

CMMSE: analysis and comparison of some numerical methods to solve a nonlinear fractional Gross–Pitaevskii system

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Abstract

In this work, we introduce and theoretically analyze various computational techniques to approximate the solutions of solve a fractional extension of a double condensate system. More precisely, the continuous model extends the well-known Gross–Pitaevskii equation to the fractional scenario, and considering two interacting condensates. The mathematical system considers two complex-valued regimes with coupling, and a mass and energy functions are associated to this model. Both are constant in time. Here, various discretizations are analyzed

to solve this system. Some of them are able to preserve the mass and the energy, some are not. We discuss the existence of solutions, the consistency of the models, the stability and the convergence. Finally, from the computational point of view, some algorithms are simpler to code than others. In fact, those for which the mass and the energy are conserved are more difficult to implement. We discuss here pros and cons.

Keywords: fractional Bose–Einstein model; double-fractional system; fully discrete model; stability and convergence analysis

MSC Classification: 65Mxx; 65Qxx

1 Introduction

In this manuscript, we let $p \in \mathbb{N}$ be the number of spatial dimensions and $T \in \mathbb{R}^+$ corresponds to a final time. We agree that $I_n = \{k \in \mathbb{N} : k \leq n\}$, while \bar{I}_n , the so-called ‘closure of I_n ’, is defined by $\{0\} \cup I_n$, for each $n \in \mathbb{N}$. We will let a_i and b_i be real numbers which must satisfy $a_i < b_i$, for all $i \in I_p$. Define $\Omega_i = (a_i, b_i) \subseteq \mathbb{R}$, the spatial domain $\Omega = \prod_{i=1}^p \Omega_i$ and the spatio-temporal domain $\Omega_T = \Omega \times (0, T)$. Suppose that $\psi_1 : \bar{\Omega}_T \rightarrow \mathbb{C}$ and $\psi_2 : \bar{\Omega}_T \rightarrow \mathbb{C}$, and let $x = (x_1, \dots, x_p) \in \Omega$. throughout, Γ will denote the Gamma function.

Definition 1 Let $\psi : \bar{\Omega}_T \rightarrow \mathbb{C}$, and $i \in I_p$ fixed. Let $n \in \mathbb{N} \cup \{0\}$ and $\alpha \in \mathbb{R}$ such that $n - 1 < \alpha < n$. For each $(x, t) \in \Omega_T$, we define

$$\frac{\partial^\alpha \psi(x, t)}{\partial |x_i|^\alpha} = \frac{-1}{2 \cos(\frac{\pi\alpha}{2}) \Gamma(n - \alpha)} \frac{\partial^n}{\partial x_i^n} \int_{-\infty}^{\infty} \frac{\psi(x_1, \dots, x_{i-1}, \eta, x_{i+1}, \dots, x_p, t)}{|\eta - x_i|^{\alpha-1}} d\eta. \quad (1)$$

Define the associated fractional Laplacian [1, 2] as

$$\Delta^\alpha \psi(x, t) = \sum_{i=1}^p \frac{\partial^\alpha \psi}{\partial |x_i|^\alpha}(x, t). \quad (2)$$

Let $1 < \alpha_1, \alpha_2 \leq 2$, and consider complex-valued functions $\phi_1 : \bar{\Omega} \rightarrow \mathbb{C}$ and $\phi_2 : \bar{\Omega} \rightarrow \mathbb{C}$. In this work, we will consider the following coupled system of nonlinear partial differential equations with non-negative constant coefficients and fractional derivatives in space:

$$\begin{aligned} i \frac{\partial \psi_1}{\partial t} &= \lambda \psi_2 + \left[V(x) + D + \beta_{11} |\psi_1|^2 + \beta_{12} |\psi_2|^2 - \frac{1}{2} \Delta^{\alpha_1} \right] \psi_1, \\ i \frac{\partial \psi_2}{\partial t} &= \lambda \psi_1 + \left[V(x) + \beta_{12} |\psi_1|^2 + \beta_{22} |\psi_2|^2 - \frac{1}{2} \Delta^{\alpha_2} \right] \psi_2, \end{aligned} \quad (3)$$

subjected to $\begin{cases} \psi_i(x, 0) = \phi_i(x), \quad \forall i \in I_2, \quad \forall x \in \bar{\Omega}, \\ \psi_i(x, t) = 0, \quad \forall i \in I_2, \quad \forall (x, t) \in (\mathbb{R}^p \setminus \Omega) \times (0, T). \end{cases}$

Obviously, this system represents a generalization of the Gross–Pitaevski system [3, 4]. One of the main properties of (3) is the existence of invariant quantities. One of them is the energy function which is constant in time. In fact, the energy is given by the following expression:

$$\begin{aligned} \mathcal{E}(t) = \int_{\Omega} \left[-\frac{1}{2} \sum_{i=1}^p \frac{\partial^{\alpha_1} \psi_1}{\partial |x_i|^{\alpha_1}} \bar{\psi}_1 - \frac{1}{2} \sum_{i=1}^p \frac{\partial^{\alpha_2} \psi_2}{\partial |x_i|^{\alpha_2}} \bar{\psi}_2 + D|\psi_1|^2 \right. \\ \left. + \lambda \operatorname{Re} \left(\psi_1 \bar{\psi}_2 \right) + V(x) \left(|\psi_1|^2 + |\psi_2|^2 \right) + \frac{1}{2} \beta_{11} |\psi_1|^4 \right. \\ \left. + \frac{1}{2} \beta_{22} |\psi_2|^4 + \beta_{12} |\psi_1|^2 |\psi_2|^2 \right] dx, \quad \forall t \in [0, T]. \end{aligned} \quad (4)$$

Obviously, the fractional Hamiltonian for this system at each point $(x, t) \in \Omega_T$ is given by the formula

$$\begin{aligned} \mathcal{H}(x, t) = -\frac{1}{2} \sum_{i=1}^p \frac{\partial^{\alpha_1} \psi_1}{\partial |x_i|^{\alpha_1}} \bar{\psi}_1 - \frac{1}{2} \sum_{i=1}^p \frac{\partial^{\alpha_2} \psi_2}{\partial |x_i|^{\alpha_2}} \bar{\psi}_2 + D|\psi_1|^2 \\ + 2\lambda \operatorname{Re} \left(\psi_1 \bar{\psi}_2 \right) + V(x) \left(|\psi_1|^2 + |\psi_2|^2 \right) + \frac{1}{2} \beta_{11} |\psi_1|^4 \\ + \frac{1}{2} \beta_{22} |\psi_2|^4 + \beta_{12} |\psi_1|^2 |\psi_2|^2. \end{aligned} \quad (5)$$

The second invariant is the total mass. The individual masses of the continuous system (3) at the time t are defined as $\mathcal{M}_i(t) = \|\psi_i\|_{x,2}^2$, for each $i \in I_2$. Meanwhile, the total mass is the sum of the individual masses, that is,

$$\mathcal{M}(t) = \mathcal{M}_1(t) + \mathcal{M}_2(t), \quad \forall t \in (0, T), \quad (6)$$

and it is also constant in time. The total energy and mass of (3) satisfy the following properties (see []).

Lemma 1 *The energy function (4) has the alternative form*

$$\begin{aligned} \mathcal{E}(t) = \frac{1}{2} \sum_{i=1}^p \left\| \frac{\partial^{\alpha_1/2} \psi_1}{\partial |x_i|^{\alpha_1/2}} \right\|_{x,2}^2 + \frac{1}{2} \sum_{i=1}^p \left\| \frac{\partial^{\alpha_2/2} \psi_2}{\partial |x_i|^{\alpha_2/2}} \right\|_{x,2}^2 + D\|\psi_1\|_{x,2}^2 \\ + 2\lambda \operatorname{Re} \langle \psi_1, \psi_2 \rangle_x + \left\langle V(x), |\psi_1|^2 + |\psi_2|^2 \right\rangle_x + \frac{1}{2} \beta_{11} \|\psi_1\|_{x,4}^4 \\ + \frac{1}{2} \beta_{22} \|\psi_2\|_{x,4}^4 + \beta_{12} \|\psi_1 \psi_2\|_{x,2}^2, \end{aligned} \quad (7)$$

for each $t \in (0, T)$. □

Theorem 2 (Energy conservation) *If ψ_1 and ψ_2 satisfy the problem (3) then the energy function $\mathcal{E}(t)$ is constant.* □

Theorem 3 (Mass conservation) *If ψ_1 and ψ_2 are solutions of (3), then the mass function $\mathcal{M}(f)$ is constant. If $\lambda = 0$, then the individual masses are constant.* \square

The following is a direct consequence from Theorem 3.

Corollary 4 (Boundedness) *If ψ_1 and ψ_2 satisfy (3), then there exists a constant $M_0 \geq 0$ such that $\max \{ \|\psi_1\|_2^2, \|\psi_2\|_2^2 \} \leq M_0$, for each $t \in (0, T)$.* \square

In this work, we compare four finite-difference methods to solve system (3). Two of those methods conserve the main structural properties of the continuous system, namely, they conserve the mass and the energy. The other two schemes have the advantage of being easier to implement computationally. All four schemes are numerically analyzed for consistency, stability and convergence. Our main goal is to study the advantages and disadvantages of each method on theoretical and numerical grounds. The discretizations for fractional derivatives will hinge on the following definition.

Definition 2 (Ortigueira [5]) Suppose that $h, \alpha \in \mathbb{R}^+$ and assume that $f : \mathbb{R} \rightarrow \mathbb{R}$. We define the discrete operator

$$\Delta_h^{(\alpha)} f(x) = \sum_{k=-\infty}^{\infty} f(x - kh) g_k^{(\alpha)}, \quad \forall x \in \mathbb{R}, \quad (8)$$

where

$$g_k^{(\alpha)} = \frac{(-1)^k \Gamma(\alpha + 1)}{\Gamma(\frac{\alpha}{2} + k + 1) \Gamma(\frac{\alpha}{2} - k + 1)}, \quad \forall k \in \mathbb{Z}. \quad (9)$$

It is important to note that if f is sufficiently smooth and $\alpha \in (0, 1) \cup (1, 2]$, then

$$\frac{\partial^\alpha f(x)}{\partial |x|^\alpha} = -\frac{\Delta_h^\alpha f(x)}{h^\alpha} + \mathcal{O}(h^2), \quad (10)$$

for almost all $x \in \mathbb{R}$ (see [6]).

2 Numerical algorithms

For the remainder, we will let N and M_i be natural numbers, with $i \in I_p$. Define $\tau = T/N$ and $h_i = (b_i - a_i)/M_i$, and let

$$x_{i,j_i} = j_i h_i + a_i, \quad \forall i \in I_p, \forall j_i \in \bar{I}_{M_i}, \quad (11)$$

$$t_n = n\tau, \quad \forall n \in \bar{I}_N. \quad (12)$$

Let $\bar{J} = \prod_{i=1}^p \bar{I}_{M_i}$, where $J = \prod_{i=1}^p I_{M_i-1}$. If $j = (j_1, \dots, j_p) \in \bar{J}$, we define x_j as $(x_{1,j_1}, \dots, x_{p,j_p})$. For each $(j, n) \in \bar{J} \times \bar{I}_N$, we use (u_j^n, v_j^n) to denote a computational approximation to $(U_j^n, V_j^n) = (\psi_1(x_j, t_n), \psi_2(x_j, t_n))$. Finally, let ∂J represent the collection of all $j \in J$ with the property that $x_j \in \partial\Omega$.

Definition 3 For each $\alpha \in (0, 1) \cup (1, 2]$, $(j, n) \in J \times I_{N-1}$ and $w = u, v$, define

$$\mu_t w_j^n = \frac{w_j^{n+1} + w_j^n}{2}, \quad (13)$$

$$\mu_t^{(1)} w_j^n = \frac{w_j^{n-1} + w_j^{n+1}}{2} \quad (14)$$

$$\mu_t^{(2)} w_j^n = \frac{3w_j^n - w_j^{n-1}}{2}. \quad (15)$$

We introduce also the difference operators

$$\delta_t w_j^n = \frac{w_j^{n+1} - w_j^n}{\tau}, \quad (16)$$

$$\delta_t^{(1)} w_j^n = \frac{w_j^{n+1} - w_j^{n-1}}{2\tau}, \quad (17)$$

$$\delta_{x_i}^{(\alpha)} w_j^n = -\frac{1}{h_i^\alpha} \sum_{k=0}^{M_i} g_{j_i-k}^{(\alpha)} w(x_{1,j_1}, \dots, x_{i-1,j_{i-1}}, x_{i,k}, x_{i+1,j_{i+1}}, \dots, x_{p,j_p}, t_n). \quad (18)$$

Moreover, we agree that

$$\Delta_h^{(\alpha)} w_j^n = \delta_{x_1}^{(\alpha)} w_j^n + \delta_{x_2}^{(\alpha)} w_j^n + \dots + \delta_{x_p}^{(\alpha)} w_j^n, \quad (19)$$

$$\nabla_h^{(\alpha)} = (\delta_{x_1}^{(\alpha)} w_j^n, \delta_{x_2}^{(\alpha)} w_j^n, \dots, \delta_{x_p}^{(\alpha)} w_j^n). \quad (20)$$

Method 1

We define the first discretization of (3) as follows [7], for each $(j, n) \in J \times \bar{I}_{N-1}$:

$$\begin{aligned} i\delta_t u_j^n &= \mu_t \lambda v_j^n + \left[V_j + D + \mu_t \left[\beta_{11} |u_j^n|^2 + \beta_{12} |v_j^n|^2 \right] - \frac{1}{2} \Delta_h^{(\alpha_1)} \right] \mu_t u_j^n, \\ i\delta_t v_j^n &= \mu_t \lambda u_j^n + \left[V_j + \mu_t \left[\beta_{12} |u_j^n|^2 + \beta_{22} |v_j^n|^2 \right] - \frac{1}{2} \Delta_h^{(\alpha_2)} \right] \mu_t v_j^n, \end{aligned} \quad (21)$$

$$\text{such that } \begin{cases} u_j^0 = \phi_1(x_j), \quad \forall j \in \bar{J}, \\ v_j^0 = \phi_2(x_j), \quad \forall j \in \bar{J}, \\ u_j^n = v_j^n = 0, \quad \forall (j, n) \in \partial J \times \bar{I}_N. \end{cases}$$

This is a two-step implicit and conservative finite-difference scheme. Like the continuous system, this discrete model has discrete Hamiltonian, energy and mass functions. For its implementation, it is necessary to solve a two equation nonlinear system at each iteration of the numerical model.

Method 2

The following is the second discretization [8], which solves some of the computational difficulties inherent to the first method:

$$\begin{aligned}
 i\delta_t^{(1)} u_j^n &= \lambda v_j^n + \left[V_j + D + \beta_{11} |u_j^n|^2 + \beta_{12} |v_j^n|^2 - \frac{1}{2} \Delta_h^{(\alpha_1)} \right] \mu_t^{(1)} u_j^n, \\
 i\delta_t^{(1)} v_j^n &= \lambda u_j^n + \left[V_j + \beta_{22} |v_j^n|^2 + \beta_{12} |u_j^n|^2 - \frac{1}{2} \Delta_h^{(\alpha_2)} \right] \mu_t^{(1)} v_j^n, \\
 \text{such that } &\begin{cases} u_j^0 = \mu_t^{(1)} u_j^0 = \phi_1(x_j), \quad \forall j \in \bar{J}, \\ v_j^0 = \mu_t^{(1)} v_j^0 = \phi_2(x_j), \quad \forall j \in \bar{J}, \\ u_j^n = v_j^n = 0, \quad \forall (j, n) \in \partial J \times \bar{I}_N, \end{cases}
 \end{aligned} \tag{22}$$

Here, $(j, n) \in J \times I_{N-1}$. This is an implicit method, it is uncoupled and linear, so its implementation is much easier than the first. Moreover, the present technique also preserves the invariants. Notice that being a three-step method, it cannot start with only the initial conditions, so we could use Taylor's expansion for the second step or artificial initial conditions.

Method 3

The two previous systems depend on the former steps to define the coefficient matrices. This issue can be solved also, at the cost losing the conservation of mass and energy [9]. Such method is given by the third discretization:

$$\begin{aligned}
 i\delta_t u_j^n &= \mu_t^{(2)} \lambda v_j^n + \left[V_j + D - \frac{1}{2} \Delta_h^{(\alpha_1)} \right] \mu_t u_j^n \\
 &\quad + \left[\beta_{11} |\mu_t^{(2)} u_j^n|^2 + \beta_{12} |\mu_t^{(2)} v_j^n|^2 \right] \mu_t^{(2)} u_j^n, \\
 i\delta_t v_j^n &= \mu_t^{(2)} \lambda u_j^n + \left[V_j - \frac{1}{2} \Delta_h^{(\alpha_2)} \right] \mu_t v_j^n \\
 &\quad + \left[\beta_{12} |\mu_t^{(2)} u_j^n|^2 + \beta_{22} |\mu_t^{(2)} v_j^n|^2 \right] \mu_t^{(2)} v_j^n, \\
 \text{such that } &\begin{cases} u_j^0 = \mu_t u_j^0 = \mu_t^{(2)} u_j^0 = \phi_1(x_j), \quad \forall j \in J, \\ v_j^0 = \mu_t v_j^0 = \mu_t^{(2)} v_j^0 = \phi_2(x_j), \quad \forall j \in J, \\ u_j^n = v_j^n = 0, \quad \forall (j, n) \in \partial J \times \bar{I}_N. \end{cases}
 \end{aligned} \tag{23}$$

Obviously, this is a semi-explicit, decoupled and linear system, and it possesses no invariants. However, the computer implementation is much easier than the two previous methods. Once again, we have a three-step method, so we could use Taylor's approximation for the second step.

Method 4

Finally, we introduce our fourth numerical algorithm [10] to approximate the solution of (3) on $\bar{\Omega} \times [0, T]$:

$$\begin{aligned} i\delta_t^{(1)} u_j^n &= \lambda v_j^n + \left[V_j + D - \frac{1}{2} \Delta_h^{(\alpha_1)} \right] \mu_t^{(1)} u_j^n \\ &\quad + \left[\beta_{11} |u_j^n|^2 + \beta_{12} |v_j^n|^2 \right] u_j^n, \\ i\delta_t^{(1)} v_j^n &= \lambda u_j^n + \left[V_j - \frac{1}{2} \Delta_h^{(\alpha_2)} \right] \mu_t^{(1)} v_j^n + \left[\beta_{12} |u_j^n|^2 + \beta_{22} |v_j^n|^2 \right] v_j^n, \quad (24) \\ \text{such that } &\begin{cases} u_j^0 = \mu_t^{(1)} u_j^0 = \phi_1(x_j), \quad \forall j \in J, \\ v_j^0 = \mu_t^{(1)} v_j^0 = \phi_2(x_j), \quad \forall j \in J, \\ u_j^n = v_j^n = 0, \quad \forall (j, n) \in \partial J \times \bar{I}_N, \end{cases} \end{aligned}$$

This scheme is a semi-explicit, decoupled and linear system. The main difference with respect to the previous method is the number of steps. In the present discretization, it is not necessary to use additional approximations around t_0 .

Clearly, systems (22) and (23) miss explicit forms of the initial approximations u^1 , and v^1 . To solve this limitation, we make use of the initial conditions $\mu_t^{(i)} u_j^0 = \phi_1(x_j)$ and $\mu_t^{(i)} v_j^0 = \phi_2(x_j)$, for all $j \in J$, $i \in \bar{I}_2$, which yield

$$\delta_t^{(i)} u_j^0 = \frac{u_j^1 - \phi_1(x_j)}{\tau}, \quad \forall j \in J, i \in \bar{I}_1 \quad (25)$$

$$\delta_t^{(i)} v_j^0 = \frac{v_j^1 - \phi_2(x_j)}{\tau}, \quad \forall j \in J, i \in \bar{I}_1. \quad (26)$$

As a consequence, we obtain

$$\begin{aligned} u_j^1 &= \phi_1(x_j) - i\tau \left[\beta_{11} |\phi_1(x_j)|^2 + \beta_{12} |\phi_2(x_j)|^2 \right] \phi_1(x_j) \\ &\quad - i\tau \lambda \phi_2(x_j) + i\tau \left[-V_j - D + \frac{1}{2} \Delta_h^{(\alpha_1)} \right] \phi_1(x_j), \quad \forall j \in J, \end{aligned} \quad (27)$$

and

$$\begin{aligned} v_j^1 &= \phi_2(x_j) - i\tau \left[\beta_{12} |\phi_1(x_j)|^2 + \beta_{22} |\phi_2(x_j)|^2 \right] \phi_2(x_j) \\ &\quad - i\tau \lambda \phi_1(x_j) + i\tau \left[-V_j + \frac{1}{2} \Delta_h^{(\alpha_2)} \right] \phi_2(x_j), \quad \forall j \in J. \end{aligned} \quad (28)$$

3 Structural properties

In this section, we provide the results that guarantee the existence of solutions of the numerical methods presented in the previous section, and present properties on the conservation of energy and mass of those discrete systems.

8 CMMSE: analysis and comparison of some numerical methods

For convenience, we let $h = (h_1, \dots, h_p)$, and \mathcal{V}_h will be the collection of all complex-valued functions with domains $\{x_j : j \in \bar{J}\}$. Finally, set $w_j = w(x_j)$.

Lemma 5 (Brouwer fixed-point theorem [11, 12]) *Let $(H, \langle \cdot, \cdot \rangle)$ be a finite-dimensional inner product space, let $\|\cdot\|$ be the associated norm and let $g : H \rightarrow H$ be a continuous function. Assume that the following condition is satisfied:*

$$\exists \beta > 0, \forall z \in H, \|z\| = \beta, \operatorname{Re}\langle g(z), z \rangle > 0. \quad (29)$$

Then there exists $z^ \in H$ such that $g(z^*) = 0$ and $\|z^*\| \leq \beta$.*

Theorem 6 (Existence of solutions) *For any set of initial conditions, the systems (21)–(22) are solvable.*

Proof Let us start with system (21) firstly. For convenience, let us define the function $G = (G_1, G_2) : (\eta, \nu) \in \mathcal{V}_h \times \mathcal{V}_h \rightarrow (G_1(\eta, \nu), G_2(\eta, \nu)) \in \mathcal{V}_h \times \mathcal{V}_h$, where

$$\begin{aligned} G_1(\eta, \nu)_j &= \frac{\lambda i \tau}{2} \nu_j + \frac{i \tau}{2} \left[V_j + D + \frac{\beta_{11}}{2} \left(|u_j^n|^2 + |2\eta_j - u_j^n|^2 \right) \right. \\ &\quad \left. + \frac{\beta_{12}}{2} \left(|v_j^n|^2 + |2\nu_j - v_j^n|^2 \right) - \frac{1}{2} \Delta_h^{\alpha_1} \right] \eta_j + \eta_j - u_j^n, \end{aligned} \quad (30)$$

and

$$\begin{aligned} G_2(\eta, \nu)_j &= \frac{\lambda i \tau}{2} \eta_j + \frac{i \tau}{2} \left[V_j + \frac{\beta_{22}}{2} \left(|v_j^n|^2 + |2\nu_j - v_j^n|^2 \right) \right. \\ &\quad \left. + \frac{\beta_{12}}{2} \left(|u_j^n|^2 + |2\eta_j - u_j^n|^2 \right) - \frac{1}{2} \Delta_h^{\alpha_2} \right] \nu_j + \nu_j - v_j^n, \end{aligned} \quad (31)$$

for each $j \in J$. Here, G_1 and G_2 are obtained from (3) after some algebraic manipulation. Take the real part of the inner product of G_1 and η as well as the real part of the inner product of G_2 and ν , to obtain

$$\operatorname{Re}\langle G_1(\eta, \nu), \eta \rangle = \|\eta\|^2 + \operatorname{Re} \left(\frac{\lambda i \tau}{2} \langle \nu, \eta \rangle - \langle u^n, \eta \rangle \right), \quad (32)$$

$$\operatorname{Re}\langle G_2(\eta, \nu), \nu \rangle = \|\nu\|^2 + \operatorname{Re} \left(\frac{\lambda i \tau}{2} \langle \eta, \nu \rangle - \langle v^n, \nu \rangle \right). \quad (33)$$

Using then the Cauchy–Schwarz inequality we see that

$$\begin{aligned} \operatorname{Re}\langle G(\eta, \nu), (\eta, \nu) \rangle &= \|(\eta, \nu)\|^2 + \operatorname{Re} \left[\frac{\lambda i \tau}{2} \left(\langle \nu, \eta \rangle + \overline{\langle \nu, \eta \rangle} \right) - \langle (u^n, v_n), (\eta, \nu) \rangle \right] \\ &\geq \|(\eta, \nu)\|^2 - \|(u_n, v_n)\| \|(\eta, \nu)\|. \end{aligned} \quad (34)$$

Letting $\beta = \|(u_n, v_n)\| + 1$ and using Lemma (5), we conclude that there exists $(\eta^*, \nu^*) \in \mathcal{V}_h \times \mathcal{V}_h$ such that $(G_1(\eta^*, \nu^*)_j, G_2(\eta^*, \nu^*)_j) = (0, 0)$, for each $j \in J$. Thus the system (21) is solvable. A similar argument applies for system (22). \square

Lemma 7 (Desplanques [13]) *Let A be a square complex matrix. If A is strictly diagonally dominant, then A is invertible.* \square

Theorem 8 (Existence of solutions) *The systems (23)–(24) are uniquely solvable for any set of initial conditions.*

Proof We provide the proof for the existence of solutions of system (24). The proof for system (23) is similar. Rewrite the first equation of (24) in vector form as

$$-\frac{1}{2}Au^{n+1} = b(u^{n-1}) + a(u^n, v^n), \quad (35)$$

where

$$a(u_j^n, v_j^n) = (\beta_{11}|u_j^n|^2 + \beta_{12}|v_j^n|^2)u_j^n + \lambda v_j^n, \quad (36)$$

$$b(u_j^n) = \frac{1}{2} \left(V_j + D + \frac{i}{\tau} - \frac{1}{2}\delta_{x_1}^{(\alpha_1)} \right) u_j^n. \quad (37)$$

$$A = \begin{pmatrix} V_0 + D - \frac{i}{\tau} + \frac{g_0^{(\alpha_1)}}{2h_1^{\alpha_1}} & \frac{g_{-1}^{(\alpha_1)}}{2h_1^{\alpha_1}} & \cdots & \frac{g_{2-M_1}^{(\alpha_1)}}{2h_1^{\alpha_1}} \\ \frac{g_1^{(\alpha_1)}}{2h_1^{\alpha_1}} & V_1 + D - \frac{i}{\tau} + \frac{g_0^{(\alpha_1)}}{2h_1^{\alpha_1}} & \cdots & \frac{g_{3-M_1}^{(\alpha_1)}}{2h_1^{\alpha_1}} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{g_{M_1-2}^{(\alpha_1)}}{2h_1^{\alpha_1}} & \frac{g_{M_1-3}^{(\alpha_1)}}{2h_1^{\alpha_1}} & \cdots & V_{M_1} + D - \frac{i}{\tau} + \frac{g_0^{(\alpha_1)}}{2h_1^{\alpha_1}} \end{pmatrix}. \quad (38)$$

It is easy to prove that:

$$\sum_{j \neq i}^{M_1} |a_{ij}| = \sum_{j \neq i}^{M_1} \left| \frac{g_{l-j}^{(\alpha_1)}}{2h_1^{\alpha_1}} \right| = - \sum_{j \neq i}^{M_1} \frac{g_{l-j}^{\alpha_1}}{2h_1^{\alpha_1}} < - \sum_{\substack{l=-\infty \\ l \neq j}}^{\infty} \frac{g_{l-j}^{\alpha_1}}{2h_1^{\alpha_1}} = \frac{g_0^{\alpha_1}}{2h_1^{\alpha_1}} \leq |a_{ii}|. \quad (39)$$

By Lemma (7), the matrix A is invertible. It follows that (23) is uniquely solvable for u^{n+1} . A similar argument can be employed to show the existence and the uniqueness of the approximation v^{n+1} . The conclusion follows now by induction. \square

Now that the existence of a solutions for the four discretizations has been proved, we turn our attention to the invariant properties of (21)–(22).

Theorem 9 (Energy conservation) *Let $(u^n, v^n)_{n=0}^N$ be a solution of (21), and define*

$$E^n = \frac{1}{2} \|\nabla_h^{\alpha_1} u^n\|_2^2 + \frac{1}{2} \|\nabla_h^{\alpha_2} v^n\|_2^2 + D\|u^n\|_2^2 + 2\lambda \operatorname{Re} \langle u^n, v^n \rangle + \langle V, |u^n|^2 + |v^n|^2 \rangle + \frac{\beta_{11}}{2} \|u^n\|_4^4 + \frac{\beta_{22}}{2} \|v^n\|_4^4 + \beta_{12} \langle |u^n|^2, |v^n|^2 \rangle, \quad (40)$$

for each $n \in I_{N-1}$. Then $\delta_t E^n = 0$, for each $n \in I_{N-1}$.

Theorem 10 (Mass conservation) *Let $(u^n, v^n)_{n=0}^N$ be a solution of (21), and let*

$$M^n = \|u^n\|_2^2 + \|v^n\|_2^2, \quad \forall n \in I_{N-1}. \quad (41)$$

Then $\delta_t M^n = 0$, for each $n \in I_{N-1}$.

Theorem 11 (Energy conservation) *Let $(u^n, v^n)_{n=0}^N$ be a solution of (22), and let*

$$\begin{aligned} E^n &= \frac{1}{2}\mu_t \left\| \nabla_h^{(\alpha_1/2)} u^n \right\|_2^2 + \frac{1}{2}\mu_t \left\| \nabla_h^{(\alpha_2/2)} v^n \right\|_2^2 + D\mu_t \|u^n\|_2^2 \\ &\quad + \lambda \operatorname{Re} \left(\langle u^n, v^{n+1} \rangle + \langle v^n, u^{n+1} \rangle \right) \\ &\quad + \left\langle V, \mu_t (|u^n|^2 + |v^n|^2) \right\rangle + \frac{\beta_{11}}{2} \left\langle |u^n|^2, |u^{n+1}|^2 \right\rangle \\ &\quad + \frac{\beta_{22}}{2} \left\langle |v^n|^2, |v^{n+1}|^2 \right\rangle \\ &\quad + \frac{\beta_{12}}{2} \left(\left\langle |u^n|^2, |v^{n+1}|^2 \right\rangle + \left\langle |v^n|^2, |u^{n+1}|^2 \right\rangle \right), \end{aligned} \quad (42)$$

for each $n \in I_{N-1}$. Then, $\delta_t E^n = 0$, for each $n \in I_{N-1}$.

Theorem 12 (Mass conservation) *If $(u^n, v^n)_{n=0}^N$ is a solution of ststem (22), then $\delta_t M^n = 0$, for each $n \in I_{N-2}$. Here, for each $n \in I_{N-1}$,*

$$M^n = \mu_t \left(\|u^n\|_2^2 + \|v^n\|_2^2 \right) - \lambda\tau \operatorname{Im} \left(\langle u^n, v^{n+1} \rangle + \langle v^n, u^{n+1} \rangle \right), \quad (43)$$

Moreover, if $\lambda = 0$, then the individual masses satisfy $\delta_t M_1^n = \delta_t M_2^n = 0$, where

$$M_1^n = \mu_t \|u^n\|_2^2 - \lambda\tau \operatorname{Im} \langle u^n, v^{n+1} \rangle, \quad \forall n \in I_{N-1}, \quad (44)$$

$$M_2^n = \mu_t \|v^n\|_2^2 - \lambda\tau \operatorname{Im} \langle v^n, u^{n+1} \rangle, \quad \forall n \in I_{N-1}. \quad (45)$$

It is clear that the discretizations described for (3) are not the same, starting with the first two being implicit and the second two semi-explicit, following with the number of steps needed for each iteration. Some properties all four of them share are the order of consistency (even if it is not around the same point), the stability of the schemes and quadratic order of convergence, obviously our goal is to compare them convergence-wise but all of the previous properties will be proved in the next section.

Before closing this section, it is worth highlighting that various mathematical models have the property that they conserve important mathematical functionals, like the energy or the mass of the system. Proposing discrete models which preserve those characteristics has been an important direction of investigation in numerical analysis. Indeed, since various decades ago, there have been articles which strive to preserve the energy of nonlinear wave equations with periodic potentials [14–16], symplectic techniques for systems in quantum mechanics [17], variational methodologies in the discrete domain which provide efficient and fast computational results [18, 19], Galerkin techniques which are capable of preserving the dissipation or the conservation of energy in nonlinear mathematical models [20, 21]. Moreover, those historic reports found generalizations to the fractional scenario a conservative techniques for energy- and mass-preserving methodologies [22–24].

4 Numerical results

In this stage, we will review the most important properties on the numerical models introduced in previous sections. More precisely, we will examine the properties of consistency, stability and convergence of the schemes. In particular, to prove the consistency, we define the continuous operators

$$\mathcal{L}_1 = i \frac{\partial \psi_1}{\partial t} - \lambda \psi_2 + \left[-V(x) - D - \beta_{11} |\psi_1|^2 - \beta_{12} |\psi_2|^2 + \frac{1}{2} \Delta^{\alpha_1} \right] \psi_1, \quad (46)$$

$$\mathcal{L}_2 = i \frac{\partial \psi_2}{\partial t} - \lambda \psi_1 + \left[-V(x) - \beta_{12} |\psi_1|^2 - \beta_{22} |\psi_2|^2 + \frac{1}{2} \Delta^{\alpha_2} \right] \psi_2, \quad (47)$$

for each $(x, t) \in \Omega_T$. It is obvious that both operators depend on (ψ_1, ψ_2) . Associated with the numerical method (21), we set

$$L_{1,1} = i \delta_t u_j^n - \lambda \mu_t v_j^n + \left[-V_j - D - \beta_{11} \mu_t |u_j^n|^2 - \beta_{12} \mu_t |v_j^n|^2 + \frac{1}{2} \Delta_h^{(\alpha_1)} \right] \mu_t u_j^n, \quad (48)$$

and

$$L_{1,2} = i \delta_t v_j^n - \lambda \mu_t u_j^n - \left[V_j + \beta_{22} \mu_t |v_j^n|^2 + \beta_{12} \mu_t |u_j^n|^2 - \frac{1}{2} \Delta_h^{(\alpha_2)} \right] \mu_t v_j^n, \quad (49)$$

both of which depend on (u_j^n, v_j^n) . In similar fashion, we introduce discrete operators $L_{i,1}$ and $L_{i,2}$ for Model j , where $i = 2, 3, 4$. As a final step, for each $(x, t) \in \Omega_T$, $(j, n) \in J \times I_{N-1}$ and $i \in I_4$, we let

$$\mathcal{L}(\psi_1, \psi_2) = (\mathcal{L}_1(\psi_1, \psi_2), \mathcal{L}_2(\psi_1, \psi_2)), \quad (50)$$

$$L_i(\psi_1, \psi_2) = (L_{i,1}(\psi_1, \psi_2), L_{i,2}(\psi_1, \psi_2)). \quad (51)$$

Theorem 13 (Consistency) *If $\psi_1, \psi_2 \in \mathcal{C}_{x,t}^{5,4}(\overline{\Omega_T})$, then the numerical models (21)–(24) yield quadratically consistent approximations to the solutions of (3).*

Proof The result is an application of Taylor's theorem. □

Next, we consider initial data of the form (ϕ_1, ϕ_2) and $(\tilde{\phi}_1, \tilde{\phi}_2)$. Here, $\tilde{\phi}_1$ and $\tilde{\phi}_2$ are both complex functions, and the numerical approximations associated to each of these pairs is represented as (u, v) and (\tilde{u}, \tilde{v}) , respectively.

Lemma 14 For each $i \in I_4$, let $P_{i,j}^n$ and $Q_{i,j}^n$ represent the nonlinear terms of Model i , and let $\epsilon^n = u^n - \tilde{u}^n$ and $\zeta^n = v^n - \tilde{v}^n$, for each $n \in \bar{I}_N$. Then there are constants $C_i \geq 0$ which depends only on τ , such that

$$\max\{|P_{1,j}^n|, |Q_{1,j}^n|\} \leq C_1(|\epsilon_j^n| + |\epsilon_j^{n+1}| + |\zeta_j^n| + |\zeta_j^{n+1}|), \quad (52)$$

$$\max\{|P_{2,j}^n|, |Q_{2,j}^n|\} \leq C_2(|\epsilon_j^{n-1}| + |\epsilon_j^n| + |\epsilon_j^{n+1}| + |\zeta_j^{n-1}| + |\zeta_j^n| + |\zeta_j^{n+1}|), \quad (53)$$

$$\max\{|P_{3,j}^n|, |Q_{3,j}^n|\} \leq C_3(|\epsilon_j^{n-1}| + |\epsilon_j^n| + |\zeta_j^{n-1}| + |\zeta_j^n|), \quad (54)$$

$$\max\{|P_{4,j}^n|, |Q_{4,j}^n|\} \leq C_4(|\epsilon_j^n| + |\zeta_j^n|), \quad (55)$$

for each $(j, n) \in J \times I_{N-1}$.

Proof The conclusions are applications of the Mean Value Theorem. \square

Next we tackle the convergence of the numerical models presented in the previous section. It is worth pointing out that the stability properties are established in similar fashion.

Theorem 15 (Convergence) Let ϵ^n and ζ^n be the differences of the previous lemma, associated with each of the numerical methods of the previous section

• **Method 1.** There exists $C_1'' \geq 0$ such that, if $2C_1''\tau < 1$, then

$$\|\epsilon^n\|_2^2 + \|\zeta^n\|_2^2 \leq 2(\|\epsilon^0\|_2^2 + \|\zeta^0\|_2^2)e^{4C_1''T}, \quad \forall n \in I_N. \quad (56)$$

• **Method 2.** There exists $C_2'' \geq 0$ such that, if $(2\lambda + 4C_2'' + 1)\tau < 1$, then

$$\mu_t \left(\|\epsilon^n\|_2^2 + \|\zeta^n\|_2^2 \right) \leq \mu_t (\|\epsilon^0\|_2^2 + \|\zeta^0\|_2^2) e^{\left(\lambda + \frac{4C_2''+1}{2} \right) T}, \quad \forall n \in I_N. \quad (57)$$

• **Method 3.** There exists $C_3'' \geq 0$ such that, if $(C_3'' + \lambda)\tau < \frac{1}{2}$, then

$$\|\epsilon^n\|_2^2 + \|\zeta^n\|_2^2 \leq \left[1 + \left(C_3'' + \frac{\lambda}{4} \right) \tau \right] (\|\epsilon^0\|_2^2 + \|\zeta^0\|_2^2) e^{2C_3''T}, \quad \forall n \in I_N. \quad (58)$$

• **Method 4.** There exists $C_4'' \geq 0$ such that, if $2C_4''\tau < 1$, then

$$\mu_t (\|\epsilon^n\|_2^2 + \|\zeta^n\|_2^2) \leq 2\mu_t (\|\epsilon^0\|_2^2 + \|\zeta^0\|_2^2) e^{2C_4''T}, \quad \forall n \in I_N. \quad (59)$$

Proof Subtract the equations satisfied by (u, v) and (\tilde{u}, \tilde{v}) using (21), in order to obtain the equations associated to (ϵ^n, ζ^n) . By the previous lemma, there exists $C_1' \in \mathbb{R}^+$ with the property that

$$\max\{\|P^n\|_2^2, \|Q^n\|_2^2\} \leq C_1' \left(\|\epsilon^n\|_2^2 + \|\zeta^n\|_2^2 \right), \quad \forall n \in I_{N-1}. \quad (60)$$

Rearranging terms, we can readily obtain

$$\delta_t \|\epsilon^n\|_2^2 = 2 \operatorname{Im} \langle P^n, \mu_t \epsilon^n \rangle + 2 \operatorname{Im} \langle \mu_t \zeta^n, \mu_t \epsilon^n \rangle, \quad \forall n \in I_{N-1}, \quad (61)$$

$$\delta_t \|\zeta^n\|_2^2 = 2 \operatorname{Im} \langle Q^n, \mu_t \zeta^n \rangle + 2 \operatorname{Im} \langle \mu_t \epsilon^n, \mu_t \zeta^n \rangle, \quad \forall n \in I_{N-1}. \quad (62)$$

The next step is to show the existence of $C_1'' \in \mathbb{R}^+$ that satisfies our conclusion. To that end, observe that

$$\begin{aligned} \|\epsilon^{m+1}\|_2^2 + \|\zeta^{m+1}\|_2^2 &= \|\epsilon^0\|_2^2 + \|\zeta^0\|_2^2 + 2\tau \sum_{n=0}^m \operatorname{Im} \langle P^n, \mu_t \epsilon^n \rangle \\ &\quad + 2\tau \sum_{n=0}^m \operatorname{Im} \langle Q^n, \mu_t \zeta^n \rangle \\ &\leq \|\epsilon^0\|_2^2 + \|\zeta^0\|_2^2 + 2C''\tau \sum_{n=0}^m \left(\|\epsilon^n\|_2^2 + \|\zeta^n\|_2^2 \right) \\ &\quad + \frac{1}{2} \left(\|\epsilon^{m+1}\|_2^2 + \|\zeta^{m+1}\|_2^2 \right). \end{aligned} \quad (63)$$

Subtract the term $\frac{1}{2}(\|\epsilon^{m+1}\|_2^2 + \|\zeta^{m+1}\|_2^2)$ from both ends, and multiply both sides by 2. It follows that a discrete form of Gronwall's inequality [25] is satisfied, for each $m \in I_{N-1}$. Here, we used $\omega^m = \|\epsilon^m\|_2^2 + \|\zeta^m\|_2^2$ for each $m \in I_N$, as well as $C_0 = 4C''$ and $\rho^m = 2(\|\epsilon^0\|_2^2 + \|\zeta^0\|_2^2)$. The proofs for (22)–(24) are very similar. \square

5 Conclusions

In this work, we compared various numerical models to approximate the solutions of a fractional extension of the Gross-Pitaevskii system. That model has been used to describe the interaction between a two-component system, and we consider here a fractional extension using derivatives of the Riesz type, with two differentiation orders. It is well known that the system is capable of preserving the mass and the total energy with respect to time. Four discretizations based on the use of fractional-order centered differences are presented here. The existence of solutions is established using fixed-point theorems, and two of the schemes have associated discrete mass and energy functionals which are conserved throughout time. The numerical properties of the schemes were also considered, and it was found out that they were second-order discretizations of the continuous model, as well as conditionally stable and convergent. Various incomparable conditions need to be imposed upon the computational parameters in order to guarantee the stability and the convergence of the schemes. Finally, it is worth pointing out that the schemes which were not capable of preserving the mass or the energy were those with the easiest implementations. Some simulations were provided to illustrate some of the properties.

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