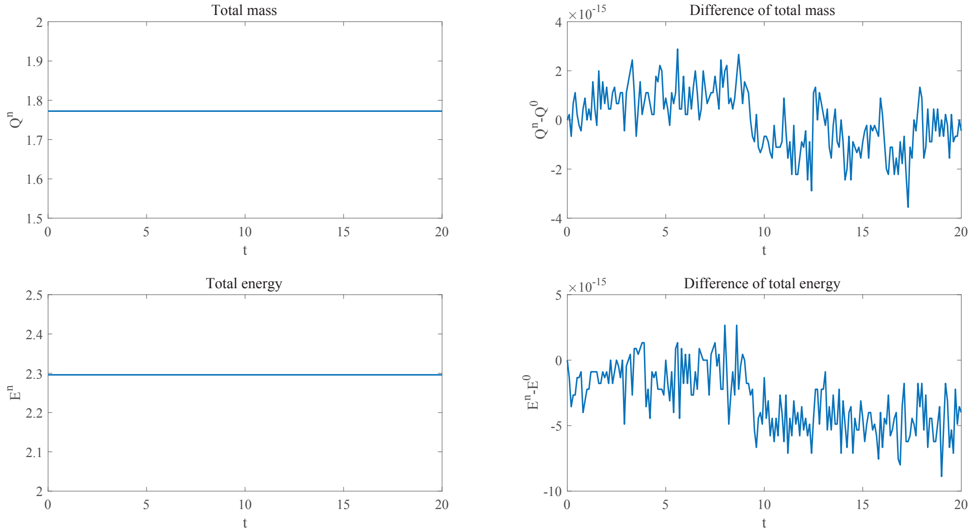

Fig. 3: Total mass (top) and energy (bottom) at different time computed by the CN-2 scheme under $-a = b = 50, T = 20, \tau = h = 0.1$.

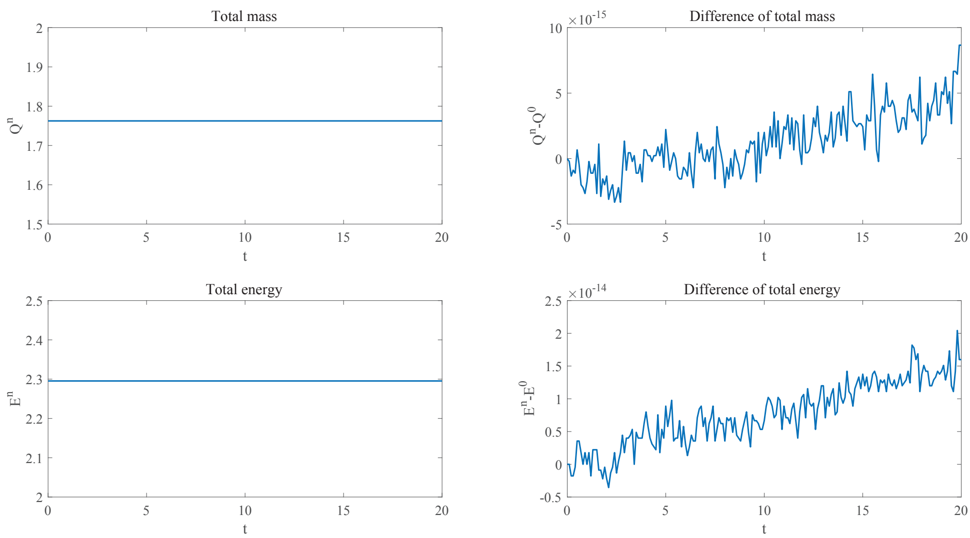

Fig. 4: Total mass (top) and energy (bottom) at different time computed by the LCN scheme under $-a = b = 50, T = 20, \tau = h = 0.1$.

that all the seven schemes preserve the total mass and energy with the same values.

3. Among the six schemes, the CN-1 scheme and the LCN-1 scheme are the most accurate ones (see Tables 1-2). As far as both the accuracy and the efficiency are

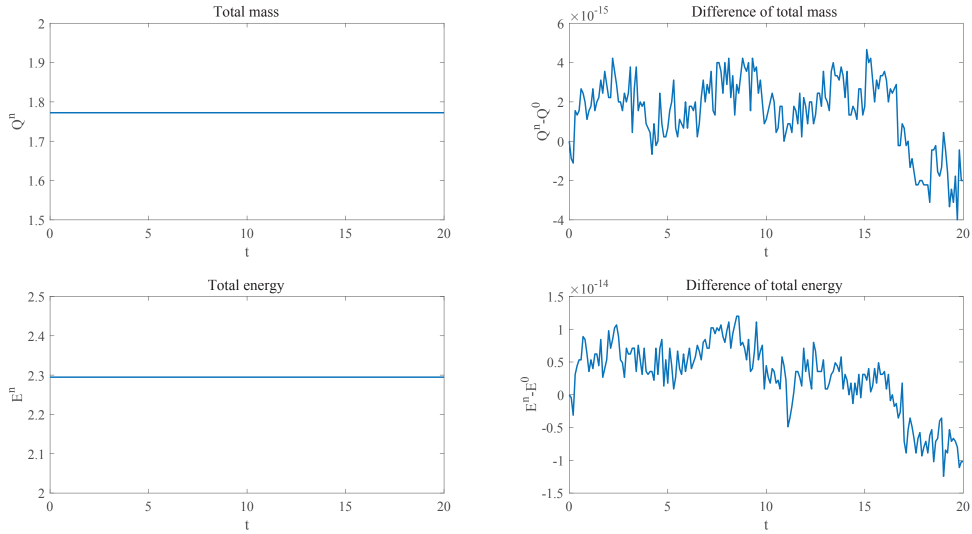

Fig. 5: Total mass (top) and energy (bottom) at different time computed by the LCN-1 scheme under $-a = b = 50, T = 20, \tau = h = 0.1$.

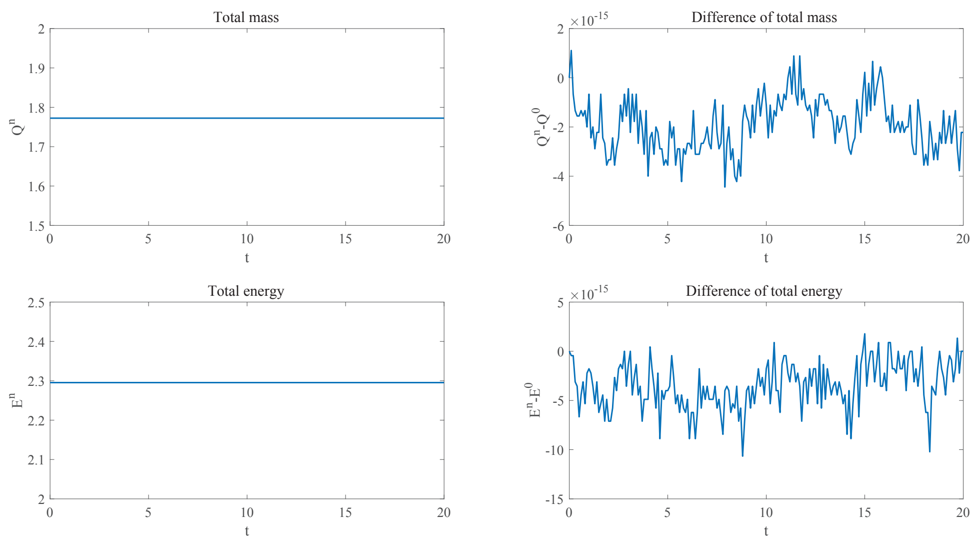

Fig. 6: Total mass (top) and energy (bottom) at different time computed by the LCN-2 scheme under $-a = b = 50, T = 20, \tau = h = 0.1$.

concerned (see Table 3), it is seen that the LCN-1 scheme is the best scheme among the six ones in the practical computation.

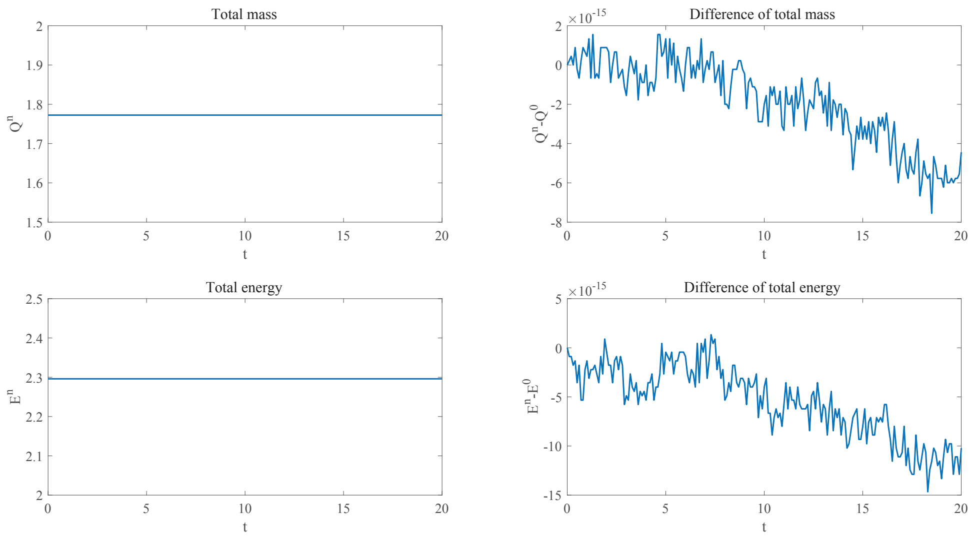

Fig. 7: Total mass (top) and energy (bottom) at different time computed by the scheme (2.1)-(2.3) under $-a = b = 50, T = 20, \tau = h = 0.1$.

5. Conclusion. In this paper, we revisit and analyze several classical finite difference schemes for solving the NLS/GP equations. By introducing a different type of energy functional, we prove that these classical schemes preserve the total mass and energy in the discrete sense. Furthermore, by using a 'cut-off' technique and a 'lifting' technique, we establish the optimal error estimates of the numerical solutions without any restriction on the grid ratios. Numerical results are reported to verify our results.

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