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A CONSERVATIVE SCHEME WITH OPTIMAL ERROR ESTIMATES FOR A MULTIDIMENSIONAL SPACE–FRACTIONAL GROSS–PITAEVSKII EQUATION

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The present work departs from an extended form of the classical multi-dimensional Gross–Pitaevskii equation, which considers fractional derivatives of the Riesz type in space, a generalized potential function and angular momentum rotation. It is well known that the classical system possesses functionals which are preserved throughout time. It is easy to check that the generalized fractional model considered in this work also possesses conserved quantities, whence the development of conservative and efficient numerical schemes is pragmatically justified. Motivated by these facts, we propose a finite-difference method based on weighted-shifted Grünwald differences to approximate the solutions of the generalized Gross–Pitaevskii system. We provide here a discrete extension of the uniform Sobolev inequality to multiple dimensions, and show that the proposed method is capable of preserving discrete forms of the mass and the energy of the model. Moreover, we establish thoroughly the stability and the convergence of the technique, and provide some illustrative simulations to show that the method is capable of preserving the total mass and the total energy of the generalized system.

Keywords: generalized Gross–Pitaevskii system, Riesz fractional diffusion, discrete uniform Sobolev inequality, conservative method, optimal error bounds.

1. Introduction

In recent years, fractional derivatives have been introduced to mathematical models in order to provide more realistic descriptions of physical phenomena. For instance, many fractional systems have been obtained as continuous limits of discrete systems of particles with long-range interactions (Tarasov, 2006; Tarasov and Zaslavsky, 2008). However, independently of that, fractional derivatives have been successfully used in the theory of viscoelasticity (Koeller, 1984), the theory of thermoelasticity (Povstenko, 2009), financial problems under a continuous time frame (Scalas *et al.*, 2000), self-similar protein dynamics (Glöckle and Nonnenmacher, 1995) and quantum mechanics (Namias, 1980). Moreover, some distributed-order fractional diffusion-wave equations are used in the modeling of groundwater flow to and from wells (Su *et al.*, 2015; Pimenov *et al.*, 2017), among other interesting applications (Oprzędkiewicz *et al.*, 2016).

From the mathematical point of view, the investigation of fractional systems turns out to be a fruitful (though challenging) task. Methods from mathematics and computer science were employed to establish suitable results on the existence and uniqueness of solutions of fractional partial differential equations. As examples, Morse's theory was employed to establish existence

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results of fractional p-Laplacian problems (Iannizzotto *et al.*, 2016), state feedbacks were used to prove the positivity of a class of nonlinear continuous-time models (Kaczorek, 2015), a penalization method was employed to show the concentration of solutions for a class of multidimensional fractional elliptic equations (Alves and Miyagaki, 2016), and even neural networks were exploited to prove the existence and uniform stability of complex-valued systems with delay (Rakkiyappan *et al.*, 2015).

As expected, the complexity of fractional problems is considerably higher than that of integer-order models, whence the need to design reliable numerical techniques to approximate the solutions is pragmatically justified. In this direction, the literature reports various methods to approximate the solutions of fractional systems. For example, some numerical methods were proposed to solve fractional partial differential equations (Macías-Díaz, 2018; 2019), the time-fractional diffusion equation (Alikhanov, 2015), the fractional Schrödinger equation in multiple spatial dimensions (Bhrawy and Abdelkawy, 2015), the nonlinear fractional Korteweg-de Vries–Burgers equation (El-Ajou *et al.*, 2015), the fractional FitzHugh–Nagumo monodomain model in two spatial dimensions (Liu *et al.*, 2015), distributed-order time-fractional diffusion-wave equations in bounded domains (Ye *et al.*, 2015), time-fractional diffusion equations with delay (Pimenov and Hendy, 2017) and some Hamiltonian hyperbolic fractional differential equations that generalize various well-known wave equations from relativistic quantum mechanics (Macías-Díaz, 2017).

It is important to point out that the development of Hamiltonian finite-difference schemes is an important research direction in numerical analysis. Many nonlinear partial differential equations of integer order are known to posses energy functionals that are preserved under suitable boundary conditions, including models like the Schrödinger, the sine-Gordon and the nonlinear Klein–Gordon equations from relativistic quantum mechanics, just to mention some wave equations of physical relevance. Several groups of researchers developed reliable numerical techniques to approximate the solutions of these and other nonlinear conservative systems as well as constant energy functionals associated to them. Historically, the most notable contributions were the energy-preserving finite-difference methodologies proposed for the Schrödinger (Tang *et al.*, 1996), the sine-Gordon (Ben-Yu *et al.*, 1986; Fei and Vázquez, 1991) and the nonlinear Klein–Gordon regimes (Strauss and Vazquez, 1978). Those works were the sources of motivation for the numerical investigation carried out in many papers published later on (Furihata, 2001; Matsuo and Furihata, 2001).

In the present work, we propose a numerical method to solve a fractional Gross–Pitaevskii equation. The continuous system has conserved quantities, whence the development of conservative schemes to solve it is justified. We propose a methodology based on weighted-shifted Grünwald operators, and show rigorously that the numerical model preserves discrete forms of the mass and the energy of the system. The main contribution of this work is summarized as the numerical model (36) and (37). Moreover, as one of the most important results of this manuscript, we propose a discrete uniform Sobolev inequality in multiple dimensions. Using this result, we have been able to provide optimal error estimates, in the sense that the constraints do not depend on quotients of the discrete norms. As a consequence, we prove that the technique proposed in this work is convergent and stable. Some numerical simulations show that the discrete quantities of interest are preserved at each time-step.

2. Mathematical model

Throughout this work, we let $d = 2, 3$, and consider an open and bounded domain $\Omega \subseteq \mathbb{R}^d$. The symbols β and γ will represent dimensionless and nonnegative constants, and $\varphi_0 : \overline{\Omega} \to \mathbb{C}$ will denote a smooth function. Meanwhile, $V : \overline{\Omega} \to \mathbb{R}$ represents a differentiable function, and $\varphi : \overline{\Omega} \times [0, \infty) \to \mathbb{C}$ will be a sufficiently smooth function satisfying the nonlinear fractional partial differential equation

$$i\frac{\partial \varphi(x,t)}{\partial t} = \Big[\tfrac{1}{2}(-\Delta)^{\alpha/2} + V(x) - \gamma L_z + \beta|\varphi(x,t)|^2\Big]\varphi(x,t), \tag{1}$$

for each $(x, t) \in \Omega \times (0, \infty)$, such that

$$\begin{cases} \varphi(x,0) = \varphi_0(x), & \forall x \in \Omega, \\ \varphi(x,t) = 0, & \forall (x,t) \in \partial\Omega \times [0,\infty). \end{cases} \tag{2}$$

For compatibility reasons, we suppose that $\varphi_0(x) = 0$ for each $x \in \partial\Omega$. On the other hand, the operator L_z is here the z-component of the angular momentum, given by

$$L_z = -i(x\partial_y - y\partial_x) = -i\partial_\theta. \tag{3}$$

Various remarks are in order. To start with, it is important to note that the system (1) is equivalent to the original form of the classical Gross–Pitaevskii (GP) system when $\alpha = 2$. It is worth recalling that the classical GP system is a mathematical model that preserves the total mass and the total energy. The functions of mass and energy associated with (1) take on the forms

$$M(\varphi(\cdot,t)) = \|\varphi(\cdot,t)\|^2_{L^2}, \tag{4}$$

and

$$E(\varphi(\cdot,t)) = \tfrac{1}{2}\|(-\Delta)^{\alpha/4}\|^2_{L^2} + \int_\Omega \big[V(x)|\varphi(x,t)|^2 + F(|\varphi(x,t)|^2) - \gamma\overline{\varphi}(x,t)L_z\varphi(x,t)\big]\,\mathrm{d}x, \tag{5}$$

for each $t \geq 0$, respectively, where $\overline{z}$ denotes the conjugate for any $z \in \mathbb{C}$, and

$$F(a) = \frac{1}{2}\beta a^2, \tag{6}$$

for each $a \in \mathbb{R}$. As a consequence, $M(\varphi(\cdot,t)) = M(\varphi_0)$ and $E(\varphi(\cdot,t)) = E(\varphi_0)$, for each $t \geq 0$.

From the physical point of view, the GP equation describes the ground state of a quantum system of identical bosons using the Hartree–Fock approximation and the pseudo-potential interaction model (Gross, 1961; Pitaevskii, 1961). This model has been used to describe the single-particle wave-function in a Bose–Einstein condensate, and it is similar in form to the Ginzburg–Landau equation. It is worth mentioning that the GP equation has been sometimes referred to as a nonlinear Schrödinger equation. Indeed, the GP equation has the form of the Schrödinger equation with the addition of a nonlinear interaction term. In the standard literature the GP equation is usually obtained in the framework of the second quantization formalism. However, it can also be derived in the context of statistical physics, thus yielding a number of applications ranging from the dynamics of a Bose–Einstein condensate to the excitations of gas clouds (Raman *et al*., 1999).

The difficulty in solving and analyzing the solutions of the integer-order GP model has open prospective research directions in numerical analysis. For example, an unconditional and optimal H^1-error estimate of a finite-difference scheme were proposed for the GP equation with an angular momentum rotation term (Wang *et al*., 2018), optimal l^∞ error estimates of finite-difference methods for the coupled GP equations were derived (Wang and Zhao, 2014) and optimal point-wise error estimates of a compact difference scheme for the coupled GP equations in one dimension were reported (Wang and Zhao, 2014), while other methods were proposed to investigate nonlinear Schrödinger–GP equations with a rotation term and nonlocal nonlinear interactions (Antoine *et al*., 2016). Most of the reports available in the literature investigate one-dimensional forms of the GP equation, and the efficiency analysis of those techniques heavily relies on the conservation laws. As a consequence, the arguments are difficult to extend to the higher-dimensional case. Moreover, there are some efficient finite-difference schemes for high-dimensional GP equations, but the error estimates come with constraints on the grid ratios.

Recently, Wang *et al*. (2018) developed a different approach to analyze a Crank–Nicolson method for a GP equation. The approach relied on two different techniques called 'cut-off' and 'lifting', along with the use of a discrete Sobolev inequality. In this way, error estimates in the H^1-norm were established. The goal of this work is to employ the same techniques to provide unconstrained optimal error estimates for a discretization of (1). To this end, we will propose a suitable discrete fractional Sobolev-type inequality in higher dimensions, and applications of this inequality will be used to establish the stability and convergence of the numerical technique. Moreover, we will show that the proposed scheme is capable of preserving discrete forms of (4) and (5), in agreement with the properties of the continuous model (1).

3. Numerical model

The numerical model proposed in this work is valid for both the two- and the three-dimensional cases. However, we will provide the description only for the case $d = 2$. To this end, assume that $\Omega = (x_L, x_R) \times (y_L, y_R) \subseteq \mathbb{R}^2$, where $x_L < x_R$ and $y_L < y_R$. We will approximate solutions for $t \in [0, T]$, where $0 < T < T_{\max}$ and $T_{\max}$ is the maximal time for which the solution of (1) exists. For convenience, let $\mathcal{I}_n = \{1, \ldots, n\}$ and $\mathring{\mathcal{I}}_n = \mathcal{I}_n \cup \{0\}$, for each $n \in \mathbb{N}$.

Let $N, M_1, M_2 \in \mathbb{N}$, and define the partition steps $\tau = T/N$, $h_1 = (x_R - x_L)/M_1$, $h_2 = (y_R - y_L)/M_2$ and $h = \max\{h_1, h_2\}$. For each $n \in \mathring{\mathcal{I}}_N$, assume that $t_n = n\tau$. Moreover, let $(x_j, y_k) = (x_L + jh_1, y_L + kh_2)$ for each $(j,k) \in \mathring{\mathcal{T}}_h$, and define $\mathring{\mathcal{T}}_h = \mathring{\mathcal{I}}_{M_1} \times \mathring{\mathcal{I}}_{M_2}$ and $\mathcal{T}_h = \mathcal{I}_{M_1 - 1} \times \mathcal{I}_{M_2 - 1}$. Let $\mathcal{W}_h$ be the space of all complex functions defined on $\mathring{\mathcal{T}}_h$ which vanish at the boundary of the grid, that is, let

$$\mathcal{W}_h = \Big\{ u : \mathring{\mathcal{T}}_h \to \mathbb{C} \,|\, u_{jk} = 0,\ \forall (j,k) \notin \mathcal{T}_h \Big\}. \tag{7}$$

Clearly, $\mathcal{W}_h \subseteq \mathbb{C}^{(M_1+1)\times(M_2+1)}$. Here, we use the convention that $u_{j,k} = u(j,k)$, for each $(j,k) \in \mathring{\mathcal{T}}_h$. Moreover, we will use the symbols $\phi^n_{j,k}$ and $\psi^n_{j,k}$ to represent, respectively, the exact solution and a numerical approximation to the exact solution of the problem (1) at (x_j, y_k, t_n), for each $(j,k,n) \in \mathring{\mathcal{T}}_h \times \mathring{\mathcal{I}}_N$. In turn, $\phi^n, \psi^n \in \mathcal{W}_h$ will represent, respectively, the exact and the numerical vector solutions at the time t_n, for each $n \in \mathring{\mathcal{I}}_N$. Finally, $V_{j,k}$ represents the number $V(x_j, y_k)$, for each $(j,k) \in \mathcal{T}_h$.

Remark 1. For future reference, it is important to recall that 'τ' denotes the temporal step-size. On the other hand, '$\mathcal{T}_h$' represents the set of pairs of indexes described above.

Let $(u^n)_{n=0}^N \in \mathcal{W}_h$. We define the following linear difference operators, for all $(j,k,n) \in \mathcal{T}_h \times \mathcal{I}_{N-1}$:

$$\delta_t^+ u^n_{j,k} = \frac{u^{n+1}_{j,k} - u^n_{j,k}}{\tau}, \tag{8}$$

$$\delta_t u_{j,k}^n = \frac{u_{j,k}^{n+1} - u_{j,k}^{n-1}}{2\tau}, \tag{9}$$

$$\delta_x^+ u_{j,k}^n = \frac{u_{j+1,k}^n - u_{j,k}^n}{h_1}, \tag{10}$$

$$\delta_x u_{j,k}^n = \frac{u_{j+1,k}^n - u_{j-1,k}^n}{2h_1}, \tag{11}$$

$$\delta_y^+ u_{j,k}^n = \frac{u_{j,k+1}^n - u_{j,k}^n}{h_2}, \tag{12}$$

$$\delta_y u_{j,k}^n = \frac{u_{j,k+1}^n - u_{j,k-1}^n}{2h_2}, \tag{13}$$

$$\delta_x^2 u_{j,k}^n = \frac{u_{j+1,k}^n - 2u_{j,k}^n + u_{j-1,k}^{n-1}}{h_1^2}, \tag{14}$$

$$\delta_y^2 u_{j,k}^n = \frac{u_{j,k+1}^n - 2u_{j,k}^n + u_{j,k-1}^{n-1}}{h_2^2}, \tag{15}$$

$$L_z^h u_{j,k}^n = -i(x_j \delta_y - y_k \delta_x) u_{j,k}^n \tag{16}$$

$$\nabla_h u_{j,k}^n = (\delta_x^+ u_{j,k}, \delta_y u_{j,k}^n)^\top, \tag{17}$$

$$\mu_t^+ u_{j,k}^n = \frac{1}{2}(u_{j,k}^{n+1} + u_{j,k}^n). \tag{18}$$

Definition 1. For any function $f : \mathbb{R} \to \mathbb{R}$, any $h > 0$ and any $\alpha \in (1, 2]$ we define the *weighted-shifted Grünwald difference* of order α of f at the point x as

$$\Delta_h^\alpha f(x) = \frac{1}{2\cos(\frac{\pi\alpha}{2})} \left({}_L\Delta_h^\alpha f(x) + {}_R\Delta_h^\alpha f(x) \right), \tag{19}$$

where ${}_L\Delta_h^\alpha$ and ${}_R\Delta_h^\alpha$ are, respectively, the *left* and the *right weighted-shifted Grünwald operators*, given by

$${}_L\Delta_h^\alpha f(x) = \frac{1}{h^\alpha} \sum_{i=0}^{\infty} \omega_i^\alpha f(x - (i+1)h), \tag{20}$$

$${}_R\Delta_h^\alpha f(x) = \frac{1}{h^\alpha} \sum_{i=0}^{\infty} \omega_i^\alpha f(x + (i+1)h), \tag{21}$$

respectively. The coefficients $(\omega_i^\alpha)_{i=0}^\infty$ are defined by

$$\begin{cases} \omega_0^\alpha = \dfrac{\alpha}{2} g_0^\alpha, \\ \omega_i^\alpha = \dfrac{\alpha}{2} g_i^\alpha + \dfrac{2-\alpha}{2} g_{i-1}^\alpha, \quad \forall i \in \mathbb{N}. \end{cases} \tag{22}$$

Here,

$$\begin{cases} g_0^\alpha = 1, \\ g_i^\alpha = (1 - \dfrac{\alpha+1}{i}) g_{i-1}^\alpha, \quad \forall i \in \mathbb{N}. \end{cases} \tag{23}$$

The left and right weighted-shifted Grünwald operators in Definition 1 approximate consistently the left and right Riemann–Liouville fractional derivatives of $f \in L_1(\mathbb{R})$ of order α at x, respectively, with the order of consistency $\mathcal{O}(h^2)$ (Tian *et al.*, 2015). Moreover, for a function f defined on a bounded domain B,

$$\begin{aligned} \Delta_h^\alpha f(x_j) &= \frac{1}{2h^\alpha \cos(\frac{\pi\alpha}{2})} \left(\sum_{i=0}^{\infty} \omega_i^\alpha f(x_{j-i+1}) \right. \\ &\quad \left. + \sum_{i=0}^{\infty} \omega_i^\alpha f(x_{j+i+1}) \right) \\ &= \frac{\mathrm{d}^\alpha f(x_j)}{\mathrm{d}|x|^\alpha} + \mathcal{O}(h^2). \end{aligned} \tag{24}$$

Let $(u^n)_{n=0}^N \in \mathcal{W}_h$. Define the difference operators

$$\begin{aligned} \delta_x^\alpha u_{j,k}^n &= \frac{1}{2h_1^\alpha \cos(\frac{\pi\alpha}{2})} \left(\sum_{l=0}^{j+1} \omega_l^\alpha u_{j-l+1,k}^n \right. \\ &\quad \left. + \sum_{l=0}^{M_1-j+1} \omega_l^\alpha u_{j+l+1,k}^n \right), \end{aligned} \tag{25}$$

$$\begin{aligned} \delta_y^\alpha u_{j,k}^n &= \frac{1}{2h_2^\alpha \cos(\frac{\pi\alpha}{2})} \left(\sum_{l=0}^{k+1} \omega_l^\alpha u_{j,k-l+1}^n \right. \\ &\quad \left. + \sum_{l=0}^{M_2-k+1} \omega_l^\alpha u_{j,k+l+1}^n \right), \end{aligned} \tag{26}$$

for each $(j, k, n) \in \mathcal{T}_h \times \mathcal{I}_{N-1}$. Moreover, let

$$\delta_h^\alpha u_{j,k}^n = (\delta_x^\alpha + \delta_y^\alpha) u_{j,k}^n. \tag{27}$$

Obviously, $\delta_h^\alpha u_{j,k}^n = (-\Delta)^{\alpha/2} u_{j,k}^n + \mathcal{O}(h^2)$. We define $\langle \cdot, \cdot \rangle : \mathcal{W}_h \times \mathcal{W}_h \to \mathbb{C}$ and $\langle \cdot, \cdot \rangle_* : \mathcal{W}_h \times \mathcal{W}_h \to \mathbb{C}$ by

$$\langle u, v \rangle = h_1 h_2 \sum_{j=1}^{M_1-1} \sum_{k=1}^{M_2-1} u_{j,k} \overline{v}_{j,k}, \tag{28}$$

$$\langle u, v \rangle_* = h_1 h_2 \sum_{j=0}^{M_1-1} \sum_{k=0}^{M_2-1} u_{j,k} \overline{v}_{j,k}, \tag{29}$$

for each $u, v \in \mathcal{W}_h$.

For each $u \in \mathcal{W}_h$, let

$$\|u\|^2 = \langle u, u \rangle, \tag{30}$$

$$\|\delta_x^+ u\|^2 = \langle \delta_x^+ u_{j,k}, \delta_x^+ u_{j,k} \rangle_*, \tag{31}$$

$$\|\delta_y^+ u\|^2 = \langle \delta_y^+ u_{j,k}, \delta_y^+ u_{j,k} \rangle_*. \tag{32}$$

$$\|u\|_\infty = \max\{|u_{j,k}| : (j,k) \in \mathcal{T}_h\}. \tag{33}$$

Moreover, set

$$\|w\|_p = \left(h_1 h_2 \sum_{j=1}^{M_1-1} \sum_{k=1}^{M_2-1} |w_{j,k}|^p \right)^{1/p}, \tag{34}$$

$$\|\nabla_h w\|^2 = \|\delta_x^+ u\|^2 + \|\delta_y^+ u\|^2, \tag{35}$$

for all $w \in \mathcal{W}_h$. With this notation, the finite-difference method to approximate the solutions of (1) is given by

$$\begin{aligned} i\delta_t^+ \psi_{j,k}^n = &\left(\frac{1}{2}\delta_h^\alpha + V_{j,k} - \gamma L_z^h\right)\mu_t^+ \psi_{j,k}^n \\ &+ \beta\mu_t^+(|\psi_{j,k}^n|^2 \psi_{j,k}^n), \end{aligned} \tag{36}$$

for each $(j,k,n) \in \mathcal{T}_h \times \mathcal{I}_{N-1}$. We impose the condition

$$\psi_{j,k}^0 = \psi_0(x_j, y_k), \quad \forall (j,k) \in \mathring{\mathcal{T}}_h. \tag{37}$$

It is easy to check that this finite-difference scheme is an implicit method. Moreover, the extension to the three-dimensional scenario is a straightforward task. In the following sections we will establish that (36) is a consistent and stable discretization of the model (1), which converges to the solution with quadratic order. Moreover, we will provide discrete forms of (4) and (5) which, as the continuous counterparts, are invariant.

4. Auxiliary lemmas

The analysis of the finite-difference method (36) will rely on the use of a suitable Sobolev inequality for the two-dimensional scenario. To this end, assume that $h_1, h_2 \in \mathbb{R}^+$, and define $x_j = jh_1$ and $y_k = kh_2$, for all $j,k \in \mathbb{Z}$. Let $\mathcal{W}_h^*$ denote the set of all functions $u : \mathbb{Z}^2 \to \mathbb{C}$, and assume that $u_{j,k} = u(j,k)$ for each $(j,k) \in \mathbb{Z}^2$. In this section, we define $\langle \cdot,\cdot \rangle : \mathcal{W}_h^* \times \mathcal{W}_h^* \to \mathbb{C}$ and $\|\cdot\| : \mathcal{W}_h^* \to \mathbb{R}$ by

$$\langle u, v\rangle = h_1 h_2 \sum_{j\in\mathbb{Z}}\sum_{k\in\mathbb{Z}} u_{j,k}\overline{v}_{j,k}, \tag{38}$$

$$\|u\|^2 = \langle u, u\rangle, \tag{39}$$

for each $u, v \in \mathcal{W}_h^*$, whenever these numbers exist. Moreover, let $L_h^2 = \{u \in \mathcal{W}_h^* : \|u\|^2 < \infty\}$.

Definition 2. For each $u \in L_h^2$, define the *semi-discrete Fourier transform* by

$$\hat{u}(\kappa_1, \kappa_2) = \frac{h_1 h_2}{2\pi} \sum_{k\in\mathbb{Z}} u_{j,k} e^{-i(\kappa_1 x_j + \kappa_2 y_k)}, \tag{40}$$

for each $(\kappa_1, \kappa_2) \in \mathbb{R}^2$.

Notice now that the condition $u \in L_h^2$ guarantees that $\hat{u} \in L^2([-\pi/h, \pi/h] \times [-\pi/h, \pi/h])$. Moreover, the inversion formula and Parseval's identity in two dimensions are respectively given by

$$u_{j,k} = \frac{1}{2\pi}\int_{-\pi/h_1}^{\pi/h_1}\int_{-\pi/h_2}^{\pi/h_2} \hat{u}(\kappa_1,\kappa_2) e^{i(\kappa_1 x_j, \kappa_2 y_k)} \mathrm{d}\kappa_2 \mathrm{d}\kappa_1, \tag{41}$$

$$\langle u, v\rangle = \int_{-\pi/h_1}^{\pi/h_1}\int_{-\pi/h_2}^{\pi/h_2} \hat{u}(\kappa_1,\kappa_2)\overline{\hat{v}}(\kappa_1,\kappa_2) \mathrm{d}\kappa_1 \mathrm{d}\kappa_2, \tag{42}$$

for each $(j,k) \in \mathbb{Z}^2$ and $u, v \in L_h^2$.

Definition 3. Let $0 \le \sigma \le 1$. Define the *fractional Sobolev norm* $\|\cdot\|_{H^\sigma} : \mathcal{W}_h^* \to \mathbb{R}$ and the *semi-norm* $|\cdot|_{H^\sigma} : \mathcal{W}_h^* \to \mathbb{R}$, respectively, by

$$\begin{aligned} \|u\|_{H^\sigma}^2 = &\int_{-\pi/h_1}^{\pi/h_1}\int_{-\pi/h_2}^{\pi/h_2} \left(1 + |\kappa_1|^{2\sigma}|\kappa_2|^{2\sigma}\right) \\ &\cdot |\hat{u}(\kappa_1,\kappa_2)|^2 \mathrm{d}\kappa_1 \mathrm{d}\kappa_2, \end{aligned} \tag{43}$$

$$\begin{aligned} |u|_{H^\sigma}^2 = &\int_{-\pi/h_1}^{\pi/h_1}\int_{-\pi/h_2}^{\pi/h_2} \left(|\kappa_1|^{2\sigma} + |\kappa_2|^{2\sigma}\right) \\ &\cdot |\hat{u}(\kappa_1,\kappa_2)|^2 \mathrm{d}\kappa_1 \mathrm{d}\kappa_2. \end{aligned} \tag{44}$$

Obviously, it readily follows that

$$\|u\|_{H^\sigma}^2 = \|u\|^2 + |u|_{H^\sigma}^2, \quad |u|_{H^0}^2 = \|u\|^2, \tag{45}$$

for each $u \in \mathcal{W}_h^*$. The discrete L^p and L^∞ norms on $\mathcal{W}_h^*$ are defined in the classical ways.

Lemma 1. (Discrete uniform Sobolev inequality) *For every $1/2 < \sigma \le 1$, there is a constant $C_\sigma = C(\sigma) > 0$ independent of $h_1, h_2 > 0$, such that $\|u\|_{L^\infty} \le C_\sigma \|u\|_{H^\sigma}$ for each $u \in \mathcal{W}_h^*$.*

Proof. The result readily follows after noting that

$$\begin{aligned} \|u\|_{L^\infty} \le &\frac{1}{2\pi}\int_{-\pi/h_1}^{\pi/h_1}\int_{-\pi/h_2}^{\pi/h_2} |\hat{u}(\kappa_1,\kappa_2)| \,\mathrm{d}\kappa_1 \mathrm{d}\kappa_2 \\ \le &\frac{1}{2\pi}\sqrt{\int_{-\pi/h_1}^{\pi/h_1}\int_{-\pi/h_2}^{\pi/h_2} \frac{\mathrm{d}\kappa_1 \mathrm{d}\kappa_2}{\sqrt{1 + |\kappa_1\kappa_2|^{2\sigma}}}} \\ &\cdot \sqrt{\int_{-\pi/h_1}^{\pi/h_1}\int_{-\pi/h_2}^{\pi/h_2} \frac{|\hat{u}(\kappa_1,\kappa_2)| \,\mathrm{d}\kappa_1 \mathrm{d}\kappa_2}{(1 + |\kappa_1\kappa_2|^{2\sigma})^{-1/2}}} \\ \le &\frac{\|u\|_{H^\sigma}}{2\pi}\sqrt{\int_{-\pi/h_1}^{\pi/h_1}\int_{-\pi/h_2}^{\pi/h_2} \frac{\mathrm{d}z_1 \mathrm{d}z_2}{\sqrt{1 + |z_1 z_2|^{2\sigma}}}} \end{aligned} \tag{46}$$

hold for any $u \in \mathcal{W}_h^*$, and that the coefficient of $\|u\|_{H^\sigma}$ is independent of h_1 and h_2. ■

Lemma 2. *Let $u, v \in \mathcal{W}_h^*$.*

(a) $\langle \delta_x u, v\rangle = -\langle u, \delta_x v\rangle$ *and* $\langle \delta_y u, v\rangle = -\langle u, \delta_y v\rangle$.

(b) $\langle \delta_x^2 u, v\rangle = -\langle \delta_x^+ u, \delta_x^+ v\rangle$, $\langle \delta_y^2 u, v\rangle = -\langle \delta_y^+ u, \delta_y^+ v\rangle$.

(c) *For each $1 < \alpha < 2$ there is $C > 0$ which depends on α, such that $C|u|_{H^{\alpha/2}}^2 \le \langle \delta_h^\alpha u, u\rangle \le |u|_{H^{\alpha/2}}^2$.*

(d) *If $1 < \alpha < 2$ then $\langle \delta_h^\alpha u, v\rangle \le |u|_{H^{\alpha/2}}|v|_{H^{\alpha/2}}$.*

Proof. Properties (a) and (b) are well known.

(c) First, observe that the one-dimensional case (Wang *et al.*, 2016) guarantees that

$$\begin{aligned} &\frac{2^\alpha(1-\alpha)}{\pi^\alpha \cos(\frac{\pi\alpha}{2})}\left(|\kappa_1|^\alpha + |\kappa_2|^\alpha\right) \\ &\quad \le h_1^{-\alpha} f(\alpha, h_1\kappa_1) + h_2^{-\alpha} f_2(\alpha, h_2\kappa_2) \\ &\quad \le |\kappa_1|^\alpha + |\kappa_2|^\alpha, \end{aligned} \tag{47}$$

where

$$f(\beta,z)=\frac{1}{2\cos(\frac{\pi\beta}{2})}\left(\sum_{l=0}^{\infty}\omega_l^{\beta}e^{i(l-1)z}+\sum_{l=0}^{\infty}\omega_l^{\beta}e^{-i(l-1)z}\right), \tag{48}$$

for each $\beta\in(1,2]$ and $z\in\mathbb{R}$. Multiplying all the three terms of (47) by $|\hat{u}(\kappa_1,\kappa_2)|^2$, integrating over all $(\kappa_1,\kappa_2)\in[-\pi/h_1,\pi/h_1]\times[-\pi/h_2,\pi/h_2]$ and using Parseval's identity in two dimensions, we note that there exists $C>0$ such that

$$\begin{aligned}C|u|^2_{H^{\alpha/2}}&\le\int_{-\pi/h_1}^{\pi/h_1}\int_{-\pi/h_2}^{\pi/h_2}\Big[h_1^{-\alpha}f(\alpha,h_1\kappa_1)\\&\quad+\frac{f(\alpha,h_2\kappa_2)}{h_2^{\alpha}}\Big]|\hat{u}(\kappa_1,\kappa_2)|^2\,\mathrm{d}\kappa_1\mathrm{d}\kappa_2\\&=\langle\delta_h^{\alpha}u,u\rangle\le|u|^2_{H^{\alpha/2}},\end{aligned} \tag{49}$$

where clearly $C=2^{\alpha}\pi^{-\alpha}(1-\alpha)/\cos(\pi\alpha/2)$.

The proof of (d) is similar to that of (c). ■

Lemma 3. *If $\alpha\in(1,2]$ then there exists a linear operator $\Lambda_h^{\alpha}:\mathcal{W}_h\to\mathcal{W}_h$ such that $\langle\delta_h^{\alpha}u,v\rangle=\langle\Lambda_h^{\alpha}u,\Lambda_h^{\alpha}v\rangle$, for each $u,v\in\mathcal{W}_h$.*

Proof. Let $\mathbf{D}=h_1^{-\alpha}\mathbf{I}_{M_2-1}\otimes\mathbf{C}+h_2^{-\alpha}\widetilde{\mathbf{C}}\otimes\mathbf{I}_{M_1-1}$, where $\oplus$ is the Kronecker product of matrices, $\mathbf{I}_M$ is the identity matrix of size $M\times M$ for each $M\in\mathbb{Z}$,

$$\begin{aligned}u^n=\big(&u^n_{1,1},\dots,u_{M_1-1,1},\\&u^n_{1,2},\dots,u_{M_1-1,2},\dots,\\&u^n_{1,M_2-1},\dots,u_{M_1-1,M_2-1}\big)^{\top},\end{aligned} \tag{50}$$

where, clearly, $u^n\in\mathbb{C}^{(M_1-1)\times(M_2-1)}$,

$$\mathbf{C}=\frac{1}{2\cos(\frac{\pi\alpha}{2})}(\mathbf{W}+\mathbf{W}^{\top}), \tag{51}$$

$$\widetilde{\mathbf{C}}=\frac{1}{2\cos(\frac{\pi\alpha}{2})}(\widetilde{\mathbf{W}}+\widetilde{\mathbf{W}}^{\top}), \tag{52}$$

and the matrices $\mathbf{W},\widetilde{\mathbf{W}}\in\mathbb{C}^{(M_1-1)\times(M_1-1)}$ are given by

$$\mathbf{W}=\begin{pmatrix}\omega_1^{\alpha}&\omega_0^{\alpha}&0&\cdots&0\\\omega_2^{\alpha}&\omega_1^{\alpha}&\omega_0^{\alpha}&\cdots&0\\\omega_3^{\alpha}&\omega_2^{\alpha}&\omega_1^{\alpha}&\cdots&0\\\vdots&\vdots&\vdots&\ddots&\vdots\\\omega_{M_1-2}^{\alpha}&\omega_{M_1-3}^{\alpha}&\omega_{M_1-4}^{\alpha}&\cdots&\omega_0^{\alpha}\\\omega_{M_1-1}^{\alpha}&\omega_{M_1-2}^{\alpha}&\omega_{M_1-3}^{\alpha}&\cdots&\omega_1^{\alpha}\end{pmatrix}, \tag{53}$$

$$\widetilde{\mathbf{W}}=\begin{pmatrix}\omega_1^{\alpha}&\omega_0^{\alpha}&0&\cdots&0\\\omega_2^{\alpha}&\omega_1^{\alpha}&\omega_0^{\alpha}&\cdots&0\\\omega_3^{\alpha}&\omega_2^{\alpha}&\omega_1^{\alpha}&\cdots&0\\\vdots&\vdots&\vdots&\ddots&\vdots\\\omega_{M_2-2}^{\alpha}&\omega_{M_2-3}^{\alpha}&\omega_{M_2-4}^{\alpha}&\cdots&\omega_0^{\alpha}\\\omega_{M_2-1}^{\alpha}&\omega_{M_2-2}^{\alpha}&\omega_{M_2-3}^{\alpha}&\cdots&\omega_1^{\alpha}\end{pmatrix}. \tag{54}$$

Obviously, $\mathbf{C}$ and $\widetilde{\mathbf{C}}$ are symmetric and positive definite matrices. As a consequence, $\mathbf{D}$ is likewise symmetric and positive definite. Thus, there exists a real orthogonal matrix $\mathbf{P}$ and a real diagonal matrix $\mathbf{A}$, such that

$$\mathbf{D}=\mathbf{P}\mathbf{A}\mathbf{P}^{\top}=\mathbf{L}^{\top}\mathbf{L}, \tag{55}$$

where $\mathbf{L}=\mathbf{P}\mathbf{A}^{1/2}\mathbf{P}^{\top}$. Finally, let now $u,v\in\mathcal{W}_h$ and note that $\delta_h^{\alpha}u^n=(\delta_x^{\alpha}+\delta_y^{\alpha})u^n=\mathbf{D}u^n$. It follows that $\langle\delta_h^{\alpha}u,v\rangle=\langle\mathbf{L}^{\top}\mathbf{L}u,v\rangle=\langle\mathbf{L}u,\mathbf{L}v\rangle$, and the conclusion is reached letting $\Lambda_h^{\alpha}=\mathbf{P}\mathbf{A}^{1/2}\mathbf{P}^{\top}$. ■

The following result will be a useful tool to prove the invariance of some quantities associated to (36).

Lemma 4. (Bao and Cai, 2013) *Let $u,v\in\mathcal{W}_h$.*

(a) $\langle-\delta_x^2u,v\rangle=\langle\delta_xu,\delta_xv\rangle$, *and there exists $C\ge0$ such that $\|u\|\le C\|\nabla_hu\|$.*

(b) $\langle\delta_x^{\alpha}u,u\rangle\le0$ *and* $\langle\delta_y^{\alpha}u,u\rangle\le0$, *for each $1<\alpha<2$.*

(c) $\langle L_z^hu,v\rangle=\langle v,L_z^hu\rangle$.

(d) $\frac{1}{2}(1-\frac{\gamma^2}{\mu^2})\|\nabla_hu\|^2\le\mathcal{E}(u)\le C\|\nabla_hu\|^2$, *where*

$$\begin{aligned}\mathcal{E}(u)=\tfrac{1}{2}\|\nabla_hu\|^2+h_1h_2\sum_{j=1}^{M_1-1}\sum_{k=1}^{M_2-1}\big[V_{j,k}|u_{j,k}|^2\\-\gamma\overline{u}_{j,k}L_z^hu_{j,k}\big].\end{aligned} \tag{56}$$

5. Numerical properties

In the present section, we will prove that the numerical scheme (36) has some associated quantities which are preserved throughout the discrete time. Suppose that $(\psi^n)_{n=0}^N$ is a solution of (36). Let $Q^0_{j,k}=0$ and $F^0_{j,k}=\frac{1}{2}\beta|\psi^0_{j,k}|^4$, for each $(j,k)\in\mathring{\mathcal{T}}_h$. Suppose that $Q^n,F^n\in\mathcal{W}_h$ have been constructed for some $n\in\mathring{\mathcal{I}}_{N-1}$. For each $(j,k)\in\mathring{\mathcal{T}}_h$, let

$$S^n_{j,k}=\mu_t^+\left(|\psi^n_{j,k}|^2\psi^n_{j,k}\right)\mu_t^+\overline{\psi}^n_{j,k}, \tag{57}$$

and define

$$Q^{n+1}_{j,k}=Q^n_{j,k}+2\beta\operatorname{Im}S^n_{j,k}, \tag{58}$$

$$F^{n+1}_{j,k}=F^n_{j,k}+2\tau\beta\operatorname{Re}S^n_{j,k}. \tag{59}$$

Definition 4. We define respectively the *total mass* and the *total energy* of (36) at the time t_n by

$$M^n = \|\psi^n\|^2 - \tau\langle Q^n, 1\rangle, \tag{60}$$

$$\begin{aligned} E^n = \frac{1}{2}\|\Lambda^\alpha \psi^n\|^2 + h_1 h_2 \sum_{j=1}^{M_1-1}\sum_{k=1}^{M_2-1} \Big[V_{j,k}|\psi^n_{j,k}|^2 \\ + F^n_{j,k} - \gamma \overline{\psi}^n_{j,k} L^h_z \psi^n_{j,k}\Big], \end{aligned} \tag{61}$$

for each $n \in \mathring{\mathcal{I}}_N$. Here, '1' in (60) is the vector of the same size of Q^n, whose all components are equal to 1.

Theorem 1. (Invariant quantities) *If* $(\psi^n)_{n=0}^N$ *is a solution of* (36) *then the quantities* (60) *and* (61) *are conserved.*

Proof. Take the inner product of $\mu_t^+\psi^n$ with (36), take the imaginary part and then use Lemma 4 to obtain

$$\begin{aligned} \delta_t^+\|\psi^n\|^2 =& 2\beta \sum_{j=1}^{M_1-1}\sum_{k=1}^{M_2-1} \operatorname{Im} S^n_{j,k} \\ =& \langle Q^{n+1} - Q^n, 1\rangle, \end{aligned} \tag{62}$$

for each $n \in \mathring{\mathcal{I}}_{N-1}$. As a consequence, it follows that $M^{n+1} = M^n$, for each $n \in \mathring{\mathcal{I}}_{N-1}$. Calculate now the inner product of $2\delta_t^+\psi^n$ with the equations of (36), take the real part, use Lemma 4 and rearrange terms to obtain

$$\begin{aligned} &\frac{1}{2}\delta_t^+\|\Lambda_h^\alpha\psi^n\|^2 + h_1h_2 \sum_{j=1}^{M_1-1}\sum_{k=1}^{M_2-1} \Big\{\delta_t^+\left(V_{j,k}|\psi^n_{j,k}|^2\right) \\ &\quad -\gamma\delta_t^+\left(\overline{\psi}^n_{j,k}L^h_z\psi^n_{j,k}\right) + 2\beta \operatorname{Re} S^n_{j,k}\Big\} \\ &= \frac{1}{2}\delta_t^+\|\Lambda_h^\alpha\psi^n\|^2 + h_1h_2 \sum_{j=1}^{M_1-1}\sum_{k=1}^{M_2-1} \delta_t^+\left[\left(V_{j,k}|\psi^n_{j,k}|^2\right)\right. \\ &\quad \left. -\gamma\left(\overline{\psi}^n_{j,k}L^h_z\psi^n_{j,k}\right)\right] + \delta_t^+\langle F^n, 1\rangle = 0. \end{aligned} \tag{63}$$

Here, Λ_h^α is as in Lemma 3. As a conclusion, $E^{n+1} = E^n$ for each $n \in \mathring{\mathcal{I}}_{N-1}$, as desired. Finally, note that the condition $Q^0 = 0$ yields that $M^n = M^0 = \|\psi^0\|^2$, which is a convenient expression for the constant mass. ■

Example 1. We provide now a numerical proof that the discrete model (36) is capable of preserving the discrete mass and energy. The simulations were obtained using an implementation of (36) in ©Matlab 8.5.0.197613 (R2015a) on a ©Hewlett-Packard 6005 Pro Microtower computer with the Linux Mint 18 "Sylvia" Cinnamon edition. Let $T = 10$, $\Omega = [-20, 20] \times [-20, 20]$,

$$V(x) = \frac{1}{2}(x^2 + y^2), \tag{64}$$

$$\phi_0 = \frac{2}{\sqrt{\pi}}(x + iy)e^{-8(x^2+y^2)}, \tag{65}$$

$\beta = 1$ and $\gamma = 0.5$. Computationally, let $h = 0.001$ and $\tau = 0.0001$. Figure 1 shows the graphs of Q^n and E^n for various values α. The graphs show that the total mass and the total energy are approximately constant, confirming the conclusion of Theorem 1. ♦

We establish next the stability and convergence properties of the finite-difference method (36). Moreover, as we mentioned in the introduction, we will establish the optimal $H^{\alpha/2}$-error estimate of the proposed scheme without requiring additional conditions on the grid ratios. To this end, we will assume the following:

A$_1$. $V \in \mathcal{C}^1(\Omega)$, and there exists $\mu > |\gamma| > 0$ such that $V(x) \geq \frac{1}{2}\mu^2|x|^2$, for all $x \in \Omega$.

A$_2$. The solution of (1) satisfies the condition $\phi \in W^{4,\infty}([0,T]; L^\infty(\Omega)) \cap W^{3,\infty}([0,T]; W^{2,\infty}(\Omega)) \cap W^{1,\infty}([0,T]; W^{4,\infty}(\Omega) \cap H^1_0(\Omega))$.

Let $\eta^n \in \mathcal{W}_h$ be the vector of local truncation errors of the method at the n-th temporal step, for each $n \in \mathring{\mathcal{I}}_{N-1}$. More precisely, let

$$\begin{aligned} \eta^n_{j,k} = i\delta_t^+\phi^n_{j,k} - \left(\frac{1}{2}\delta_h^\alpha + V_{j,k} - \gamma L^h_z\right)\mu_t^+\phi^n_{j,k} \\ - \beta\mu_t^+(|\phi^n_{j,k}|^2\phi^n_{j,k}), \end{aligned} \tag{66}$$

for each $(j, k, n) \in \mathcal{T}_h \times \mathcal{I}_{N-1}$. The following result can be easily established using standard arguments with Taylor series and a discrete Gronwall inequality.

Theorem 2. (Consistency) *If Assumptions* A_1 *and* A_2 *are satisfied, then there exists a constant* $C_0 \geq 0$ *independent of* τ *and* h*, such that the following hold, for each* $n \in \mathring{\mathcal{I}}_{N-1}$*:*

$$\|\eta^n\| \leq C_0(\tau^2 + h^2), \tag{67}$$

$$\|\delta_t^+\eta^n\| \leq C_0(\tau^2 + h^2). \tag{68}$$

Let $1/2 < \sigma \leq 1$. Use of the discrete uniform Sobolev inequality and Lemmas 2 and 3 show that there is a constant $C > 0$ such that, for any $u \in \mathcal{W}_h$,

$$\begin{aligned} \|u\|^2_{L^\infty} \leq& C_\sigma\|u\|^2_{H^\sigma} = C_\sigma\left(\|u\|^2 + |u|^2_{H^\sigma}\right) \\ \leq& C_\sigma\left(\|u\|^2 + \frac{1}{C'}\langle\delta_h^\alpha u, u\rangle\right) \\ \leq& C\left(\|u\|^2 + \|\Lambda_h^\alpha u\|^2\right). \end{aligned} \tag{69}$$

Here, C' represents the constant of Lemma 2(c). This remark will be employed to prove the convergence of (36). Also, for each $(j, k, n) \in \mathring{\mathcal{T}}_j \times \mathring{\mathcal{I}}_N$, let

$$\epsilon^n_{j,k} = \phi^n_{j,k} - \psi^n_{j,k}, \tag{70}$$

The symbol 'C' will represent a nonnegative constant whose value may change from place to place.

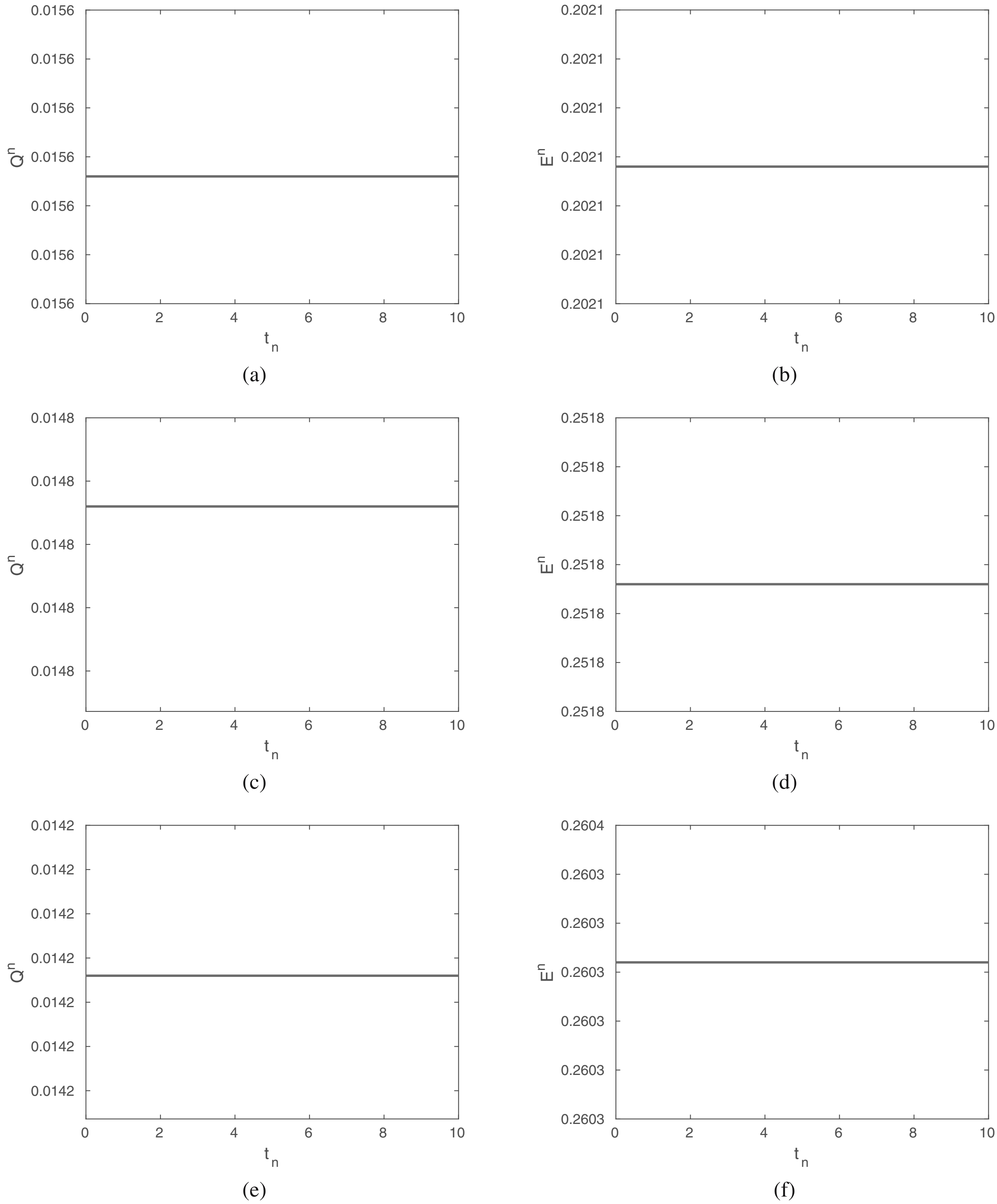

Fig. 1. Graphs of the values of Q^n (left column) and E^n (right column) versus t_n obtained using the finite-difference method (36) with $T = 10$, $\Omega = [-20, 20] \times [-20, 20]$, $\beta = 1$, $\gamma = 0.5$ and $V(x) = \frac{1}{2}(x^2 + y^2)$ and $\phi_0 = \frac{2}{\sqrt{\pi}}(x + iy)e^{-8(x^2+y^2)}$. Various values of α were employed, namely, $\alpha = 2$ (top row), $\alpha = 1.8$ (middle row) and $\alpha = 1.6$ (bottom row). The graphs show that the discrete total mass Q^n and total energy E^n are approximately constant, confirming the conclusion of Theorem 1.

Theorem 3. (Convergence) *Let Assumptions* A_1 *and* A_2 *hold. Then there exist* $h_0, \tau_0 \in \mathbb{R}^+$ *and a constant* $C > 0$ *such that* $\|\epsilon^n\|_{L^\infty} \leq C(h^2 + \tau^2)$*, for all* $0 < h \leq h_0$*,* $0 < \tau \leq \tau_0$.

Proof. Let $\rho : \mathbb{R} \to [0, 1]$ be any function in $\mathcal{C}^\infty(\mathbb{R})$, with

$$\rho(s) = \begin{cases} 1, & \forall |s| \leq 1, \\ 0, & \forall |s| \geq 2. \end{cases} \tag{71}$$

Note that $M_0 = \|\phi\|_{L^\infty} \in \mathbb{R}$, so $B = (M_0 + 1)^2 > 0$. Let $f_B : [0, \infty) \to \mathbb{R}$ be the globally Lipschitz function given by $f_B(s) = s\rho(s/B)$, for each $s \in [0, \infty)$, and assume that $\hat{\psi}^0 = \psi^0$. Define $\hat{\psi}^n \in \mathcal{W}_h$ by

$$\begin{aligned} i\delta_t^+ \hat{\psi}_{j,k}^n = & \left(\tfrac{1}{2}\delta_h^\alpha + V_{j,k} - \gamma L_z^h\right) \mu_t^+ \hat{\psi}_{j,k}^n \\ & + \beta \mu_t^+ \left[f_B(|\hat{\psi}_{j,k}^n|^2) \hat{\psi}_{j,k}^n \right], \end{aligned} \tag{72}$$

for each $(j, k, n) \in \mathring{\mathcal{T}}_h \times \mathring{\mathcal{I}}_{N-1}$. Using the facts that $f_B(|\phi_{j,k}^n|^2) = |\phi_{j,k}^n|^2$ for each $(j, k, n) \in \mathring{\mathcal{T}}_h \times \mathring{\mathcal{I}}_{N-1}$, we get that (72) approximates the partial differential equation (1) with local truncation error given by (66). Let

$$\hat{\epsilon}^n = \phi^n - \hat{\psi}^n, \tag{73}$$

for each $n \in \mathring{\mathcal{I}}_N$, and subtract (72) from (66).

After some algebraic reductions, we obtain

$$\begin{aligned} i\delta_t^+ \hat{\epsilon}_{j,k}^n = & \left(\tfrac{1}{2}\delta_h^\alpha + V_{j,k} - \gamma L_z^h\right) \mu_t^+ \epsilon_{j,k}^n \\ & + \xi_{j,k}^{n+1} - \eta_{j,k}^n, \end{aligned} \tag{74}$$

for each $(j, k, n) \in \mathring{\mathcal{T}}_h \times \mathring{\mathcal{I}}_{N-1}$. Here

$$\begin{aligned} \xi_{j,k}^n = & \beta \mu_t^+ \left[\left(f_B(|\phi_{j,k}^n|^2) - f_B(|\hat{\psi}_{j,k}^n|^2 \right) \phi_{j,k}^n \right. \\ & \left. + f_B(|\psi_{j,k}^n|^2) \hat{\epsilon}_{j,k}^n \right]. \end{aligned} \tag{75}$$

This and the global Lipschitz property of f_B imply that there exists a constant $C_1 \geq 0$ such that

$$|\xi_{j,k}^{n+1}| \leq C_1(|\hat{\epsilon}_{j,k}^n| + |\hat{\epsilon}_{j,k}^{n+1}|), \tag{76}$$

for all $(j, k, n) \in \mathring{\mathcal{T}}_h \times \mathring{\mathcal{I}}_{N-1}$. On the other hand, computing the inner product of $2\mu_t^+ \hat{\epsilon}^n$ with the vector difference equations (72), taking then the imaginary part and using Lemma 2, the Cauchy–Schwarz inequality and the bound of $|\xi_{j,k}^n|$, we readily obtain

$$\begin{aligned} & \|\hat{\epsilon}^{n+1}\|^2 - \|\hat{\epsilon}^{n+1}\|^2 \leq \tau \left| \delta_t^+ \|\hat{\epsilon}^n\|^2 \right| \\ & = \tau \left| \mathrm{Im}\langle \xi^{n+1}, \hat{\epsilon}^n + \hat{\epsilon}^{n+1} \rangle + \mathrm{Im}\langle \eta^n, \hat{\epsilon}^n + \hat{\epsilon}^{n+1} \rangle \right| \\ & \leq C_0 \tau (\tau^2 + h^2)^2 + C_1 \tau \left(\|\hat{\epsilon}^n\|^2 + \|\hat{\epsilon}^{n+1}\|^2 \right), \end{aligned} \tag{77}$$

where C_0 is the constant of Theorem 2. An application of Gronwall's inequality shows now that there exists a constant $C_2 > 0$ independent of τ and h, such that

$$\|\hat{\epsilon}^n\| \leq C_2(\tau^2 + h^2), \tag{78}$$

for each $n \in \mathring{\mathcal{I}}_N$. On the other hand, using the assumptions of the theorem and the definition of f_B, calculating the inner product of $\tau\delta_t^+ \hat{\epsilon}^n$ with (72) and taking the real part, it follows that

$$\begin{aligned} & \tfrac{1}{2} \mathrm{Re}\langle \delta_h^\alpha \mu_t^+ \hat{\epsilon}^n, \tau\delta_t^+ \hat{\epsilon}^n \rangle \\ & \quad = \mathrm{Re}\langle \eta^n, \tau\delta_t^+ \hat{\epsilon}^n \rangle + \mathrm{Re}\langle \xi^{n+1}, \tau\delta_t^+ \hat{\epsilon}^n \rangle \\ & \quad - \mathrm{Re}\langle V\mu_t^+ \hat{\epsilon}^n, \tau\delta_t^+ \hat{\epsilon}^n \rangle, \end{aligned} \tag{79}$$

for each $n \in \mathring{\mathcal{I}}_{N-1}$. But notice that

$$2\,\mathrm{Re}\langle \delta_h^\alpha \mu_t^+ \hat{\epsilon}^n, \tau\delta_t^+ \hat{\epsilon}^n \rangle = \|\Lambda_h^\alpha \hat{\epsilon}^{n+1}\|^2 - \|\Lambda_h^\alpha \hat{\epsilon}^n\|^2, \tag{80}$$

$$\begin{aligned} \mathrm{Re}\langle \eta^n, \tau\delta_t^+ \hat{\epsilon}^n \rangle & \leq \tfrac{1}{2}\|\eta^n\|^2 + \|\hat{\epsilon}^{n+1}\|^2 + \|\hat{\epsilon}^n\|^2 \\ & \leq C\big[(\tau^2 + h^2)^2 + \|\hat{\epsilon}^{n+1}\|^2 \\ & \quad + \|\hat{\epsilon}^n\|^2\big], \end{aligned} \tag{81}$$

$$\begin{aligned} \mathrm{Re}\langle \xi^n, \tau\delta_t^+ \hat{\epsilon}^n \rangle & \leq \frac{1}{2}\|\xi^n\|^2 + \|\hat{\epsilon}^{n+1}\|^2 + \|\hat{\epsilon}^n\|^2 \\ & \leq C\left(\|\hat{\epsilon}^{n+1}\|^2 + \|\hat{\epsilon}^n\|^2 \right), \end{aligned} \tag{82}$$

$$\begin{aligned} \mathrm{Re}\langle V\mu_t^+ \hat{\epsilon}^n, \tau\delta_t^+ \hat{\epsilon}^n \rangle & = \tfrac{1}{2} V \left(\|\hat{\epsilon}^{n+1}\|^2 - \|\hat{\epsilon}^n\|^2 \right) \\ & \leq C\left(\|\hat{\epsilon}^{n+1}\|^2 + \|\hat{\epsilon}^n\|^2 \right). \end{aligned} \tag{83}$$

The inequality (81) was obtained using the Cauchy–Schwarz inequality and Theorem 2, while (82) and (83) were derived using the Cauchy–Schwarz inequality and the hypotheses. The expression (79) and Gronwall's inequality now yield

$$\|\Lambda^\alpha \hat{\epsilon}^n\| \leq C(\tau^2 + h^2), \tag{84}$$

for some $C \geq 0$ which is independent of τ and h. These facts and (69) are used to reach the conclusion. ■

Finally, the stability of (36) can be established using arguments similar to those in the proof of Theorem 3.

6. Conclusions

In this work, we investigated numerically a fractional extension of the Gross–Pitaevskii equation in multiple spatial dimensions. The total mass and the total energy of the system are quantities that are preserved throughout time, whence the design of mass- and energy-preserving finite-difference methods to solve the model is an interesting problem in numerical mathematics. In the present work, we propose numerical model to solve the Gross–Pitaevskii equation together with discrete forms of the total mass and the total energy, and prove mathematically that those quantities are invariants.

To carry out the efficiency analysis, we proposed and proved a multidimensional discrete form of the uniform Sobolev inequality. Perhaps this is the most important contribution of this manuscript. With such a result, we were able to provide optimal bounds for the error associated to the method. The convergence and the stability are proved thoroughly, and some simulations show the capability of the method to preserve the invariant quantities.

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